D.1: Full crystallographic Data Tables of [Au(L1)](PF_6)

Table D.1.1: Bond lengths [Å] and angles [°] for [Au(L1)](PF_6)

Au(1)-N(4)	1.976(5)
Au(1)-N(1)	1.993(5)
Au(1)-N(2)	2.005(5)
Au(1)-N(3)	2.022(5)
P-F(5)	1.588(4)
P-F(4)	1.600(4)
P-F(2)	1.605(4)
P-F(1)	1.606(4)
P-F(3)	1.617(5)
P-F(6)	1.619(4)
N(1)-C(1)	1.361(7)
N(1)-C(4)	1.386(7)
N(4)-C(13)	1.361(7)
N(4)-C(10)	1.404(8)
N(6)-C(14)	1.340(7)
N(6)-C(21)	1.355(7)
C(14)-C(15)	1.473(7)
C(14)-C(13)	1.486(8)
N(2)-C(5)	1.314(9)
N(2)-C(6)	1.467(8)
C(15)-N(5)	1.348(7)
C(15)-C(1)	1.482(8)
N(5)-C(16)	1.342(7)
C(10)-C(9)	1.403(8)
C(10)-C(11)	1.404(8)
C(1)-C(2)	1.433(8)
C(2)-C(3)	1.381(9)
C(13)-C(12)	1.419(8)
C(19)-C(20)	1.392(9)
C(19)-C(18)	1.431(9)
N(3)-C(9)	1.308(7)
N(3)-C(8)	1.480(7)
C(21)-C(20)	1.411(8)
C(21)-C(16)	1.444(8)

Table D.1.1. continued…

C(12)-C(11)	1.405(8)
C(17)-C(18)	1.358(9)
C(17)-C(16)	1.446(8)
C(3)-C(4)	1.403(9)
C(7)-C(6)	1.526(10)
C(7)-C(8)	1.537(10)
C(5)-C(4)	1.410(9)
N(4)-Au(1)-N(1)	99.23(19)
N(4)-Au(1)-N(2)	177.65(19)
N(1)-Au(1)-N(2)	81.7(2)
N(4)-Au(1)-N(3)	81.8(2)
N(1)-Au(1)-N(3)	177.71(18)
N(2)-Au(1)-N(3)	97.2(2)
F(5)-P-F(4)	89.9(2)
F(5)-P-F(2)	90.0(2)
F(4)-P-F(2)	179.9(3)
F(5)-P-F(1)	179.5(3)
F(4)-P-F(1)	90.5(3)
F(2)-P-F(1)	89.7(2)
F(5)-P-F(3)	89.9(2)
F(4)-P-F(3)	90.7(3)
F(2)-P-F(3)	89.3(2)
F(1)-P-F(3)	89.8(2)
F(5)-P-F(6)	91.5(2)
F(4)-P-F(6)	90.2(3)
F(2)-P-F(6)	89.7(2)
F(1)-P-F(6)	88.8(2)
F(3)-P-F(6)	178.3(3)
C(1)-N(1)-C(4)	108.4(5)
C(1)-N(1)-Au(1)	138.6(4)
C(4)-N(1)-Au(1)	112.6(4)
C(13)-N(4)-C(10)	108.6(5)
C(13)-N(4)-Au(1)	139.3(4)
C(10)-N(4)-Au(1)	111.6(4)
C(14)-N(6)-C(21)	120.0(5)
N(6)-C(14)-C(15)	119.6(5)

Table D.1.1. continued…

N(6)-C(14)-C(13)	109.2(4)
C(15)-C(14)-C(13)	131.1(5)
C(5)-N(2)-C(6)	124.5(5)
C(5)-N(2)-Au(1)	112.5(4)
C(6)-N(2)-Au(1)	123.0(5)
N(5)-C(15)-C(14)	119.9(5)
N(5)-C(15)-C(1)	108.6(5)
C(14)-C(15)-C(1)	131.5(5)
C(16)-N(5)-C(15)	119.7(5)
C(9)-C(10)-C(11)	134.5(6)
C(9)-C(10)-N(4)	116.1(5)
C(11)-C(10)-N(4)	109.3(5)
N(1)-C(1)-C(2)	107.6(5)
N(1)-C(1)-C(15)	129.9(5)
C(2)-C(1)-C(15)	122.5(5)
C(3)-C(2)-C(1)	108.2(6)
N(4)-C(13)-C(12)	107.4(5)
N(4)-C(13)-C(14)	129.7(5)
C(12)-C(13)-C(14)	122.9(5)
C(20)-C(19)-C(18)	120.5(6)
C(9)-N(3)-C(8)	123.8(6)
C(9)-N(3)-Au(1)	113.3(4)
C(8)-N(3)-Au(1)	122.9(4)
N(6)-C(21)-C(20)	120.1(5)
N(6)-C(21)-C(16)	120.2(5)
C(20)-C(21)-C(16)	119.7(5)
C(11)-C(12)-C(13)	109.3(5)
C(18)-C(17)-C(16)	119.5(6)
N(5)-C(16)-C(21)	120.6(5)
N(5)-C(16)-C(17)	120.3(5)
C(21)-C(16)-C(17)	119.1(5)
C(2)-C(3)-C(4)	106.5(5)
N(3)-C(9)-C(10)	117.1(6)
C(6)-C(7)-C(8)	115.4(5)
N(2)-C(5)-C(4)	118.9(6)
N(3)-C(8)-C(7)	111.6(5)
N(2)-C(6)-C(7)	113.1(5)

Table D.1.1. continued…

C(17)-C(18)-C(19)	121.5(6)
C(10)-C(11)-C(12)	105.3(5)
N(1)-C(4)-C(3)	109.3(5)
N(1)-C(4)-C(5)	114.2(6)
C(3)-C(4)-C(5)	136.4(6)
C(19)-C(20)-C(21)	119.7(6)

Table D.1.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [Au(L1)](PF_6). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	14(1)	20(1)	25(1)	-4(1)	-1(1)	3(1)
P	21(1)	35(1)	22(1)	-5(1)	5(1)	-3(1)
N(1)	23(3)	20(2)	16(2)	0(2)	-4(2)	3(2)
N(4)	18(2)	20(2)	24(2)	-3(2)	5(2)	4(2)
N(6)	17(3)	15(2)	19(2)	0(2)	1(2)	5(2)
C(14)	17(3)	10(2)	18(3)	-4(2)	4(2)	3(2)
F(5)	22(2)	58(3)	67(3)	-15(2)	10(2)	-6(2)
F(6)	43(2)	35(2)	61(3)	1(2)	13(2)	1(2)
N(2)	20(3)	30(3)	36(3)	-8(3)	-7(2)	2(2)
C(15)	17(3)	9(3)	23(3)	0(2)	4(2)	4(2)
N(5)	23(3)	16(2)	22(3)	-4(2)	8(2)	3(2)
C(10)	17(3)	25(3)	35(3)	1(3)	8(3)	2(2)
F(2)	61(3)	55(3)	36(2)	-15(2)	19(2)	2(2)
C(1)	22(3)	24(3)	20(3)	-6(3)	7(3)	7(2)
C(2)	32(4)	38(4)	17(3)	-2(3)	10(3)	6(3)
C(13)	16(3)	18(3)	19(3)	2(2)	2(2)	3(2)
F(4)	73(4)	113(4)	40(3)	-36(3)	28(3)	-45(3)
F(3)	51(3)	56(3)	67(3)	21(2)	5(2)	-11(2)
C(19)	21(3)	15(3)	48(4)	-8(3)	6(3)	3(2)
N(3)	16(3)	21(2)	33(3)	-5(2)	6(2)	-1(2)
C(21)	18(3)	10(2)	24(3)	-1(2)	8(2)	6(2)
C(12)	21(3)	33(3)	18(3)	-1(3)	3(3)	-4(3)
C(17)	26(3)	19(3)	32(3)	3(3)	16(3)	1(2)
C(16)	25(3)	16(3)	28(3)	0(2)	11(3)	9(2)
C(3)	40(4)	42(4)	16(3)	-4(3)	1(3)	7(3)
C(9)	29(4)	24(3)	31(4)	2(3)	14(3)	2(3)
C(7)	13(3)	32(4)	76(5)	-3(4)	-5(3)	-1(3)
C(5)	28(4)	31(4)	32(4)	-6(3)	-7(3)	5(3)
C(8)	14(3)	38(4)	52(4)	-17(3)	8(3)	-5(3)
F(1)	23(2)	63(3)	69(3)	6(2)	2(2)	-1(2)
C(6)	15(3)	44(4)	47(4)	-6(3)	-12(3)	-2(3)
C(18)	24(3)	22(3)	45(4)	-4(3)	19(3)	0(3)
C(11)	25(3)	35(3)	19(3)	1(3)	9(2)	-4(3)
C(4)	30(4)	27(3)	16(3)	-3(3)	-3(3)	7(3)
C(20)	14(3)	25(3)	33(3)	-5(3)	-2(3)	4(2)

Table D.1.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [Au(L1)](PF_6).

	x	y	z	U(eq)
H(2)	5125	1269	1919	34
H(19)	1552	740	-1393	35
H(12)	5002	2916	-1817	30
H(17)	2833	525	761	29
H(3)	6498	1794	2848	41
H(9)	7996	4855	-1043	32
H(7A)	9207	2593	934	52
H(7B)	9924	4115	1188	52
H(5)	8121	3240	2621	40
H(8A)	8987	6460	458	42
H(8B)	9260	4854	-13	42
H(6A)	9330	3815	2143	47
H(6B)	9038	5819	1790	47
H(18)	1614	107	-153	34
H(11)	6345	3939	-2091	31
H(20)	2741	1773	-1719	31

Table D.1.4: Torsion angles [°] for [Au(L1)](PF_6)

N(4)-Au(1)-N(1)-C(1)	4.0(6)
N(2)-Au(1)-N(1)-C(1)	-173.8(6)
N(4)-Au(1)-N(1)-C(4)	175.4(4)
N(2)-Au(1)-N(1)-C(4)	-2.4(4)
N(1)-Au(1)-N(4)-C(13)	-3.9(6)
N(3)-Au(1)-N(4)-C(13)	174.0(6)
N(1)-Au(1)-N(4)-C(10)	-174.4(4)
N(3)-Au(1)-N(4)-C(10)	3.5(4)
C(21)-N(6)-C(14)-C(15)	-1.0(7)
C(21)-N(6)-C(14)-C(13)	176.6(4)
N(1)-Au(1)-N(2)-C(5)	2.2(4)
N(3)-Au(1)-N(2)-C(5)	-175.7(4)
N(1)-Au(1)-N(2)-C(6)	-179.6(5)
N(3)-Au(1)-N(2)-C(6)	2.4(5)
N(6)-C(14)-C(15)-N(5)	1.0(7)
C(13)-C(14)-C(15)-N(5)	-176.1(5)
N(6)-C(14)-C(15)-C(1)	178.8(5)
C(13)-C(14)-C(15)-C(1)	1.7(9)
C(14)-C(15)-N(5)-C(16)	0.3(7)
C(1)-C(15)-N(5)-C(16)	-178.0(4)
C(13)-N(4)-C(10)-C(9)	-177.0(5)
Au(1)-N(4)-C(10)-C(9)	-3.5(6)
C(13)-N(4)-C(10)-C(11)	0.5(6)
Au(1)-N(4)-C(10)-C(11)	174.0(4)
C(4)-N(1)-C(1)-C(2)	0.4(6)
Au(1)-N(1)-C(1)-C(2)	172.1(4)
C(4)-N(1)-C(1)-C(15)	180.0(5)
Au(1)-N(1)-C(1)-C(15)	-8.3(10)
N(5)-C(15)-C(1)-N(1)	-175.2(5)
C(14)-C(15)-C(1)-N(1)	6.8(10)
N(5)-C(15)-C(1)-C(2)	4.4(7)
C(14)-C(15)-C(1)-C(2)	-173.7(5)
N(1)-C(1)-C(2)-C(3)	0.0(7)
C(15)-C(1)-C(2)-C(3)	-179.6(5)
C(10)-N(4)-C(13)-C(12)	-0.3(6)
Au(1)-N(4)-C(13)-C(12)	-171.0(4)

Table D.1.4. continued…

C(10)-N(4)-C(13)-C(14)	179.6(5)
Au(1)-N(4)-C(13)-C(14)	8.9(10)
N(6)-C(14)-C(13)-N(4)	173.6(5)
C(15)-C(14)-C(13)-N(4)	-9.1(10)
N(6)-C(14)-C(13)-C(12)	-6.6(7)
C(15)-C(14)-C(13)-C(12)	170.7(5)
N(4)-Au(1)-N(3)-C(9)	-3.2(4)
N(2)-Au(1)-N(3)-C(9)	174.7(4)
N(4)-Au(1)-N(3)-C(8)	178.6(5)
N(2)-Au(1)-N(3)-C(8)	-3.5(5)
C(14)-N(6)-C(21)-C(20)	-178.8(5)
C(14)-N(6)-C(21)-C(16)	-0.1(7)
N(4)-C(13)-C(12)-C(11)	0.0(7)
C(14)-C(13)-C(12)-C(11)	-179.9(5)
C(15)-N(5)-C(16)-C(21)	-1.4(7)
C(15)-N(5)-C(16)-C(17)	179.5(5)
N(6)-C(21)-C(16)-N(5)	1.3(8)
C(20)-C(21)-C(16)-N(5)	-179.9(5)
N(6)-C(21)-C(16)-C(17)	-179.5(5)
C(20)-C(21)-C(16)-C(17)	-0.8(8)
C(18)-C(17)-C(16)-N(5)	179.7(5)
C(18)-C(17)-C(16)-C(21)	0.5(8)
C(1)-C(2)-C(3)-C(4)	-0.4(7)
C(8)-N(3)-C(9)-C(10)	-179.7(5)
Au(1)-N(3)-C(9)-C(10)	2.1(7)
C(11)-C(10)-C(9)-N(3)	-175.8(6)
N(4)-C(10)-C(9)-N(3)	1.0(8)
C(6)-N(2)-C(5)-C(4)	-179.7(6)
Au(1)-N(2)-C(5)-C(4)	-1.6(7)
C(9)-N(3)-C(8)-C(7)	-144.9(6)
Au(1)-N(3)-C(8)-C(7)	33.1(7)
C(6)-C(7)-C(8)-N(3)	-69.5(7)
C(5)-N(2)-C(6)-C(7)	146.4(6)
Au(1)-N(2)-C(6)-C(7)	-31.5(8)
C(8)-C(7)-C(6)-N(2)	69.1(7)
C(16)-C(17)-C(18)-C(19)	-0.3(8)
C(20)-C(19)-C(18)-C(17)	0.3(8)

Table D.1.4. continued…

C(9)-C(10)-C(11)-C(12)	176.4(7)
N(4)-C(10)-C(11)-C(12)	-0.5(7)
C(13)-C(12)-C(11)-C(10)	0.3(7)
C(1)-N(1)-C(4)-C(3)	-0.7(7)
Au(1)-N(1)-C(4)-C(3)	-174.7(4)
C(1)-N(1)-C(4)-C(5)	176.3(5)
Au(1)-N(1)-C(4)-C(5)	2.3(6)
C(2)-C(3)-C(4)-N(1)	0.6(7)
C(2)-C(3)-C(4)-C(5)	-175.3(7)
N(2)-C(5)-C(4)-N(1)	-0.4(8)
N(2)-C(5)-C(4)-C(3)	175.4(7)
C(18)-C(19)-C(20)-C(21)	-0.6(8)
N(6)-C(21)-C(20)-C(19)	179.6(5)
C(16)-C(21)-C(20)-C(19)	0.8(8)

D.2: Full crystallographic Data Tables of [Au(L2)](CF_3SO_3)

Table D.2.1: Bond lengths [Å] and angles [°] for [Au(L2)](CF_3SO_3).

C(1A)-C(2A)	1.43(3)
C(1A)-N(1A)	1.43(3)
C(1A)-C(047)	1.46(4)
C(1B)-C(2B)	1.33(4)
C(1B)-N(2B)	1.38(3)
C(1B)-C(21B)	1.39(4)
C(2A)-C(3A)	1.35(3)
C(2B)-C(3B)	1.40(3)
C(3A)-C(4A)	1.41(3)
C(3B)-C(4B)	1.38(3)
C(4A)-C(5A)	1.34(3)
C(4A)-N(1A)	1.39(3)
C(4B)-N(2B)	1.38(3)
C(4B)-C(5B)	1.41(3)
C(5A)-N(2A)	1.39(3)
C(5B)-N(1B)	1.38(4)
C(6A)-N(2A)	1.40(3)
C(6A)-C(7A)	1.59(3)
C(6B)-N(1B)	1.35(4)
C(6B)-C(7B)	1.52(5)
C(7A)-C(22A)	1.52(3)
C(7A)-C(23A)	1.52(3)
C(7A)-C(8A)	1.64(4)
C(7B)-C(8B)	1.43(4)
C(7B)-C(23B)	1.47(4)
C(7B)-C(22B)	1.58(3)
C(8A)-N(3A)	1.43(3)
C(8B)-N(4B)	1.54(3)
C(9A)-C(11A)	1.32(4)
C(9A)-N(3A)	1.32(3)
C(9B)-N(4B)	1.21(3)
C(9B)-C(10B)	1.47(3)
C(10A)-C(12A)	1.37(4)
C(10A)-C(11A)	1.41(3)

Table D.2.1. continued…

C(10B)-C(11B)	1.31(3)
C(10B)-N(3B)	1.41(3)
C(11A)-N(4A)	1.37(3)
C(11B)-C(13B)	1.41(3)
C(12A)-C(13A)	1.44(3)
C(13A)-N(4A)	1.36(3)
C(13A)-C(14A)	1.47(3)
C(13B)-N(027)	1.42(5)
C(14A)-N(6A)	1.28(3)
C(14A)-C(047)	1.51(3)
C(14B)-N(5B)	1.40(5)
C(14B)-C(21B)	1.46(6)
C(14B)-N(027)	1.57(6)
C(15A)-C(16A)	1.34(3)
C(15A)-N(6A)	1.36(3)
C(15A)-C(21A)	1.44(4)
C(15B)-C(20B)	1.36(3)
C(15B)-N(5B)	1.40(3)
C(15B)-C(16B)	1.46(4)
C(16A)-C(17A)	1.24(4)
C(16B)-C(17B)	1.33(3)
C(17A)-C(19A)	1.42(4)
C(17B)-C(18B)	1.42(3)
C(18B)-C(19B)	1.21(3)
C(19A)-C(20A)	1.36(3)
C(19B)-C(20B)	1.39(3)
C(20A)-C(21A)	1.39(3)
C(20B)-N(6B)	1.43(3)
C(21A)-N(5A)	1.30(3)
C(21B)-N(6B)	1.23(3)
C(24A)-F(2A)	1.26(5)
C(24A)-F(3A)	1.39(4)
C(24A)-F(1A)	1.43(3)
C(24A)-S(1A)	1.72(6)
C(24B)-F(2B)	0.83(12)
C(24B)-F(3B)	1.43(7)
C(24B)-F(1B)	1.53(7)

Table D.2.1. continued…

C(24B)-S(1B)	2.04(8)
C(047)-N(5A)	1.24(3)
N(1A)-Au(1A)	1.981(18)
N(1B)-Au(1B)	2.02(2)
N(2A)-Au(1A)	1.989(18)
N(2B)-Au(1B)	1.94(2)
N(3A)-Au(1A)	1.98(2)
N(3B)-N(027)	1.34(4)
N(3B)-Au(1B)	2.01(2)
N(4A)-Au(1A)	1.993(18)
N(4B)-Au(1B)	2.07(3)
O(1A)-S(1A)	1.419(18)
O(1B)-S(1B)	1.52(3)
O(2A)-S(1A)	1.48(2)
O(2B)-S(1B)	1.48(5)
O(3A)-S(1A)	1.47(2)
O(3B)-S(1B)	1.46(3)
C(2A)-C(1A)-N(1A)	102(2)
C(2A)-C(1A)-C(047)	121.9(19)
N(1A)-C(1A)-C(047)	136(2)
C(2B)-C(1B)-N(2B)	109(2)
C(2B)-C(1B)-C(21B)	118(3)
N(2B)-C(1B)-C(21B)	132(3)
C(3A)-C(2A)-C(1A)	111.3(18)
C(1B)-C(2B)-C(3B)	110(2)
C(2A)-C(3A)-C(4A)	108.9(17)
C(4B)-C(3B)-C(2B)	104(2)
C(5A)-C(4A)-N(1A)	114.4(19)
C(5A)-C(4A)-C(3A)	139(2)
N(1A)-C(4A)-C(3A)	106.3(15)
N(2B)-C(4B)-C(3B)	109.9(19)
N(2B)-C(4B)-C(5B)	117(3)
C(3B)-C(4B)-C(5B)	133(3)
C(4A)-C(5A)-N(2A)	118.5(19)
N(1B)-C(5B)-C(4B)	114(2)
N(2A)-C(6A)-C(7A)	113.7(19)

Table D.2.1. continued…

N(1B)-C(6B)-C(7B)	116(3)
C(22A)-C(7A)-C(23A)	110(2)
C(22A)-C(7A)-C(6A)	110.7(18)
C(23A)-C(7A)-C(6A)	107.9(18)
C(22A)-C(7A)-C(8A)	110.8(19)
C(23A)-C(7A)-C(8A)	106.5(18)
C(6A)-C(7A)-C(8A)	110.8(19)
C(8B)-C(7B)-C(23B)	109(2)
C(8B)-C(7B)-C(6B)	115(3)
C(23B)-C(7B)-C(6B)	112(3)
C(8B)-C(7B)-C(22B)	100(2)
C(23B)-C(7B)-C(22B)	111(2)
C(6B)-C(7B)-C(22B)	110(2)
N(3A)-C(8A)-C(7A)	110.5(19)
C(7B)-C(8B)-N(4B)	117(2)
C(11A)-C(9A)-N(3A)	118(2)
N(4B)-C(9B)-C(10B)	122(3)
C(12A)-C(10A)-C(11A)	110(2)
C(11B)-C(10B)-N(3B)	107(2)
C(11B)-C(10B)-C(9B)	140(2)
N(3B)-C(10B)-C(9B)	113(2)
C(9A)-C(11A)-N(4A)	119(2)
C(9A)-C(11A)-C(10A)	136(3)
N(4A)-C(11A)-C(10A)	105(2)
C(10B)-C(11B)-C(13B)	109(2)
C(10A)-C(12A)-C(13A)	107(2)
N(4A)-C(13A)-C(12A)	106(2)
N(4A)-C(13A)-C(14A)	132.5(18)
C(12A)-C(13A)-C(14A)	121.5(19)
C(11B)-C(13B)-N(027)	108(2)
N(6A)-C(14A)-C(13A)	110.3(19)
N(6A)-C(14A)-C(047)	118(2)
C(13A)-C(14A)-C(047)	131.3(19)
N(5B)-C(14B)-C(21B)	125(2)
N(5B)-C(14B)-N(027)	99(4)
C(21B)-C(14B)-N(027)	136(3)
C(16A)-C(15A)-N(6A)	125(3)

Table D.2.1. continued…

C(16A)-C(15A)-C(21A)	117(3)
N(6A)-C(15A)-C(21A)	118(2)
C(20B)-C(15B)-N(5B)	119.1(19)
C(20B)-C(15B)-C(16B)	122(2)
N(5B)-C(15B)-C(16B)	118(2)
C(17A)-C(16A)-C(15A)	129(3)
C(17B)-C(16B)-C(15B)	115(3)
C(16A)-C(17A)-C(19A)	118(2)
C(16B)-C(17B)-C(18B)	122(3)
C(19B)-C(18B)-C(17B)	118(2)
C(20A)-C(19A)-C(17A)	118(2)
C(18B)-C(19B)-C(20B)	129(2)
C(19A)-C(20A)-C(21A)	124(2)
C(15B)-C(20B)-C(19B)	113.6(19)
C(15B)-C(20B)-N(6B)	121(2)
C(19B)-C(20B)-N(6B)	125(2)
N(5A)-C(21A)-C(20A)	124(2)
N(5A)-C(21A)-C(15A)	121(2)
C(20A)-C(21A)-C(15A)	115(2)
N(6B)-C(21B)-C(1B)	117(3)
N(6B)-C(21B)-C(14B)	116(2)
C(1B)-C(21B)-C(14B)	127(2)
F(2A)-C(24A)-F(3A)	112(4)
F(2A)-C(24A)-F(1A)	104(3)
F(3A)-C(24A)-F(1A)	102(3)
F(2A)-C(24A)-S(1A)	112(3)
F(3A)-C(24A)-S(1A)	112(3)
F(1A)-C(24A)-S(1A)	114(3)
F(2B)-C(24B)-F(3B)	118(8)
F(2B)-C(24B)-F(1B)	132(9)
F(3B)-C(24B)-F(1B)	95(6)
F(2B)-C(24B)-S(1B)	121(7)
F(3B)-C(24B)-S(1B)	93(5)
F(1B)-C(24B)-S(1B)	88(5)
N(5A)-C(047)-C(1A)	111.9(19)
N(5A)-C(047)-C(14A)	121(2)
C(1A)-C(047)-C(14A)	127(2)

Table D.2.1. continued…

C(4A)-N(1A)-C(1A)	111.1(18)
C(4A)-N(1A)-Au(1A)	114.2(13)
C(1A)-N(1A)-Au(1A)	134.5(16)
C(6B)-N(1B)-C(5B)	121(3)
C(6B)-N(1B)-Au(1B)	125(3)
C(5B)-N(1B)-Au(1B)	113.4(16)
C(5A)-N(2A)-C(6A)	122.9(19)
C(5A)-N(2A)-Au(1A)	111.7(14)
C(6A)-N(2A)-Au(1A)	123.8(15)
C(1B)-N(2B)-C(4B)	106(2)
C(1B)-N(2B)-Au(1B)	139.8(19)
C(4B)-N(2B)-Au(1B)	113.9(16)
C(9A)-N(3A)-C(8A)	122(2)
C(9A)-N(3A)-Au(1A)	111.7(16)
C(8A)-N(3A)-Au(1A)	124.9(18)
N(027)-N(3B)-C(10B)	112(3)
N(027)-N(3B)-Au(1B)	137(2)
C(10B)-N(3B)-Au(1B)	111.6(14)
C(13A)-N(4A)-C(11A)	112.5(19)
C(13A)-N(4A)-Au(1A)	137.8(14)
C(11A)-N(4A)-Au(1A)	109.3(16)
C(9B)-N(4B)-C(8B)	130(3)
C(9B)-N(4B)-Au(1B)	112.0(18)
C(8B)-N(4B)-Au(1B)	116.9(19)
C(047)-N(5A)-C(21A)	121(2)
C(14B)-N(5B)-C(15B)	115(3)
C(14A)-N(6A)-C(15A)	120.3(19)
C(21B)-N(6B)-C(20B)	124(3)
N(3B)-N(027)-C(13B)	104(3)
N(3B)-N(027)-C(14B)	127(4)
C(13B)-N(027)-C(14B)	129(3)
O(1A)-S(1A)-O(3A)	115.1(13)
O(1A)-S(1A)-O(2A)	115.7(13)
O(3A)-S(1A)-O(2A)	114.7(14)
O(1A)-S(1A)-C(24A)	103.9(16)
O(3A)-S(1A)-C(24A)	101.7(15)
O(2A)-S(1A)-C(24A)	103(2)

Table D.2.1. continued…

O(3B)-S(1B)-O(2B)	113(2)
O(3B)-S(1B)-O(1B)	111(3)
O(2B)-S(1B)-O(1B)	125(3)
O(3B)-S(1B)-C(24B)	97(2)
O(2B)-S(1B)-C(24B)	90(3)
O(1B)-S(1B)-C(24B)	115(3)
N(1A)-Au(1A)-N(3A)	174.0(8)
N(1A)-Au(1A)-N(2A)	80.8(7)
N(3A)-Au(1A)-N(2A)	96.7(8)
N(1A)-Au(1A)-N(4A)	100.1(7)
N(3A)-Au(1A)-N(4A)	81.8(8)
N(2A)-Au(1A)-N(4A)	173.5(7)
N(2B)-Au(1B)-N(3B)	100.3(8)
N(2B)-Au(1B)-N(1B)	81.7(8)
N(3B)-Au(1B)-N(1B)	174.8(8)
N(2B)-Au(1B)-N(4B)	176.5(9)
N(3B)-Au(1B)-N(4B)	81.7(8)
N(1B)-Au(1B)-N(4B)	96.0(9)

Table D.2.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for [Au(L2)](CF_3SO_3). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	54(15)	59(16)	32(12)	26(11)	37(12)	45(13)
C(1B)	51(16)	36(14)	27(12)	6(10)	15(11)	4(12)
C(2A)	34(11)	36(11)	29(11)	-2(8)	15(9)	9(9)
C(2B)	47(14)	66(18)	58(15)	20(13)	30(13)	16(13)
C(3A)	20(9)	45(13)	25(10)	-14(8)	9(8)	-11(8)
C(3B)	45(12)	59(15)	44(13)	12(11)	25(11)	15(12)
C(4A)	36(11)	12(9)	49(12)	10(8)	27(10)	10(8)
C(4B)	39(12)	71(17)	32(11)	23(11)	12(9)	28(12)
C(5A)	44(12)	19(10)	25(10)	7(8)	12(9)	1(9)
C(5B)	58(16)	61(17)	40(14)	20(12)	29(12)	20(13)
C(6A)	43(11)	35(10)	64(18)	-1(11)	28(12)	0(11)
C(6B)	70(20)	180(40)	80(20)	50(20)	50(20)	90(30)
C(7A)	27(10)	61(15)	54(14)	6(11)	10(10)	-5(10)
C(7B)	34(12)	84(18)	53(15)	20(13)	22(11)	-4(12)
C(8A)	35(12)	76(19)	33(13)	13(12)	16(11)	14(12)
C(8B)	38(14)	100(20)	59(17)	-9(16)	1(12)	18(15)
C(9A)	24(10)	54(15)	34(11)	-7(11)	10(9)	-5(11)
C(9B)	29(11)	80(20)	41(12)	-20(13)	17(10)	-6(13)
C(10A)	61(16)	33(12)	23(11)	-1(9)	1(10)	-16(11)
C(10B)	58(15)	41(12)	27(11)	-1(10)	17(11)	-3(11)
C(11A)	90(20)	46(15)	43(15)	-15(12)	42(16)	-9(15)
C(11B)	70(16)	43(13)	49(14)	5(11)	38(13)	-5(12)
C(12A)	33(12)	72(18)	33(12)	8(11)	9(10)	0(12)
C(13A)	64(18)	49(12)	18(9)	-20(10)	23(11)	-23(12)
C(13B)	53(14)	68(18)	22(11)	9(11)	19(10)	1(13)
C(14A)	50(13)	18(10)	35(11)	4(8)	32(11)	-8(9)
C(14B)	21(17)	200(50)	40(20)	1(19)	26(16)	-17(17)
C(15A)	46(13)	38(11)	42(12)	0(9)	27(11)	8(10)
C(15B)	30(11)	58(15)	29(11)	22(10)	15(9)	19(10)
C(16A)	110(20)	28(12)	80(20)	16(13)	60(19)	7(15)
C(16B)	49(15)	130(30)	33(13)	-9(15)	14(11)	-27(17)
C(17A)	83(19)	25(12)	58(16)	2(11)	20(14)	-11(13)
C(17B)	8(9)	90(20)	66(17)	-10(14)	16(10)	9(11)
C(18B)	51(13)	42(13)	69(15)	-15(11)	44(12)	-22(11)

Table D.2.2. continued…

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(19A)	90(20)	29(13)	79(19)	0(12)	31(16)	4(13)
C(19B)	27(4)	28(4)	27(4)	1(1)	13(2)	-1(1)
C(20A)	31(11)	48(13)	33(11)	-3(9)	15(9)	-2(10)
C(20B)	37(11)	59(15)	32(11)	4(9)	16(9)	4(10)
C(21A)	45(14)	100(20)	19(10)	-3(12)	18(10)	14(14)
C(21B)	20(13)	110(30)	18(12)	32(12)	6(10)	2(13)
C(22A)	34(10)	36(11)	55(13)	13(10)	16(9)	7(9)
C(22B)	27(11)	90(19)	66(17)	22(14)	14(11)	22(12)
C(23A)	30(11)	48(14)	82(18)	13(12)	13(11)	2(10)
C(23B)	37(12)	72(17)	65(16)	4(13)	17(11)	-4(11)
C(24A)	36(16)	60(20)	210(50)	30(20)	-10(20)	-19(15)
C(24B)	120(40)	440(120)	70(30)	-30(50)	20(30)	150(60)
C(047)	19(9)	60(16)	9(9)	-5(9)	2(7)	-15(10)
N(1A)	39(9)	38(10)	38(9)	5(8)	27(8)	-3(8)
N(1B)	42(12)	88(18)	24(10)	0(10)	9(9)	16(12)
N(2A)	35(9)	52(11)	33(9)	5(8)	15(8)	1(8)
N(2B)	31(10)	64(13)	26(10)	9(9)	14(8)	0(9)
N(3A)	62(14)	52(12)	49(12)	14(10)	35(11)	21(11)
N(3B)	16(8)	91(15)	17(8)	14(9)	7(7)	-5(9)
N(4A)	34(9)	43(11)	31(9)	-19(8)	15(8)	0(8)
N(4B)	47(13)	70(16)	58(15)	22(12)	15(11)	29(12)
N(5A)	40(10)	40(10)	38(9)	2(8)	26(8)	14(8)
N(5B)	46(12)	48(13)	26(10)	12(9)	8(9)	0(10)
N(6A)	27(8)	42(10)	22(7)	8(6)	7(6)	-8(7)
N(6B)	32(10)	75(14)	40(11)	2(10)	20(9)	-3(10)
N(027)	100(20)	170(40)	21(13)	26(17)	24(14)	20(20)
O(1A)	35(9)	84(13)	78(14)	-19(11)	1(9)	5(9)
O(1B)	230(40)	58(17)	390(70)	30(30)	200(40)	-20(20)
O(2A)	39(10)	150(20)	140(20)	-54(17)	13(12)	31(12)
O(2B)	360(60)	500(80)	250(50)	190(50)	230(50)	370(70)
O(3A)	47(10)	93(14)	116(18)	-37(13)	29(11)	-18(10)
O(3B)	270(40)	120(20)	76(17)	40(16)	80(20)	110(30)
F(1A)	88(12)	66(11)	160(20)	17(12)	36(13)	7(10)
F(1B)	130(20)	220(30)	180(30)	110(30)	-20(20)	-50(20)
F(2A)	74(12)	79(13)	180(20)	11(13)	31(14)	27(11)
F(2B)	210(40)	160(30)	400(80)	100(40)	80(40)	-70(30)

Table D.2.2. continued…

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(3A)	58(10)	135(18)	114(15)	14(13)	19(10)	8(11)
F(3B)	190(30)	150(30)	200(30)	-70(20)	80(30)	20(20)
S(1A)	45(4)	80(5)	92(6)	-19(4)	3(4)	6(4)
S(1B)	184(12)	109(8)	112(8)	34(6)	83(9)	82(9)
Au(1A)	25(1)	30(1)	29(1)	2(1)	11(1)	0(1)
Au(1B)	28(1)	62(1)	27(1)	0(1)	10(1)	5(1)

Table D.2.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [Au(L2)](CF_3SO_3).

	x	y	z	U(eq)
H(2A)	12266	389	3715	40
H(2B)	-1103	8722	3526	66
H(3A)	12271	1344	3698	37
H(3B)	305	8182	4590	57
H(5A)	10768	2087	2352	38
H(5B)	2148	8533	6117	61
H(6A1)	9074	2239	179	56
H(6A2)	9310	2505	1354	56
H(6B1)	3472	9037	6928	127
H(6B2)	3229	9344	7764	127
H(8A1)	6839	1728	-648	58
H(8A2)	7581	1771	-1041	58
H(8B1)	3855	10589	7276	91
H(8B2)	3446	10286	7946	91
H(9A)	6690	802	-852	47
H(9B)	2561	11247	6548	60
H(10A)	6826	-330	-666	56
H(11B)	821	11822	5122	60
H(12A)	8127	-910	443	59
H(13B)	-737	11465	3901	57
H(16A)	10022	-1908	1890	77
H(16B)	-3168	11113	1676	87
H(17A)	11159	-2394	2859	74
H(17B)	-4531	10694	759	69
H(18B)	-4626	9768	760	57
H(19A)	12596	-1987	3954	82
H(19B)	-3470	9326	1783	33
H(20A)	12661	-1087	4011	46
H(22A)	8436	2214	2263	66
H(22B)	7915	1679	1721	66
H(22C)	7369	2214	1511	66
H(22D)	4975	10151	7969	97
H(22E)	5009	9534	7775	97
H(22F)	4698	9743	8640	97
H(23A)	7034	2727	105	89

Table D.2.3 continued…

	x	y	z	U(eq)
H(23B)	7413	2679	-758	89
H(23C)	7994	2966	424	89
H(23D)	3017	9876	5258	92
H(23E)	3950	9571	5741	92
H(23F)	3938	10196	5819	92

Table D.4.4: Torsion angles [°] for [Au(L2)](CF_3SO_3).

N(1A)-C(1A)-C(2A)-C(3A)	1(2)
C(047)-C(1A)-C(2A)-C(3A)	178.2(18)
N(2B)-C(1B)-C(2B)-C(3B)	1(3)
C(21B)-C(1B)-C(2B)-C(3B)	178(2)
C(1A)-C(2A)-C(3A)-C(4A)	-1(2)
C(1B)-C(2B)-C(3B)-C(4B)	0(3)
C(2A)-C(3A)-C(4A)-C(5A)	-177(3)
C(2A)-C(3A)-C(4A)-N(1A)	1(2)
C(2B)-C(3B)-C(4B)-N(2B)	-1(2)
C(2B)-C(3B)-C(4B)-C(5B)	178(2)
N(1A)-C(4A)-C(5A)-N(2A)	3(3)
C(3A)-C(4A)-C(5A)-N(2A)	-178(2)
N(2B)-C(4B)-C(5B)-N(1B)	-1(3)
C(3B)-C(4B)-C(5B)-N(1B)	180(2)
N(2A)-C(6A)-C(7A)-C(22A)	55(3)
N(2A)-C(6A)-C(7A)-C(23A)	176(2)
N(2A)-C(6A)-C(7A)-C(8A)	-68(3)
N(1B)-C(6B)-C(7B)-C(8B)	66(4)
N(1B)-C(6B)-C(7B)-C(23B)	-58(4)
N(1B)-C(6B)-C(7B)-C(22B)	178(3)
C(22A)-C(7A)-C(8A)-N(3A)	-56(3)
C(23A)-C(7A)-C(8A)-N(3A)	-176(2)
C(6A)-C(7A)-C(8A)-N(3A)	67(3)
C(23B)-C(7B)-C(8B)-N(4B)	58(3)
C(6B)-C(7B)-C(8B)-N(4B)	-68(4)
C(22B)-C(7B)-C(8B)-N(4B)	174(3)
N(4B)-C(9B)-C(10B)-C(11B)	-174(3)
N(4B)-C(9B)-C(10B)-N(3B)	3(3)
N(3A)-C(9A)-C(11A)-N(4A)	-2(3)
N(3A)-C(9A)-C(11A)-C(10A)	-178(3)
C(12A)-C(10A)-C(11A)-C(9A)	177(3)
C(12A)-C(10A)-C(11A)-N(4A)	1(3)
N(3B)-C(10B)-C(11B)-C(13B)	2(3)
C(9B)-C(10B)-C(11B)-C(13B)	179(3)
C(11A)-C(10A)-C(12A)-C(13A)	-2(3)
C(10A)-C(12A)-C(13A)-N(4A)	3(3)

Table D.4.4. continued…

C(10A)-C(12A)-C(13A)-C(14A)	179(2)
C(10B)-C(11B)-C(13B)-N(027)	-3(3)
N(4A)-C(13A)-C(14A)-N(6A)	178(2)
C(12A)-C(13A)-C(14A)-N(6A)	3(3)
N(4A)-C(13A)-C(14A)-C(047)	-6(4)
C(12A)-C(13A)-C(14A)-C(047)	179(2)
N(6A)-C(15A)-C(16A)-C(17A)	179(3)
C(21A)-C(15A)-C(16A)-C(17A)	5(4)
C(20B)-C(15B)-C(16B)-C(17B)	2(3)
N(5B)-C(15B)-C(16B)-C(17B)	-178(2)
C(15A)-C(16A)-C(17A)-C(19A)	-5(5)
C(15B)-C(16B)-C(17B)-C(18B)	-3(4)
C(16B)-C(17B)-C(18B)-C(19B)	4(4)
C(16A)-C(17A)-C(19A)-C(20A)	2(4)
C(17B)-C(18B)-C(19B)-C(20B)	-3(4)
C(17A)-C(19A)-C(20A)-C(21A)	0(4)
N(5B)-C(15B)-C(20B)-C(19B)	178.7(19)
C(16B)-C(15B)-C(20B)-C(19B)	-1(3)
N(5B)-C(15B)-C(20B)-N(6B)	0(3)
C(16B)-C(15B)-C(20B)-N(6B)	-179(2)
C(18B)-C(19B)-C(20B)-C(15B)	1(3)
C(18B)-C(19B)-C(20B)-N(6B)	179(2)
C(19A)-C(20A)-C(21A)-N(5A)	-180(2)
C(19A)-C(20A)-C(21A)-C(15A)	0(3)
C(16A)-C(15A)-C(21A)-N(5A)	178(2)
N(6A)-C(15A)-C(21A)-N(5A)	3(3)
C(16A)-C(15A)-C(21A)-C(20A)	-3(3)
N(6A)-C(15A)-C(21A)-C(20A)	-177.0(18)
C(2B)-C(1B)-C(21B)-N(6B)	7(3)
N(2B)-C(1B)-C(21B)-N(6B)	-178(3)
C(2B)-C(1B)-C(21B)-C(14B)	-175(2)
N(2B)-C(1B)-C(21B)-C(14B)	1(4)
N(5B)-C(14B)-C(21B)-N(6B)	-6(4)
N(027)-C(14B)-C(21B)-N(6B)	170(3)
N(5B)-C(14B)-C(21B)-C(1B)	175(3)
N(027)-C(14B)-C(21B)-C(1B)	-9(4)
C(2A)-C(1A)-C(047)-N(5A)	3(3)

Table D.4.4. continued…

N(1A)-C(1A)-C(047)-N(5A)	179(2)
C(2A)-C(1A)-C(047)-C(14A)	179.1(18)
N(1A)-C(1A)-C(047)-C(14A)	-5(4)
N(6A)-C(14A)-C(047)-N(5A)	-3(3)
C(13A)-C(14A)-C(047)-N(5A)	-179(2)
N(6A)-C(14A)-C(047)-C(1A)	-178.5(19)
C(13A)-C(14A)-C(047)-C(1A)	5(4)
C(5A)-C(4A)-N(1A)-C(1A)	178.3(18)
C(3A)-C(4A)-N(1A)-C(1A)	-1(2)
C(5A)-C(4A)-N(1A)-Au(1A)	2(2)
C(3A)-C(4A)-N(1A)-Au(1A)	-176.9(12)
C(2A)-C(1A)-N(1A)-C(4A)	0(2)
C(047)-C(1A)-N(1A)-C(4A)	-177(2)
C(2A)-C(1A)-N(1A)-Au(1A)	175.1(13)
C(047)-C(1A)-N(1A)-Au(1A)	-1(3)
C(7B)-C(6B)-N(1B)-C(5B)	153(3)
C(7B)-C(6B)-N(1B)-Au(1B)	-31(4)
C(4B)-C(5B)-N(1B)-C(6B)	176(2)
C(4B)-C(5B)-N(1B)-Au(1B)	-1(2)
C(4A)-C(5A)-N(2A)-C(6A)	-173(2)
C(4A)-C(5A)-N(2A)-Au(1A)	-7(2)
C(7A)-C(6A)-N(2A)-C(5A)	-155(2)
C(7A)-C(6A)-N(2A)-Au(1A)	41(3)
C(2B)-C(1B)-N(2B)-C(4B)	-2(3)
C(21B)-C(1B)-N(2B)-C(4B)	-178(3)
C(2B)-C(1B)-N(2B)-Au(1B)	177.5(18)
C(21B)-C(1B)-N(2B)-Au(1B)	1(5)
C(3B)-C(4B)-N(2B)-C(1B)	2(2)
C(5B)-C(4B)-N(2B)-C(1B)	-177(2)
C(3B)-C(4B)-N(2B)-Au(1B)	-177.5(14)
C(5B)-C(4B)-N(2B)-Au(1B)	3(2)
C(11A)-C(9A)-N(3A)-C(8A)	172(2)
C(11A)-C(9A)-N(3A)-Au(1A)	5(3)
C(7A)-C(8A)-N(3A)-C(9A)	153(2)
C(7A)-C(8A)-N(3A)-Au(1A)	-42(3)
C(11B)-C(10B)-N(3B)-N(027)	-1(3)
C(9B)-C(10B)-N(3B)-N(027)	-178(2)

Table D.4.4. continued…

C(11B)-C(10B)-N(3B)-Au(1B)	176.7(16)
C(9B)-C(10B)-N(3B)-Au(1B)	-1(2)
C(12A)-C(13A)-N(4A)-C(11A)	-2(2)
C(14A)-C(13A)-N(4A)-C(11A)	-178(2)
C(12A)-C(13A)-N(4A)-Au(1A)	-174.1(17)
C(14A)-C(13A)-N(4A)-Au(1A)	10(4)
C(9A)-C(11A)-N(4A)-C(13A)	-176(2)
C(10A)-C(11A)-N(4A)-C(13A)	1(3)
C(9A)-C(11A)-N(4A)-Au(1A)	-2(3)
C(10A)-C(11A)-N(4A)-Au(1A)	175.2(16)
C(10B)-C(9B)-N(4B)-C(8B)	-172(3)
C(10B)-C(9B)-N(4B)-Au(1B)	-3(3)
C(7B)-C(8B)-N(4B)-C(9B)	-157(3)
C(7B)-C(8B)-N(4B)-Au(1B)	34(4)
C(1A)-C(047)-N(5A)-C(21A)	-180.0(18)
C(14A)-C(047)-N(5A)-C(21A)	4(3)
C(20A)-C(21A)-N(5A)-C(047)	176(2)
C(15A)-C(21A)-N(5A)-C(047)	-4(3)
C(21B)-C(14B)-N(5B)-C(15B)	4(3)
N(027)-C(14B)-N(5B)-C(15B)	-174(2)
C(20B)-C(15B)-N(5B)-C(14B)	-1(3)
C(16B)-C(15B)-N(5B)-C(14B)	179(2)
C(13A)-C(14A)-N(6A)-C(15A)	179.1(18)
C(047)-C(14A)-N(6A)-C(15A)	2(3)
C(16A)-C(15A)-N(6A)-C(14A)	-176(2)
C(21A)-C(15A)-N(6A)-C(14A)	-2(3)
C(1B)-C(21B)-N(6B)-C(20B)	-176(2)
C(14B)-C(21B)-N(6B)-C(20B)	6(3)
C(15B)-C(20B)-N(6B)-C(21B)	-3(3)
C(19B)-C(20B)-N(6B)-C(21B)	179(2)
C(10B)-N(3B)-N(027)-C(13B)	-1(3)
Au(1B)-N(3B)-N(027)-C(13B)	-177.3(15)
C(10B)-N(3B)-N(027)-C(14B)	179(2)
Au(1B)-N(3B)-N(027)-C(14B)	2(4)
C(11B)-C(13B)-N(027)-N(3B)	2(3)
C(11B)-C(13B)-N(027)-C(14B)	-178(2)
N(5B)-C(14B)-N(027)-N(3B)	-175(3)

Table D.4.4. continued…

C(21B)-C(14B)-N(027)-N(3B)	8(5)
N(5B)-C(14B)-N(027)-C(13B)	4(3)
C(21B)-C(14B)-N(027)-C(13B)	-172(3)
F(2A)-C(24A)-S(1A)-O(1A)	-55(3)
F(3A)-C(24A)-S(1A)-O(1A)	177(2)
F(1A)-C(24A)-S(1A)-O(1A)	62(3)
F(2A)-C(24A)-S(1A)-O(3A)	64(2)
F(3A)-C(24A)-S(1A)-O(3A)	-63(3)
F(1A)-C(24A)-S(1A)-O(3A)	-178(2)
F(2A)-C(24A)-S(1A)-O(2A)	-176(2)
F(3A)-C(24A)-S(1A)-O(2A)	56(3)
F(1A)-C(24A)-S(1A)-O(2A)	-59(3)
F(2B)-C(24B)-S(1B)-O(3B)	48(8)
F(3B)-C(24B)-S(1B)-O(3B)	-77(4)
F(1B)-C(24B)-S(1B)-O(3B)	-172(3)
F(2B)-C(24B)-S(1B)-O(2B)	-66(8)
F(3B)-C(24B)-S(1B)-O(2B)	169(4)
F(1B)-C(24B)-S(1B)-O(2B)	74(4)
F(2B)-C(24B)-S(1B)-O(1B)	165(7)
F(3B)-C(24B)-S(1B)-O(1B)	39(4)
F(1B)-C(24B)-S(1B)-O(1B)	-56(4)
C(4A)-N(1A)-Au(1A)-N(3A)	-70(9)
C(1A)-N(1A)-Au(1A)-N(3A)	115(8)
C(4A)-N(1A)-Au(1A)-N(2A)	-4.4(12)
C(1A)-N(1A)-Au(1A)-N(2A)	-179.6(18)
C(4A)-N(1A)-Au(1A)-N(4A)	-177.8(12)
C(1A)-N(1A)-Au(1A)-N(4A)	7.0(18)
C(9A)-N(3A)-Au(1A)-N(1A)	-113(8)
C(8A)-N(3A)-Au(1A)-N(1A)	81(9)
C(9A)-N(3A)-Au(1A)-N(2A)	-177.9(15)
C(8A)-N(3A)-Au(1A)-N(2A)	16(2)
C(9A)-N(3A)-Au(1A)-N(4A)	-4.3(14)
C(8A)-N(3A)-Au(1A)-N(4A)	-171(2)
C(5A)-N(2A)-Au(1A)-N(1A)	5.8(14)
C(6A)-N(2A)-Au(1A)-N(1A)	171.5(19)
C(5A)-N(2A)-Au(1A)-N(3A)	-179.7(15)
C(6A)-N(2A)-Au(1A)-N(3A)	-14.0(19)

Table D.4.4. continued…

C(5A)-N(2A)-Au(1A)-N(4A)	104(7)
C(6A)-N(2A)-Au(1A)-N(4A)	-90(7)
C(13A)-N(4A)-Au(1A)-N(1A)	-11(2)
C(11A)-N(4A)-Au(1A)-N(1A)	177.4(14)
C(13A)-N(4A)-Au(1A)-N(3A)	175(2)
C(11A)-N(4A)-Au(1A)-N(3A)	3.2(15)
C(13A)-N(4A)-Au(1A)-N(2A)	-108(7)
C(11A)-N(4A)-Au(1A)-N(2A)	80(7)
C(1B)-N(2B)-Au(1B)-N(3B)	3(3)
C(4B)-N(2B)-Au(1B)-N(3B)	-178.2(14)
C(1B)-N(2B)-Au(1B)-N(1B)	178(2)
C(4B)-N(2B)-Au(1B)-N(1B)	-3.0(16)
C(1B)-N(2B)-Au(1B)-N(4B)	130(15)
C(4B)-N(2B)-Au(1B)-N(4B)	-51(17)
N(027)-N(3B)-Au(1B)-N(2B)	-6(3)
C(10B)-N(3B)-Au(1B)-N(2B)	177.1(14)
N(027)-N(3B)-Au(1B)-N(1B)	-119(10)
C(10B)-N(3B)-Au(1B)-N(1B)	64(11)
N(027)-N(3B)-Au(1B)-N(4B)	176(2)
C(10B)-N(3B)-Au(1B)-N(4B)	-0.1(16)
C(6B)-N(1B)-Au(1B)-N(2B)	-175(2)
C(5B)-N(1B)-Au(1B)-N(2B)	2.3(17)
C(6B)-N(1B)-Au(1B)-N(3B)	-61(11)
C(5B)-N(1B)-Au(1B)-N(3B)	116(10)
C(6B)-N(1B)-Au(1B)-N(4B)	3(3)
C(5B)-N(1B)-Au(1B)-N(4B)	179.6(16)
C(9B)-N(4B)-Au(1B)-N(2B)	-126(15)
C(8B)-N(4B)-Au(1B)-N(2B)	45(17)
C(9B)-N(4B)-Au(1B)-N(3B)	1(2)
C(8B)-N(4B)-Au(1B)-N(3B)	172(2)
C(9B)-N(4B)-Au(1B)-N(1B)	-173.9(19)
C(8B)-N(4B)-Au(1B)-N(1B)	-3(2)

D.3: Full crystallographic Data Tables of [Au(L3)](PF_6)

Table D.3.1: Bond lengths [Å] and angles [°] for [Au(L3)](PF_6)

Au(1)-N(4A)	1.976(12)
Au(1)-N(1A)	1.990(12)
Au(1)-N(3A)	2.018(14)
Au(1)-N(2A)	2.028(11)
Au(2)-N(1B)	1.972(12)
Au(2)-N(4B)	1.980(12)
Au(2)-N(3B)	2.025(11)
Au(2)-N(2B)	2.033(13)
Au(3)-N(1C)	1.973(15)
Au(3)-N(4C)	1.982(14)
Au(3)-N(3C)	2.028(13)
Au(3)-N(2C)	2.064(13)
Au(4)-N(4D)	1.975(11)
Au(4)-N(1D)	1.997(14)
Au(4)-N(2D)	2.011(12)
Au(4)-N(3D)	2.015(12)
Au(5)-N(4E)	1.974(14)
Au(5)-N(1E)	2.002(11)
Au(5)-N(2E)	2.012(11)
Au(5)-N(3E)	2.045(12)
Au(6)-N(2F)	1.967(14)
Au(6)-N(4F)	1.985(16)
Au(6)-N(1F)	1.993(14)
Au(6)-N(3F)	2.004(13)
P(1)-F(4)	1.579(11)
P(1)-F(5)	1.583(9)
P(1)-F(2)	1.592(11)
P(1)-F(1)	1.593(11)
P(1)-F(3)	1.594(12)
P(1)-F(6)	1.608(10)
P(2)-F(9)	1.573(11)
P(2)-F(12)	1.579(10)
P(2)-F(7)	1.600(10)
P(2)-F(10)	1.607(9)

Table D.3.1 continued…

P(2)-F(8)	1.611(9)
P(2)-F(11)	1.650(12)
P(3)-F(18)	1.581(10)
P(3)-F(15)	1.584(11)
P(3)-F(14)	1.595(9)
P(3)-F(13)	1.599(12)
P(3)-F(16)	1.602(9)
P(3)-F(17)	1.609(9)
P(4)-F(23)	1.587(11)
P(4)-F(20)	1.592(10)
P(4)-F(19)	1.603(10)
P(4)-F(22)	1.610(10)
P(4)-F(21)	1.619(9)
P(4)-F(24)	1.622(12)
P(5)-F(26)	1.576(10)
P(5)-F(28)	1.582(9)
P(5)-F(30)	1.590(9)
P(5)-F(25)	1.592(9)
P(5)-F(27)	1.606(9)
P(5)-F(29)	1.609(10)
P(6)-F(31)	1.572(10)
P(6)-F(35)	1.584(10)
P(6)-F(34)	1.597(13)
P(6)-F(32)	1.598(11)
P(6)-F(33)	1.605(10)
P(6)-F(36)	1.614(9)
N(1A)-C(1A)	1.343(18)
N(1A)-C(4A)	1.394(17)
N(1B)-C(1B)	1.380(19)
N(1B)-C(4B)	1.42(2)
N(1C)-C(4C)	1.37(2)
N(1C)-C(1C)	1.38(2)
N(1D)-C(4D)	1.34(2)
N(1D)-C(1D)	1.35(2)
N(1E)-C(1E)	1.322(18)
N(1E)-C(4E)	1.381(18)
N(1F)-C(1F)	1.33(2)

Table D.3.1 continued…

N(1F)-C(4F)	1.40(2)
N(1S)-C(1S)	1.10(2)
N(2A)-C(5A)	1.303(18)
N(2A)-C(6A)	1.496(18)
N(2B)-C(5B)	1.347(19)
N(2B)-C(6B)	1.444(19)
N(2C)-C(5C)	1.29(2)
N(2C)-C(6C)	1.45(2)
N(2D)-C(5D)	1.32(2)
N(2D)-C(6D)	1.45(2)
N(2E)-C(5E)	1.282(17)
N(2E)-C(6E)	1.468(15)
N(2F)-C(5F)	1.35(2)
N(2F)-C(6F)	1.49(2)
N(2S)-C(3S)	1.15(3)
N(3A)-C(10A)	1.304(19)
N(3A)-C(9A)	1.488(19)
N(3B)-C(10B)	1.295(18)
N(3B)-C(9B)	1.467(17)
N(3C)-C(10C)	1.26(2)
N(3C)-C(9C)	1.493(19)
N(3D)-C(10D)	1.286(18)
N(3D)-C(9D)	1.492(17)
N(3E)-C(10E)	1.28(2)
N(3E)-C(9E)	1.49(2)
N(3F)-C(10F)	1.32(2)
N(3F)-C(9F)	1.48(2)
N(3S)-C(5S)	1.119(18)
N(4A)-C(14A)	1.36(2)
N(4A)-C(11A)	1.39(2)
N(4B)-C(14B)	1.347(19)
N(4B)-C(11B)	1.406(17)
N(4C)-C(11C)	1.37(2)
N(4C)-C(14C)	1.37(2)
N(4D)-C(14D)	1.393(18)
N(4D)-C(11D)	1.409(18)
N(4E)-C(14E)	1.38(2)

Table D.3.1 continued…

N(4E)-C(11E)	1.40(2)
N(4F)-C(14F)	1.35(2)
N(4F)-C(11F)	1.41(2)
N(4S)-C(7S)	1.126(19)
N(5A)-C(15A)	1.360(19)
N(5A)-C(17A)	1.36(2)
N(5B)-C(17B)	1.337(19)
N(5B)-C(15B)	1.34(2)
N(5C)-C(15C)	1.34(2)
N(5C)-C(17C)	1.35(2)
N(5E)-C(15E)	1.33(2)
N(5E)-C(17E)	1.34(3)
N(5F)-C(15F)	1.33(2)
N(5F)-C(17F)	1.34(2)
N(5S)-C(9S)	1.10(3)
N(6A)-C(16A)	1.33(2)
N(6A)-C(22A)	1.36(2)
N(6B)-C(16B)	1.327(19)
N(6B)-C(22B)	1.330(19)
N(6C)-C(16C)	1.34(2)
N(6C)-C(22C)	1.34(2)
N(6E)-C(16E)	1.33(2)
N(6E)-C(22E)	1.35(3)
N(6F)-C(22F)	1.32(2)
N(6F)-C(16F)	1.35(2)
N(6S)-C(11S)	1.16(2)
N(41)-C(15D)	1.34(2)
N(41)-C(17D)	1.38(3)
N(42)-C(22D)	1.35(3)
N(42)-C(16D)	1.35(2)
C(1A)-C(2A)	1.42(2)
C(1A)-C(16A)	1.480(19)
C(1B)-C(2B)	1.37(2)
C(1B)-C(16B)	1.48(2)
C(1C)-C(2C)	1.45(2)
C(1C)-C(16C)	1.46(2)
C(1D)-C(2D)	1.42(3)

Table D.3.1 continued…

C(1D)-C(16D)	1.49(2)
C(1E)-C(16E)	1.43(2)
C(1E)-C(2E)	1.44(2)
C(1F)-C(2F)	1.42(3)
C(1F)-C(16F)	1.49(3)
C(1S)-C(2S)	1.48(2)
C(2A)-C(3A)	1.39(2)
C(2A)-H(2A)	0.9500
C(2B)-C(3B)	1.40(2)
C(2B)-H(2B)	0.9500
C(2C)-C(3C)	1.37(2)
C(2C)-H(2C)	0.9500
C(2D)-C(3D)	1.32(3)
C(2D)-H(2D)	0.9500
C(2E)-C(3E)	1.33(2)
C(2E)-H(2E)	0.9500
C(2F)-C(3F)	1.42(3)
C(2F)-H(2F)	0.9500
C(2S)-H(2SA)	0.9800
C(2S)-H(2SB)	0.9800
C(2S)-H(2SC)	0.9800
C(3A)-C(4A)	1.41(2)
C(3A)-H(3A)	0.9500
C(3B)-C(4B)	1.37(2)
C(3B)-H(3B)	0.9500
C(3C)-C(4C)	1.37(2)
C(3C)-H(3C)	0.9500
C(3D)-C(4D)	1.42(3)
C(3D)-H(3D)	0.9500
C(3E)-C(4E)	1.40(2)
C(3E)-H(3E)	0.9500
C(3F)-C(4F)	1.42(3)
C(3F)-H(3F)	0.9500
C(3S)-C(4S)	1.43(3)
C(4A)-C(5A)	1.38(2)
C(4B)-C(5B)	1.35(2)
C(4C)-C(5C)	1.40(2)

Table D.3.1 continued…

C(4D)-C(5D)	1.44(3)
C(4E)-C(5E)	1.429(19)
C(4F)-C(5F)	1.41(2)
C(4S)-H(4SA)	0.9800
C(4S)-H(4SB)	0.9800
C(4S)-H(4SC)	0.9800
C(5A)-H(5A)	0.9500
C(5B)-H(5B)	0.9500
C(5C)-H(5C)	0.9500
C(5D)-H(5D)	0.9500
C(5E)-H(5E)	0.9500
C(5F)-H(5F)	0.9500
C(5S)-C(6S)	1.48(2)
C(6A)-C(7A)	1.51(2)
C(6A)-H(6AA)	0.9900
C(6A)-H(6AB)	0.9900
C(6B)-C(7B)	1.51(2)
C(6B)-H(6BA)	0.9900
C(6B)-H(6BB)	0.9900
C(6C)-C(7C)	1.50(2)
C(6C)-H(6CA)	0.9900
C(6C)-H(6CB)	0.9900
C(6D)-C(7D)	1.56(2)
C(6D)-H(6DA)	0.9900
C(6D)-H(6DB)	0.9900
C(6E)-C(7E)	1.524(18)
C(6E)-H(6EA)	0.9900
C(6E)-H(6EB)	0.9900
C(6F)-C(7F)	1.48(2)
C(6F)-H(6FA)	0.9900
C(6F)-H(6FB)	0.9900
C(6S)-H(6SA)	0.9800
C(6S)-H(6SB)	0.9800
C(6S)-H(6SC)	0.9800
C(7A)-C(8A)	1.48(2)
C(7A)-H(7AA)	0.9900
C(7A)-H(7AB)	0.9900

Table D.3.1 continued…

C(7B)-C(8B)	1.56(2)
C(7B)-H(7BA)	0.9900
C(7B)-H(7BB)	0.9900
C(7C)-C(8C)	1.57(2)
C(7C)-H(7CA)	0.9900
C(7C)-H(7CB)	0.9900
C(7D)-C(8D)	1.49(2)
C(7D)-H(7DA)	0.9900
C(7D)-H(7DB)	0.9900
C(7E)-C(8E)	1.52(2)
C(7E)-H(7EA)	0.9900
C(7E)-H(7EB)	0.9900
C(7F)-C(8F)	1.55(3)
C(7F)-H(7FA)	0.9900
C(7F)-H(7FB)	0.9900
C(7S)-C(8S)	1.49(2)
C(8A)-C(9A)	1.52(2)
C(8A)-H(8AA)	0.9900
C(8A)-H(8AB)	0.9900
C(8B)-C(9B)	1.543(19)
C(8B)-H(8BA)	0.9900
C(8B)-H(8BB)	0.9900
C(8C)-C(9C)	1.49(2)
C(8C)-H(8CA)	0.9900
C(8C)-H(8CB)	0.9900
C(8D)-C(9D)	1.510(18)
C(8D)-H(8DA)	0.9900
C(8D)-H(8DB)	0.9900
C(8E)-C(9E)	1.50(2)
C(8E)-H(8EA)	0.9900
C(8E)-H(8EB)	0.9900
C(8F)-C(9F)	1.50(2)
C(8F)-H(8FA)	0.9900
C(8F)-H(8FB)	0.9900
C(8S)-H(8SA)	0.9800
C(8S)-H(8SB)	0.9800
C(8S)-H(8SC)	0.9800

Table D.3.1 continued…

C(9A)-H(9AA)	0.9900
C(9A)-H(9AB)	0.9900
C(9B)-H(9BA)	0.9900
C(9B)-H(9BB)	0.9900
C(9C)-H(9CA)	0.9900
C(9C)-H(9CB)	0.9900
C(9D)-H(9DA)	0.9900
C(9D)-H(9DB)	0.9900
C(9E)-H(9EA)	0.9900
C(9E)-H(9EB)	0.9900
C(9F)-H(9FA)	0.9900
C(9F)-H(9FB)	0.9900
C(9S)-C(10S)	1.49(3)
C(10A)-C(11A)	1.43(2)
C(10A)-H(10A)	0.9500
C(10B)-C(11B)	1.412(19)
C(10B)-H(10B)	0.9500
C(10C)-C(11C)	1.37(2)
C(10C)-H(10C)	0.9500
C(10D)-C(11D)	1.39(2)
C(10D)-H(10D)	0.9500
C(10E)-C(11E)	1.40(3)
C(10E)-H(10E)	0.9500
C(10F)-C(11F)	1.41(2)
C(10F)-H(10F)	0.9500
C(10S)-H(10G)	0.9800
C(10S)-H(10H)	0.9800
C(10S)-H(10I)	0.9800
C(11A)-C(12A)	1.40(2)
C(11B)-C(12B)	1.38(2)
C(11C)-C(12C)	1.37(2)
C(11D)-C(12D)	1.41(2)
C(11E)-C(12E)	1.36(3)
C(11F)-C(12F)	1.36(3)
C(11S)-C(12S)	1.45(3)
C(12A)-C(13A)	1.36(2)
C(12A)-H(12A)	0.9500

Table D.3.1 continued…

C(12B)-C(13B)	1.39(2)
C(12B)-H(12B)	0.9500
C(12C)-C(13C)	1.38(3)
C(12C)-H(12C)	0.9500
C(12D)-C(13D)	1.37(2)
C(12D)-H(12D)	0.9500
C(12E)-C(13E)	1.43(3)
C(12E)-H(12E)	0.9500
C(12F)-C(13F)	1.38(2)
C(12F)-H(12F)	0.9500
C(12S)-H(12G)	0.9800
C(12S)-H(12H)	0.9800
C(12S)-H(12I)	0.9800
C(13A)-C(14A)	1.42(2)
C(13A)-H(13A)	0.9500
C(13B)-C(14B)	1.40(2)
C(13B)-H(13B)	0.9500
C(13C)-C(14C)	1.38(3)
C(13C)-H(13C)	0.9500
C(13D)-C(14D)	1.39(2)
C(13D)-H(13D)	0.9500
C(13E)-C(14E)	1.41(3)
C(13E)-H(13E)	0.9500
C(13F)-C(14F)	1.41(2)
C(13F)-H(13F)	0.9500
C(14A)-C(15A)	1.45(2)
C(14B)-C(15B)	1.52(2)
C(14C)-C(15C)	1.48(3)
C(14D)-C(15D)	1.48(2)
C(14E)-C(15E)	1.45(2)
C(14F)-C(15F)	1.50(2)
C(15A)-C(16A)	1.48(2)
C(15B)-C(16B)	1.41(2)
C(15C)-C(16C)	1.44(2)
C(15D)-C(16D)	1.42(3)
C(15E)-C(16E)	1.49(3)
C(15F)-C(16F)	1.43(3)

Table D.3.1 continued…

C(17A)-C(18A)	1.382(19)
C(17A)-C(22A)	1.40(2)
C(17B)-C(22B)	1.42(2)
C(17B)-C(18B)	1.43(2)
C(17C)-C(22C)	1.37(2)
C(17C)-C(18C)	1.42(2)
C(17D)-C(22D)	1.30(3)
C(17D)-C(18D)	1.45(3)
C(17E)-C(18E)	1.38(3)
C(17E)-C(22E)	1.46(3)
C(17F)-C(18F)	1.41(2)
C(17F)-C(22F)	1.42(3)
C(18A)-C(19A)	1.377(19)
C(18A)-H(18A)	0.9500
C(18B)-C(19B)	1.40(2)
C(18B)-H(18B)	0.9500
C(18C)-C(19C)	1.36(3)
C(18C)-H(18C)	0.9500
C(18D)-C(19D)	1.42(3)
C(18D)-H(18D)	0.9500
C(18E)-C(19E)	1.45(3)
C(18E)-H(18E)	0.9500
C(18F)-C(19F)	1.33(2)
C(18F)-H(18F)	0.9500
C(19A)-C(20A)	1.44(2)
C(19A)-H(19A)	0.9500
C(19B)-C(20B)	1.42(2)
C(19B)-H(19B)	0.9500
C(19C)-C(20C)	1.36(3)
C(19C)-H(19C)	0.9500
C(19D)-C(20D)	1.35(3)
C(19D)-H(19D)	0.9500
C(19E)-C(20E)	1.38(3)
C(19E)-H(19E)	0.9500
C(19F)-C(20F)	1.44(3)
C(19F)-H(19F)	0.9500
C(20A)-C(21A)	1.34(2)

Table D.3.1 continued…

C(20A)-H(20A)	0.9500
C(20B)-C(21B)	1.35(2)
C(20B)-H(20B)	0.9500
C(20C)-C(21C)	1.41(2)
C(20C)-H(20C)	0.9500
C(20D)-C(21D)	1.29(3)
C(20D)-H(20D)	0.9500
C(20E)-C(21E)	1.30(3)
C(20E)-H(20E)	0.9500
C(20F)-C(21F)	1.38(3)
C(20F)-H(20F)	0.9500
C(21A)-C(22A)	1.41(2)
C(21A)-H(21A)	0.9500
C(21B)-C(22B)	1.433(18)
C(21B)-H(21B)	0.9500
C(21C)-C(22C)	1.43(2)
C(21C)-H(21C)	0.9500
C(21D)-C(22D)	1.49(3)
C(21D)-H(21D)	0.9500
C(21E)-C(22E)	1.42(3)
C(21E)-H(21E)	0.9500
C(21F)-C(22F)	1.40(2)
C(21F)-H(21F)	0.9500

N(4A)-Au(1)-N(1A)	96.6(5)
N(4A)-Au(1)-N(3A)	82.6(5)
N(1A)-Au(1)-N(3A)	177.3(4)
N(4A)-Au(1)-N(2A)	176.8(5)
N(1A)-Au(1)-N(2A)	81.8(5)
N(3A)-Au(1)-N(2A)	99.2(5)
N(1B)-Au(2)-N(4B)	97.1(5)
N(1B)-Au(2)-N(3B)	176.3(4)
N(4B)-Au(2)-N(3B)	82.0(4)
N(1B)-Au(2)-N(2B)	82.3(5)
N(4B)-Au(2)-N(2B)	177.5(4)
N(3B)-Au(2)-N(2B)	98.8(5)
N(1C)-Au(3)-N(4C)	98.3(6)

Table D.3.1 continued…

N(1C)-Au(3)-N(3C)	177.8(5)
N(4C)-Au(3)-N(3C)	79.9(5)
N(1C)-Au(3)-N(2C)	82.1(6)
N(4C)-Au(3)-N(2C)	177.6(5)
N(3C)-Au(3)-N(2C)	99.7(6)
N(4D)-Au(4)-N(1D)	97.2(5)
N(4D)-Au(4)-N(2D)	175.5(4)
N(1D)-Au(4)-N(2D)	82.1(5)
N(4D)-Au(4)-N(3D)	81.9(5)
N(1D)-Au(4)-N(3D)	176.1(5)
N(2D)-Au(4)-N(3D)	99.2(5)
N(4E)-Au(5)-N(1E)	97.1(5)
N(4E)-Au(5)-N(2E)	177.1(5)
N(1E)-Au(5)-N(2E)	81.6(5)
N(4E)-Au(5)-N(3E)	81.9(6)
N(1E)-Au(5)-N(3E)	175.7(4)
N(2E)-Au(5)-N(3E)	99.6(5)
N(2F)-Au(6)-N(4F)	178.4(5)
N(2F)-Au(6)-N(1F)	83.2(6)
N(4F)-Au(6)-N(1F)	96.1(6)
N(2F)-Au(6)-N(3F)	98.5(6)
N(4F)-Au(6)-N(3F)	82.3(6)
N(1F)-Au(6)-N(3F)	175.5(5)
F(4)-P(1)-F(5)	88.7(6)
F(4)-P(1)-F(2)	179.2(7)
F(5)-P(1)-F(2)	91.1(6)
F(4)-P(1)-F(1)	91.3(6)
F(5)-P(1)-F(1)	89.6(6)
F(2)-P(1)-F(1)	89.4(6)
F(4)-P(1)-F(3)	89.5(6)
F(5)-P(1)-F(3)	90.0(6)
F(2)-P(1)-F(3)	89.7(6)
F(1)-P(1)-F(3)	179.0(7)
F(4)-P(1)-F(6)	91.1(6)
F(5)-P(1)-F(6)	179.6(7)
F(2)-P(1)-F(6)	89.2(6)
F(1)-P(1)-F(6)	90.1(6)

Table D.3.1 continued…

F(3)-P(1)-F(6)	90.3(6)
F(9)-P(2)-F(12)	90.2(7)
F(9)-P(2)-F(7)	179.0(8)
F(12)-P(2)-F(7)	90.8(6)
F(9)-P(2)-F(10)	88.8(7)
F(12)-P(2)-F(10)	89.8(6)
F(7)-P(2)-F(10)	90.9(5)
F(9)-P(2)-F(8)	91.0(6)
F(12)-P(2)-F(8)	90.5(5)
F(7)-P(2)-F(8)	89.3(5)
F(10)-P(2)-F(8)	179.7(6)
F(9)-P(2)-F(11)	90.8(8)
F(12)-P(2)-F(11)	178.8(7)
F(7)-P(2)-F(11)	88.3(6)
F(10)-P(2)-F(11)	89.5(7)
F(8)-P(2)-F(11)	90.2(6)
F(18)-P(3)-F(15)	90.3(7)
F(18)-P(3)-F(14)	90.1(7)
F(15)-P(3)-F(14)	90.2(6)
F(18)-P(3)-F(13)	90.6(7)
F(15)-P(3)-F(13)	178.9(7)
F(14)-P(3)-F(13)	90.4(6)
F(18)-P(3)-F(16)	90.8(6)
F(15)-P(3)-F(16)	89.7(6)
F(14)-P(3)-F(16)	179.1(7)
F(13)-P(3)-F(16)	89.7(6)
F(18)-P(3)-F(17)	179.5(6)
F(15)-P(3)-F(17)	90.0(6)
F(14)-P(3)-F(17)	90.3(6)
F(13)-P(3)-F(17)	89.1(6)
F(16)-P(3)-F(17)	88.8(6)
F(23)-P(4)-F(20)	91.8(6)
F(23)-P(4)-F(19)	91.8(6)
F(20)-P(4)-F(19)	90.3(6)
F(23)-P(4)-F(22)	89.9(6)
F(20)-P(4)-F(22)	178.3(6)
F(19)-P(4)-F(22)	90.2(5)

Table D.3.1 continued…

F(23)-P(4)-F(21)	89.6(6)
F(20)-P(4)-F(21)	90.9(5)
F(19)-P(4)-F(21)	178.2(6)
F(22)-P(4)-F(21)	88.6(6)
F(23)-P(4)-F(24)	177.2(7)
F(20)-P(4)-F(24)	90.0(6)
F(19)-P(4)-F(24)	90.3(6)
F(22)-P(4)-F(24)	88.3(6)
F(21)-P(4)-F(24)	88.2(6)
F(26)-P(5)-F(28)	178.7(6)
F(26)-P(5)-F(30)	90.3(6)
F(28)-P(5)-F(30)	90.8(6)
F(26)-P(5)-F(25)	90.6(6)
F(28)-P(5)-F(25)	90.2(5)
F(30)-P(5)-F(25)	89.6(5)
F(26)-P(5)-F(27)	89.0(5)
F(28)-P(5)-F(27)	90.2(5)
F(30)-P(5)-F(27)	89.7(5)
F(25)-P(5)-F(27)	179.2(5)
F(26)-P(5)-F(29)	88.6(7)
F(28)-P(5)-F(29)	90.4(7)
F(30)-P(5)-F(29)	178.5(7)
F(25)-P(5)-F(29)	91.5(6)
F(27)-P(5)-F(29)	89.2(6)
F(31)-P(6)-F(35)	91.8(6)
F(31)-P(6)-F(34)	90.0(6)
F(35)-P(6)-F(34)	90.6(6)
F(31)-P(6)-F(32)	90.4(6)
F(35)-P(6)-F(32)	90.6(6)
F(34)-P(6)-F(32)	178.7(6)
F(31)-P(6)-F(33)	178.8(7)
F(35)-P(6)-F(33)	89.4(6)
F(34)-P(6)-F(33)	90.0(6)
F(32)-P(6)-F(33)	89.5(5)
F(31)-P(6)-F(36)	89.7(6)
F(35)-P(6)-F(36)	178.5(6)
F(34)-P(6)-F(36)	90.0(6)

Table D.3.1 continued…

F(32)-P(6)-F(36)	88.8(5)
F(33)-P(6)-F(36)	89.1(6)
C(1A)-N(1A)-C(4A)	109.3(12)
C(1A)-N(1A)-Au(1)	140.0(9)
C(4A)-N(1A)-Au(1)	110.6(9)
C(1B)-N(1B)-C(4B)	107.1(12)
C(1B)-N(1B)-Au(2)	141.0(11)
C(4B)-N(1B)-Au(2)	111.8(9)
C(4C)-N(1C)-C(1C)	109.3(14)
C(4C)-N(1C)-Au(3)	112.0(11)
C(1C)-N(1C)-Au(3)	138.7(11)
C(4D)-N(1D)-C(1D)	108.1(15)
C(4D)-N(1D)-Au(4)	111.8(11)
C(1D)-N(1D)-Au(4)	139.8(12)
C(1E)-N(1E)-C(4E)	109.5(12)
C(1E)-N(1E)-Au(5)	139.0(11)
C(4E)-N(1E)-Au(5)	111.1(9)
C(1F)-N(1F)-C(4F)	108.0(15)
C(1F)-N(1F)-Au(6)	141.7(14)
C(4F)-N(1F)-Au(6)	109.9(11)
C(5A)-N(2A)-C(6A)	122.2(12)
C(5A)-N(2A)-Au(1)	112.0(9)
C(6A)-N(2A)-Au(1)	125.4(9)
C(5B)-N(2B)-C(6B)	121.8(13)
C(5B)-N(2B)-Au(2)	110.2(10)
C(6B)-N(2B)-Au(2)	127.7(10)
C(5C)-N(2C)-C(6C)	124.2(14)
C(5C)-N(2C)-Au(3)	109.6(11)
C(6C)-N(2C)-Au(3)	126.1(11)
C(5D)-N(2D)-C(6D)	118.5(13)
C(5D)-N(2D)-Au(4)	112.9(11)
C(6D)-N(2D)-Au(4)	128.5(10)
C(5E)-N(2E)-C(6E)	119.8(11)
C(5E)-N(2E)-Au(5)	113.7(9)
C(6E)-N(2E)-Au(5)	125.5(9)
C(5F)-N(2F)-C(6F)	117.0(14)
C(5F)-N(2F)-Au(6)	114.1(11)

Table D.3.1 continued…

C(6F)-N(2F)-Au(6)	128.2(11)
C(10A)-N(3A)-C(9A)	120.0(14)
C(10A)-N(3A)-Au(1)	112.5(11)
C(9A)-N(3A)-Au(1)	127.2(10)
C(10B)-N(3B)-C(9B)	120.4(11)
C(10B)-N(3B)-Au(2)	113.3(9)
C(9B)-N(3B)-Au(2)	125.9(9)
C(10C)-N(3C)-C(9C)	123.8(13)
C(10C)-N(3C)-Au(3)	112.2(10)
C(9C)-N(3C)-Au(3)	122.9(10)
C(10D)-N(3D)-C(9D)	121.6(12)
C(10D)-N(3D)-Au(4)	112.9(10)
C(9D)-N(3D)-Au(4)	125.1(9)
C(10E)-N(3E)-C(9E)	122.5(13)
C(10E)-N(3E)-Au(5)	111.1(11)
C(9E)-N(3E)-Au(5)	125.8(10)
C(10F)-N(3F)-C(9F)	117.9(14)
C(10F)-N(3F)-Au(6)	113.4(11)
C(9F)-N(3F)-Au(6)	128.6(12)
C(14A)-N(4A)-C(11A)	106.9(12)
C(14A)-N(4A)-Au(1)	141.4(11)
C(11A)-N(4A)-Au(1)	111.8(10)
C(14B)-N(4B)-C(11B)	108.2(12)
C(14B)-N(4B)-Au(2)	140.7(10)
C(11B)-N(4B)-Au(2)	110.9(9)
C(11C)-N(4C)-C(14C)	108.8(14)
C(11C)-N(4C)-Au(3)	112.4(11)
C(14C)-N(4C)-Au(3)	138.2(13)
C(14D)-N(4D)-C(11D)	108.2(12)
C(14D)-N(4D)-Au(4)	139.9(10)
C(11D)-N(4D)-Au(4)	110.8(9)
C(14E)-N(4E)-C(11E)	108.4(15)
C(14E)-N(4E)-Au(5)	139.4(12)
C(11E)-N(4E)-Au(5)	111.7(11)
C(14F)-N(4F)-C(11F)	106.2(15)
C(14F)-N(4F)-Au(6)	142.1(12)
C(11F)-N(4F)-Au(6)	111.7(12)

Table D.3.1 continued…

C(15A)-N(5A)-C(17A)	121.7(13)
C(17B)-N(5B)-C(15B)	118.2(13)
C(15C)-N(5C)-C(17C)	121.3(17)
C(15E)-N(5E)-C(17E)	121.1(18)
C(15F)-N(5F)-C(17F)	122.0(15)
C(16A)-N(6A)-C(22A)	120.3(13)
C(16B)-N(6B)-C(22B)	121.0(13)
C(16C)-N(6C)-C(22C)	117.2(14)
C(16E)-N(6E)-C(22E)	123.2(18)
C(22F)-N(6F)-C(16F)	120.1(17)
C(15D)-N(41)-C(17D)	115.4(18)
C(22D)-N(42)-C(16D)	117.5(18)
N(1A)-C(1A)-C(2A)	107.9(12)
N(1A)-C(1A)-C(16A)	131.5(13)
C(2A)-C(1A)-C(16A)	120.5(13)
C(2B)-C(1B)-N(1B)	109.1(14)
C(2B)-C(1B)-C(16B)	122.1(14)
N(1B)-C(1B)-C(16B)	128.8(13)
N(1C)-C(1C)-C(2C)	105.5(12)
N(1C)-C(1C)-C(16C)	132.6(15)
C(2C)-C(1C)-C(16C)	121.8(14)
N(1D)-C(1D)-C(2D)	105.8(15)
N(1D)-C(1D)-C(16D)	128.4(17)
C(2D)-C(1D)-C(16D)	125.7(17)
N(1E)-C(1E)-C(16E)	132.1(14)
N(1E)-C(1E)-C(2E)	107.2(14)
C(16E)-C(1E)-C(2E)	120.2(13)
N(1F)-C(1F)-C(2F)	109.2(18)
N(1F)-C(1F)-C(16F)	128.5(17)
C(2F)-C(1F)-C(16F)	122.3(17)
N(1S)-C(1S)-C(2S)	177.1(19)
C(3A)-C(2A)-C(1A)	108.3(13)
C(3A)-C(2A)-H(2A)	125.8
C(1A)-C(2A)-H(2A)	125.8
C(1B)-C(2B)-C(3B)	107.8(14)
C(1B)-C(2B)-H(2B)	126.1
C(3B)-C(2B)-H(2B)	126.1

Table D.3.1 continued…

C(3C)-C(2C)-C(1C)	107.4(13)
C(3C)-C(2C)-H(2C)	126.3
C(1C)-C(2C)-H(2C)	126.3
C(3D)-C(2D)-C(1D)	111.5(16)
C(3D)-C(2D)-H(2D)	124.3
C(1D)-C(2D)-H(2D)	124.3
C(3E)-C(2E)-C(1E)	108.2(13)
C(3E)-C(2E)-H(2E)	125.9
C(1E)-C(2E)-H(2E)	125.9
C(3F)-C(2F)-C(1F)	108.3(18)
C(3F)-C(2F)-H(2F)	125.8
C(1F)-C(2F)-H(2F)	125.8
C(1S)-C(2S)-H(2SA)	109.5
C(1S)-C(2S)-H(2SB)	109.5
H(2SA)-C(2S)-H(2SB)	109.5
C(1S)-C(2S)-H(2SC)	109.5
H(2SA)-C(2S)-H(2SC)	109.5
H(2SB)-C(2S)-H(2SC)	109.5
C(2A)-C(3A)-C(4A)	106.2(12)
C(2A)-C(3A)-H(3A)	126.9
C(4A)-C(3A)-H(3A)	126.9
C(4B)-C(3B)-C(2B)	108.4(15)
C(4B)-C(3B)-H(3B)	125.8
C(2B)-C(3B)-H(3B)	125.8
C(4C)-C(3C)-C(2C)	108.5(13)
C(4C)-C(3C)-H(3C)	125.7
C(2C)-C(3C)-H(3C)	125.7
C(2D)-C(3D)-C(4D)	104.0(15)
C(2D)-C(3D)-H(3D)	128.0
C(4D)-C(3D)-H(3D)	128.0
C(2E)-C(3E)-C(4E)	107.6(14)
C(2E)-C(3E)-H(3E)	126.2
C(4E)-C(3E)-H(3E)	126.2
C(4F)-C(3F)-C(2F)	104.1(17)
C(4F)-C(3F)-H(3F)	128.0
C(2F)-C(3F)-H(3F)	128.0
N(2S)-C(3S)-C(4S)	178.5(18)

Table D.3.1 continued…

C(5A)-C(4A)-N(1A)	116.7(12)
C(5A)-C(4A)-C(3A)	135.0(13)
N(1A)-C(4A)-C(3A)	108.3(12)
C(5B)-C(4B)-C(3B)	136.7(16)
C(5B)-C(4B)-N(1B)	115.3(13)
C(3B)-C(4B)-N(1B)	107.6(14)
C(3C)-C(4C)-N(1C)	109.2(14)
C(3C)-C(4C)-C(5C)	135.1(15)
N(1C)-C(4C)-C(5C)	115.7(15)
N(1D)-C(4D)-C(3D)	110.6(15)
N(1D)-C(4D)-C(5D)	117.4(16)
C(3D)-C(4D)-C(5D)	131.8(16)
N(1E)-C(4E)-C(3E)	107.4(12)
N(1E)-C(4E)-C(5E)	115.5(12)
C(3E)-C(4E)-C(5E)	136.9(14)
N(1F)-C(4F)-C(5F)	117.4(14)
N(1F)-C(4F)-C(3F)	109.9(16)
C(5F)-C(4F)-C(3F)	132.4(17)
C(3S)-C(4S)-H(4SA)	109.5
C(3S)-C(4S)-H(4SB)	109.5
H(4SA)-C(4S)-H(4SB)	109.5
C(3S)-C(4S)-H(4SC)	109.5
H(4SA)-C(4S)-H(4SC)	109.5
H(4SB)-C(4S)-H(4SC)	109.5
N(2A)-C(5A)-C(4A)	118.5(12)
N(2A)-C(5A)-H(5A)	120.7
C(4A)-C(5A)-H(5A)	120.7
N(2B)-C(5B)-C(4B)	120.1(15)
N(2B)-C(5B)-H(5B)	120.0
C(4B)-C(5B)-H(5B)	120.0
N(2C)-C(5C)-C(4C)	120.5(15)
N(2C)-C(5C)-H(5C)	119.7
C(4C)-C(5C)-H(5C)	119.7
N(2D)-C(5D)-C(4D)	115.7(15)
N(2D)-C(5D)-H(5D)	122.1
C(4D)-C(5D)-H(5D)	122.1
N(2E)-C(5E)-C(4E)	117.6(12)

Table D.3.1 continued…

N(2E)-C(5E)-H(5E)	121.2
C(4E)-C(5E)-H(5E)	121.2
N(2F)-C(5F)-C(4F)	115.0(14)
N(2F)-C(5F)-H(5F)	122.5
C(4F)-C(5F)-H(5F)	122.5
N(3S)-C(5S)-C(6S)	179.4(18)
N(2A)-C(6A)-C(7A)	112.0(11)
N(2A)-C(6A)-H(6AA)	109.2
C(7A)-C(6A)-H(6AA)	109.2
N(2A)-C(6A)-H(6AB)	109.2
C(7A)-C(6A)-H(6AB)	109.2
H(6AA)-C(6A)-H(6AB)	107.9
N(2B)-C(6B)-C(7B)	113.3(13)
N(2B)-C(6B)-H(6BA)	108.9
C(7B)-C(6B)-H(6BA)	108.9
N(2B)-C(6B)-H(6BB)	108.9
C(7B)-C(6B)-H(6BB)	108.9
H(6BA)-C(6B)-H(6BB)	107.7
N(2C)-C(6C)-C(7C)	113.4(12)
N(2C)-C(6C)-H(6CA)	108.9
C(7C)-C(6C)-H(6CA)	108.9
N(2C)-C(6C)-H(6CB)	108.9
C(7C)-C(6C)-H(6CB)	108.9
H(6CA)-C(6C)-H(6CB)	107.7
N(2D)-C(6D)-C(7D)	111.6(11)
N(2D)-C(6D)-H(6DA)	109.3
C(7D)-C(6D)-H(6DA)	109.3
N(2D)-C(6D)-H(6DB)	109.3
C(7D)-C(6D)-H(6DB)	109.3
H(6DA)-C(6D)-H(6DB)	108.0
N(2E)-C(6E)-C(7E)	112.4(10)
N(2E)-C(6E)-H(6EA)	109.1
C(7E)-C(6E)-H(6EA)	109.1
N(2E)-C(6E)-H(6EB)	109.1
C(7E)-C(6E)-H(6EB)	109.1
H(6EA)-C(6E)-H(6EB)	107.9
C(7F)-C(6F)-N(2F)	114.4(14)

Table D.3.1 continued…

C(7F)-C(6F)-H(6FA)	108.7
N(2F)-C(6F)-H(6FA)	108.7
C(7F)-C(6F)-H(6FB)	108.7
N(2F)-C(6F)-H(6FB)	108.7
H(6FA)-C(6F)-H(6FB)	107.6
C(5S)-C(6S)-H(6SA)	109.5
C(5S)-C(6S)-H(6SB)	109.5
H(6SA)-C(6S)-H(6SB)	109.5
C(5S)-C(6S)-H(6SC)	109.5
H(6SA)-C(6S)-H(6SC)	109.5
H(6SB)-C(6S)-H(6SC)	109.5
C(8A)-C(7A)-C(6A)	116.5(13)
C(8A)-C(7A)-H(7AA)	108.2
C(6A)-C(7A)-H(7AA)	108.2
C(8A)-C(7A)-H(7AB)	108.2
C(6A)-C(7A)-H(7AB)	108.2
H(7AA)-C(7A)-H(7AB)	107.3
C(6B)-C(7B)-C(8B)	114.9(11)
C(6B)-C(7B)-H(7BA)	108.5
C(8B)-C(7B)-H(7BA)	108.5
C(6B)-C(7B)-H(7BB)	108.5
C(8B)-C(7B)-H(7BB)	108.5
H(7BA)-C(7B)-H(7BB)	107.5
C(6C)-C(7C)-C(8C)	112.1(12)
C(6C)-C(7C)-H(7CA)	109.2
C(8C)-C(7C)-H(7CA)	109.2
C(6C)-C(7C)-H(7CB)	109.2
C(8C)-C(7C)-H(7CB)	109.2
H(7CA)-C(7C)-H(7CB)	107.9
C(8D)-C(7D)-C(6D)	114.1(11)
C(8D)-C(7D)-H(7DA)	108.7
C(6D)-C(7D)-H(7DA)	108.7
C(8D)-C(7D)-H(7DB)	108.7
C(6D)-C(7D)-H(7DB)	108.7
H(7DA)-C(7D)-H(7DB)	107.6
C(8E)-C(7E)-C(6E)	112.9(12)
C(8E)-C(7E)-H(7EA)	109.0

Table D.3.1 continued…

C(6E)-C(7E)-H(7EA)	109.0
C(8E)-C(7E)-H(7EB)	109.0
C(6E)-C(7E)-H(7EB)	109.0
H(7EA)-C(7E)-H(7EB)	107.8
C(6F)-C(7F)-C(8F)	114.7(17)
C(6F)-C(7F)-H(7FA)	108.6
C(8F)-C(7F)-H(7FA)	108.6
C(6F)-C(7F)-H(7FB)	108.6
C(8F)-C(7F)-H(7FB)	108.6
H(7FA)-C(7F)-H(7FB)	107.6
N(4S)-C(7S)-C(8S)	178.0(17)
C(7A)-C(8A)-C(9A)	114.3(11)
C(7A)-C(8A)-H(8AA)	108.7
C(9A)-C(8A)-H(8AA)	108.7
C(7A)-C(8A)-H(8AB)	108.7
C(9A)-C(8A)-H(8AB)	108.7
H(8AA)-C(8A)-H(8AB)	107.6
C(9B)-C(8B)-C(7B)	112.6(12)
C(9B)-C(8B)-H(8BA)	109.1
C(7B)-C(8B)-H(8BA)	109.1
C(9B)-C(8B)-H(8BB)	109.1
C(7B)-C(8B)-H(8BB)	109.1
H(8BA)-C(8B)-H(8BB)	107.8
C(9C)-C(8C)-C(7C)	115.1(14)
C(9C)-C(8C)-H(8CA)	108.5
C(7C)-C(8C)-H(8CA)	108.5
C(9C)-C(8C)-H(8CB)	108.5
C(7C)-C(8C)-H(8CB)	108.5
H(8CA)-C(8C)-H(8CB)	107.5
C(7D)-C(8D)-C(9D)	115.3(13)
C(7D)-C(8D)-H(8DA)	108.4
C(9D)-C(8D)-H(8DA)	108.4
C(7D)-C(8D)-H(8DB)	108.4
C(9D)-C(8D)-H(8DB)	108.4
H(8DA)-C(8D)-H(8DB)	107.5
C(9E)-C(8E)-C(7E)	116.3(11)
C(9E)-C(8E)-H(8EA)	108.2

Table D.3.1 continued…

C(7E)-C(8E)-H(8EA)	108.2
C(9E)-C(8E)-H(8EB)	108.2
C(7E)-C(8E)-H(8EB)	108.2
H(8EA)-C(8E)-H(8EB)	107.4
C(9F)-C(8F)-C(7F)	115.2(13)
C(9F)-C(8F)-H(8FA)	108.5
C(7F)-C(8F)-H(8FA)	108.5
C(9F)-C(8F)-H(8FB)	108.5
C(7F)-C(8F)-H(8FB)	108.5
H(8FA)-C(8F)-H(8FB)	107.5
C(7S)-C(8S)-H(8SA)	109.5
C(7S)-C(8S)-H(8SB)	109.5
H(8SA)-C(8S)-H(8SB)	109.5
C(7S)-C(8S)-H(8SC)	109.5
H(8SA)-C(8S)-H(8SC)	109.5
H(8SB)-C(8S)-H(8SC)	109.5
N(3A)-C(9A)-C(8A)	111.2(12)
N(3A)-C(9A)-H(9AA)	109.4
C(8A)-C(9A)-H(9AA)	109.4
N(3A)-C(9A)-H(9AB)	109.4
C(8A)-C(9A)-H(9AB)	109.4
H(9AA)-C(9A)-H(9AB)	108.0
N(3B)-C(9B)-C(8B)	115.3(10)
N(3B)-C(9B)-H(9BA)	108.5
C(8B)-C(9B)-H(9BA)	108.5
N(3B)-C(9B)-H(9BB)	108.5
C(8B)-C(9B)-H(9BB)	108.5
H(9BA)-C(9B)-H(9BB)	107.5
N(3C)-C(9C)-C(8C)	114.3(12)
N(3C)-C(9C)-H(9CA)	108.7
C(8C)-C(9C)-H(9CA)	108.7
N(3C)-C(9C)-H(9CB)	108.7
C(8C)-C(9C)-H(9CB)	108.7
H(9CA)-C(9C)-H(9CB)	107.6
N(3D)-C(9D)-C(8D)	113.4(10)
N(3D)-C(9D)-H(9DA)	108.9
C(8D)-C(9D)-H(9DA)	108.9

Table D.3.1 continued…

N(3D)-C(9D)-H(9DB)	108.9
C(8D)-C(9D)-H(9DB)	108.9
H(9DA)-C(9D)-H(9DB)	107.7
N(3E)-C(9E)-C(8E)	111.9(12)
N(3E)-C(9E)-H(9EA)	109.2
C(8E)-C(9E)-H(9EA)	109.2
N(3E)-C(9E)-H(9EB)	109.2
C(8E)-C(9E)-H(9EB)	109.2
H(9EA)-C(9E)-H(9EB)	107.9
N(3F)-C(9F)-C(8F)	111.3(14)
N(3F)-C(9F)-H(9FA)	109.4
C(8F)-C(9F)-H(9FA)	109.4
N(3F)-C(9F)-H(9FB)	109.4
C(8F)-C(9F)-H(9FB)	109.4
H(9FA)-C(9F)-H(9FB)	108.0
N(5S)-C(9S)-C(10S)	179(2)
N(3A)-C(10A)-C(11A)	117.9(15)
N(3A)-C(10A)-H(10A)	121.1
C(11A)-C(10A)-H(10A)	121.1
N(3B)-C(10B)-C(11B)	117.3(12)
N(3B)-C(10B)-H(10B)	121.4
C(11B)-C(10B)-H(10B)	121.4
N(3C)-C(10C)-C(11C)	120.2(15)
N(3C)-C(10C)-H(10C)	119.9
C(11C)-C(10C)-H(10C)	119.9
N(3D)-C(10D)-C(11D)	118.4(13)
N(3D)-C(10D)-H(10D)	120.8
C(11D)-C(10D)-H(10D)	120.8
N(3E)-C(10E)-C(11E)	120.3(15)
N(3E)-C(10E)-H(10E)	119.9
C(11E)-C(10E)-H(10E)	119.9
N(3F)-C(10F)-C(11F)	117.1(14)
N(3F)-C(10F)-H(10F)	121.5
C(11F)-C(10F)-H(10F)	121.5
C(9S)-C(10S)-H(10G)	109.5
C(9S)-C(10S)-H(10H)	109.5
H(10G)-C(10S)-H(10H)	109.5

Table D.3.1 continued…

C(9S)-C(10S)-H(10I)	109.5
H(10G)-C(10S)-H(10I)	109.5
H(10H)-C(10S)-H(10I)	109.5
N(4A)-C(11A)-C(12A)	110.0(14)
N(4A)-C(11A)-C(10A)	115.2(13)
C(12A)-C(11A)-C(10A)	134.5(16)
C(12B)-C(11B)-N(4B)	107.8(12)
C(12B)-C(11B)-C(10B)	135.9(13)
N(4B)-C(11B)-C(10B)	116.1(12)
C(12C)-C(11C)-C(10C)	136.4(16)
C(12C)-C(11C)-N(4C)	108.2(15)
C(10C)-C(11C)-N(4C)	114.0(14)
C(10D)-C(11D)-N(4D)	115.3(12)
C(10D)-C(11D)-C(12D)	136.3(14)
N(4D)-C(11D)-C(12D)	108.4(13)
C(12E)-C(11E)-N(4E)	108.6(15)
C(12E)-C(11E)-C(10E)	136.7(17)
N(4E)-C(11E)-C(10E)	114.7(16)
C(12F)-C(11F)-N(4F)	109.1(15)
C(12F)-C(11F)-C(10F)	135.1(16)
N(4F)-C(11F)-C(10F)	115.5(16)
N(6S)-C(11S)-C(12S)	174(2)
C(13A)-C(12A)-C(11A)	105.9(15)
C(13A)-C(12A)-H(12A)	127.1
C(11A)-C(12A)-H(12A)	127.1
C(11B)-C(12B)-C(13B)	107.5(12)
C(11B)-C(12B)-H(12B)	126.3
C(13B)-C(12B)-H(12B)	126.3
C(11C)-C(12C)-C(13C)	107.1(17)
C(11C)-C(12C)-H(12C)	126.5
C(13C)-C(12C)-H(12C)	126.5
C(13D)-C(12D)-C(11D)	105.5(14)
C(13D)-C(12D)-H(12D)	127.3
C(11D)-C(12D)-H(12D)	127.3
C(11E)-C(12E)-C(13E)	108.7(15)
C(11E)-C(12E)-H(12E)	125.6
C(13E)-C(12E)-H(12E)	125.6

Table D.3.1 continued…

C(11F)-C(12F)-C(13F)	108.6(15)
C(11F)-C(12F)-H(12F)	125.7
C(13F)-C(12F)-H(12F)	125.7
C(11S)-C(12S)-H(12G)	109.5
C(11S)-C(12S)-H(12H)	109.5
H(12G)-C(12S)-H(12H)	109.5
C(11S)-C(12S)-H(12I)	109.5
H(12G)-C(12S)-H(12I)	109.5
H(12H)-C(12S)-H(12I)	109.5
C(12A)-C(13A)-C(14A)	109.0(14)
C(12A)-C(13A)-H(13A)	125.5
C(14A)-C(13A)-H(13A)	125.5
C(12B)-C(13B)-C(14B)	107.9(13)
C(12B)-C(13B)-H(13B)	126.1
C(14B)-C(13B)-H(13B)	126.1
C(14C)-C(13C)-C(12C)	108.9(17)
C(14C)-C(13C)-H(13C)	125.5
C(12C)-C(13C)-H(13C)	125.5
C(12D)-C(13D)-C(14D)	112.0(14)
C(12D)-C(13D)-H(13D)	124.0
C(14D)-C(13D)-H(13D)	124.0
C(14E)-C(13E)-C(12E)	105.7(15)
C(14E)-C(13E)-H(13E)	127.1
C(12E)-C(13E)-H(13E)	127.1
C(12F)-C(13F)-C(14F)	105.7(14)
C(12F)-C(13F)-H(13F)	127.2
C(14F)-C(13F)-H(13F)	127.2
N(4A)-C(14A)-C(13A)	108.0(14)
N(4A)-C(14A)-C(15A)	129.3(13)
C(13A)-C(14A)-C(15A)	122.5(14)
N(4B)-C(14B)-C(13B)	108.5(12)
N(4B)-C(14B)-C(15B)	128.8(13)
C(13B)-C(14B)-C(15B)	122.6(13)
N(4C)-C(14C)-C(13C)	106.6(17)
N(4C)-C(14C)-C(15C)	130.1(16)
C(13C)-C(14C)-C(15C)	123.1(16)
C(13D)-C(14D)-N(4D)	105.9(14)

Table D.3.1 continued…

C(13D)-C(14D)-C(15D)	125.8(14)
N(4D)-C(14D)-C(15D)	127.9(14)
N(4E)-C(14E)-C(13E)	108.6(15)
N(4E)-C(14E)-C(15E)	129.9(16)
C(13E)-C(14E)-C(15E)	121.3(16)
N(4F)-C(14F)-C(13F)	110.3(14)
N(4F)-C(14F)-C(15F)	127.6(15)
C(13F)-C(14F)-C(15F)	122.1(15)
N(5A)-C(15A)-C(14A)	111.3(13)
N(5A)-C(15A)-C(16A)	116.3(14)
C(14A)-C(15A)-C(16A)	132.4(13)
N(5B)-C(15B)-C(16B)	121.4(14)
N(5B)-C(15B)-C(14B)	106.9(13)
C(16B)-C(15B)-C(14B)	131.7(14)
N(5C)-C(15C)-C(16C)	118.2(16)
N(5C)-C(15C)-C(14C)	109.1(16)
C(16C)-C(15C)-C(14C)	132.7(15)
N(41)-C(15D)-C(16D)	122.4(16)
N(41)-C(15D)-C(14D)	106.2(15)
C(16D)-C(15D)-C(14D)	131.3(15)
N(5E)-C(15E)-C(14E)	108.5(17)
N(5E)-C(15E)-C(16E)	120.8(15)
C(14E)-C(15E)-C(16E)	130.7(16)
N(5F)-C(15F)-C(16F)	119.0(15)
N(5F)-C(15F)-C(14F)	109.4(15)
C(16F)-C(15F)-C(14F)	131.5(15)
N(6A)-C(16A)-C(15A)	121.1(13)
N(6A)-C(16A)-C(1A)	110.4(13)
C(15A)-C(16A)-C(1A)	128.5(14)
N(6B)-C(16B)-C(15B)	119.1(15)
N(6B)-C(16B)-C(1B)	109.3(13)
C(15B)-C(16B)-C(1B)	131.6(14)
N(6C)-C(16C)-C(15C)	120.9(14)
N(6C)-C(16C)-C(1C)	110.7(14)
C(15C)-C(16C)-C(1C)	128.5(15)
N(42)-C(16D)-C(15D)	118.5(15)
N(42)-C(16D)-C(1D)	108.5(16)

Table D.3.1 continued…

C(15D)-C(16D)-C(1D)	133.0(16)
N(6E)-C(16E)-C(1E)	113.2(15)
N(6E)-C(16E)-C(15E)	116.6(15)
C(1E)-C(16E)-C(15E)	130.2(14)
N(6F)-C(16F)-C(15F)	119.3(17)
N(6F)-C(16F)-C(1F)	108.8(16)
C(15F)-C(16F)-C(1F)	131.9(15)
N(5A)-C(17A)-C(18A)	120.1(13)
N(5A)-C(17A)-C(22A)	120.0(13)
C(18A)-C(17A)-C(22A)	119.9(14)
N(5B)-C(17B)-C(22B)	120.9(14)
N(5B)-C(17B)-C(18B)	118.1(14)
C(22B)-C(17B)-C(18B)	121.0(13)
N(5C)-C(17C)-C(22C)	118.0(15)
N(5C)-C(17C)-C(18C)	120.2(17)
C(22C)-C(17C)-C(18C)	121.6(16)
C(22D)-C(17D)-N(41)	122.2(19)
C(22D)-C(17D)-C(18D)	121(2)
N(41)-C(17D)-C(18D)	116(2)
N(5E)-C(17E)-C(18E)	124(2)
N(5E)-C(17E)-C(22E)	119.3(18)
C(18E)-C(17E)-C(22E)	116.1(18)
N(5F)-C(17F)-C(18F)	122.2(16)
N(5F)-C(17F)-C(22F)	118.3(15)
C(18F)-C(17F)-C(22F)	119.6(14)
C(19A)-C(18A)-C(17A)	121.9(14)
C(19A)-C(18A)-H(18A)	119.0
C(17A)-C(18A)-H(18A)	119.0
C(19B)-C(18B)-C(17B)	118.0(14)
C(19B)-C(18B)-H(18B)	121.0
C(17B)-C(18B)-H(18B)	121.0
C(19C)-C(18C)-C(17C)	117.8(17)
C(19C)-C(18C)-H(18C)	121.1
C(17C)-C(18C)-H(18C)	121.1
C(19D)-C(18D)-C(17D)	115(2)
C(19D)-C(18D)-H(18D)	122.4
C(17D)-C(18D)-H(18D)	122.4

Table D.3.1 continued…

C(17E)-C(18E)-C(19E)	119(2)
C(17E)-C(18E)-H(18E)	120.5
C(19E)-C(18E)-H(18E)	120.5
C(19F)-C(18F)-C(17F)	119.4(16)
C(19F)-C(18F)-H(18F)	120.3
C(17F)-C(18F)-H(18F)	120.3
C(18A)-C(19A)-C(20A)	117.3(13)
C(18A)-C(19A)-H(19A)	121.4
C(20A)-C(19A)-H(19A)	121.4
C(18B)-C(19B)-C(20B)	120.1(14)
C(18B)-C(19B)-H(19B)	120.0
C(20B)-C(19B)-H(19B)	120.0
C(18C)-C(19C)-C(20C)	122.4(17)
C(18C)-C(19C)-H(19C)	118.8
C(20C)-C(19C)-H(19C)	118.8
C(20D)-C(19D)-C(18D)	121(2)
C(20D)-C(19D)-H(19D)	119.4
C(18D)-C(19D)-H(19D)	119.4
C(20E)-C(19E)-C(18E)	122.6(19)
C(20E)-C(19E)-H(19E)	118.7
C(18E)-C(19E)-H(19E)	118.7
C(18F)-C(19F)-C(20F)	122.5(16)
C(18F)-C(19F)-H(19F)	118.7
C(20F)-C(19F)-H(19F)	118.7
C(21A)-C(20A)-C(19A)	121.3(15)
C(21A)-C(20A)-H(20A)	119.4
C(19A)-C(20A)-H(20A)	119.4
C(21B)-C(20B)-C(19B)	122.7(13)
C(21B)-C(20B)-H(20B)	118.7
C(19B)-C(20B)-H(20B)	118.7
C(19C)-C(20C)-C(21C)	121.3(16)
C(19C)-C(20C)-H(20C)	119.3
C(21C)-C(20C)-H(20C)	119.3
C(21D)-C(20D)-C(19D)	125(2)
C(21D)-C(20D)-H(20D)	117.7
C(19D)-C(20D)-H(20D)	117.7
C(21E)-C(20E)-C(19E)	118.6(19)

Table D.3.1 continued…

C(21E)-C(20E)-H(20E)	120.7
C(19E)-C(20E)-H(20E)	120.7
C(21F)-C(20F)-C(19F)	118.3(16)
C(21F)-C(20F)-H(20F)	120.8
C(19F)-C(20F)-H(20F)	120.8
C(20A)-C(21A)-C(22A)	121.0(16)
C(20A)-C(21A)-H(21A)	119.5
C(22A)-C(21A)-H(21A)	119.5
C(20B)-C(21B)-C(22B)	119.0(13)
C(20B)-C(21B)-H(21B)	120.5
C(22B)-C(21B)-H(21B)	120.5
C(20C)-C(21C)-C(22C)	117.5(15)
C(20C)-C(21C)-H(21C)	121.3
C(22C)-C(21C)-H(21C)	121.3
C(20D)-C(21D)-C(22D)	117(2)
C(20D)-C(21D)-H(21D)	121.7
C(22D)-C(21D)-H(21D)	121.7
C(20E)-C(21E)-C(22E)	123(2)
C(20E)-C(21E)-H(21E)	118.4
C(22E)-C(21E)-H(21E)	118.4
C(20F)-C(21F)-C(22F)	120.4(18)
C(20F)-C(21F)-H(21F)	119.8
C(22F)-C(21F)-H(21F)	119.8
N(6A)-C(22A)-C(17A)	120.5(15)
N(6A)-C(22A)-C(21A)	120.9(15)
C(17A)-C(22A)-C(21A)	118.6(14)
N(6B)-C(22B)-C(17B)	119.4(12)
N(6B)-C(22B)-C(21B)	121.2(12)
C(17B)-C(22B)-C(21B)	119.3(13)
N(6C)-C(22C)-C(17C)	124.1(16)
N(6C)-C(22C)-C(21C)	116.4(15)
C(17C)-C(22C)-C(21C)	119.4(15)
C(17D)-C(22D)-N(42)	123(2)
C(17D)-C(22D)-C(21D)	121(2)
N(42)-C(22D)-C(21D)	115(2)
N(6E)-C(22E)-C(21E)	121(2)
N(6E)-C(22E)-C(17E)	118.9(17)

Table D.3.1 continued…

C(21E)-C(22E)-C(17E)	120.3(18)
N(6F)-C(22F)-C(21F)	119.0(17)
N(6F)-C(22F)-C(17F)	121.3(15)
C(21F)-C(22F)-C(17F)	119.7(16)

Table D.3.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [Au(L3)](PF_6).

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(1)	14(1)	18(1)	24(1)	-1(1)	1(1)	0(1)
Au(2)	14(1)	21(1)	22(1)	0(1)	0(1)	-1(1)
Au(3)	20(1)	25(1)	19(1)	1(1)	-3(1)	1(1)
Au(4)	15(1)	19(1)	19(1)	1(1)	0(1)	0(1)
Au(5)	15(1)	21(1)	17(1)	-1(1)	-1(1)	1(1)
Au(6)	21(1)	30(1)	22(1)	-1(1)	-1(1)	0(1)
P(1)	34(2)	25(2)	28(2)	-2(2)	0(2)	-1(2)
P(2)	22(2)	36(2)	23(2)	1(2)	-2(1)	-4(1)
P(3)	27(2)	31(2)	21(2)	4(1)	0(2)	6(1)
P(4)	20(2)	29(2)	30(3)	0(2)	3(2)	-1(1)
P(5)	16(2)	42(2)	21(2)	2(2)	2(1)	3(1)
P(6)	19(2)	33(2)	27(3)	1(2)	4(2)	0(1)
F(1)	39(6)	64(6)	28(6)	0(5)	-4(4)	-2(5)
F(2)	39(6)	38(5)	76(9)	-14(5)	-7(5)	-1(4)
F(3)	44(6)	47(5)	35(7)	-5(5)	-3(5)	-8(4)
F(4)	47(6)	53(6)	66(8)	-17(5)	4(5)	13(5)
F(5)	44(6)	32(4)	51(7)	11(4)	-15(5)	-15(4)
F(6)	30(5)	48(5)	60(7)	16(5)	-2(5)	-9(4)
F(7)	49(6)	47(5)	32(5)	-4(4)	-7(4)	13(4)
F(8)	28(5)	64(6)	20(5)	5(4)	0(3)	-8(4)
F(9)	58(8)	69(7)	43(8)	-15(6)	6(6)	27(6)
F(10)	26(5)	69(6)	37(6)	-7(5)	-8(4)	-1(4)
F(11)	54(8)	60(6)	72(10)	10(6)	9(7)	-43(5)
F(12)	33(6)	86(7)	43(6)	26(5)	-4(4)	-26(5)
F(13)	53(7)	61(6)	38(7)	-9(5)	-22(5)	19(5)
F(14)	52(6)	63(6)	43(6)	-21(5)	6(5)	27(5)
F(15)	35(6)	51(5)	29(6)	-11(4)	-6(4)	-4(4)
F(16)	32(5)	43(5)	48(6)	-16(4)	13(4)	6(4)
F(17)	25(5)	36(4)	46(6)	9(4)	5(4)	-4(3)
F(18)	49(7)	69(7)	77(9)	46(7)	17(6)	-3(5)
F(19)	24(5)	38(4)	56(7)	6(4)	13(4)	-1(3)
F(20)	31(5)	54(5)	44(7)	-18(5)	12(4)	-5(4)
F(21)	44(6)	38(5)	39(6)	18(4)	14(5)	4(4)
F(22)	34(6)	43(5)	54(7)	-23(5)	10(5)	-5(4)

Table D.3.3 continued…

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
F(23)	26(6)	57(6)	38(8)	-10(4)	-14(5)	1(4)
F(24)	37(6)	36(4)	44(8)	1(4)	-7(5)	-6(3)
F(25)	24(5)	64(6)	28(5)	7(4)	-3(4)	3(4)
F(26)	35(6)	53(5)	28(6)	-10(4)	-3(4)	14(4)
F(27)	23(4)	47(5)	37(5)	2(4)	3(4)	1(3)
F(28)	39(6)	73(6)	38(6)	-27(5)	3(4)	18(5)
F(29)	42(7)	66(6)	42(8)	25(5)	-11(5)	-23(5)
F(30)	39(6)	39(4)	46(6)	12(4)	8(4)	-4(4)
F(31)	42(6)	45(5)	45(7)	-16(5)	9(5)	4(4)
F(32)	21(5)	44(4)	33(6)	3(4)	2(4)	-2(3)
F(33)	27(5)	46(5)	47(7)	-16(4)	7(4)	-7(4)
F(34)	29(6)	55(6)	37(8)	0(4)	9(5)	-8(4)
F(35)	40(6)	50(5)	52(7)	14(5)	11(5)	-8(4)
F(36)	26(5)	31(4)	51(7)	12(4)	8(4)	0(3)
N(1A)	19(3)	12(4)	19(3)	-3(3)	-3(2)	0(3)
N(1B)	17(3)	17(4)	18(3)	0(3)	0(3)	0(3)
N(1C)	30(4)	13(4)	16(4)	2(3)	-2(3)	-1(3)
N(1D)	26(3)	20(4)	19(4)	5(4)	1(3)	-1(3)
N(1E)	18(3)	29(4)	24(3)	-3(4)	-1(3)	-3(3)
N(1F)	23(3)	34(4)	19(4)	0(4)	-1(3)	-7(4)
N(1S)	36(6)	43(7)	40(8)	0(6)	-1(5)	2(6)
N(2A)	23(5)	24(5)	32(4)	2(4)	-1(3)	4(4)
N(2B)	23(3)	22(5)	16(5)	0(4)	3(3)	2(4)
N(2C)	21(5)	24(5)	33(4)	11(4)	-5(4)	-2(4)
N(2D)	20(5)	24(4)	23(4)	1(4)	0(3)	9(4)
N(2E)	19(3)	16(4)	14(5)	3(4)	-5(3)	-3(3)
N(2F)	28(4)	38(5)	30(6)	0(5)	-1(3)	-1(4)
N(2S)	29(7)	42(7)	40(9)	2(5)	-6(5)	5(5)
N(3A)	25(3)	27(5)	26(6)	-1(5)	0(3)	3(4)
N(3B)	27(5)	15(4)	27(3)	-3(4)	4(3)	-6(4)
N(3C)	27(3)	28(3)	21(3)	-3(3)	-2(3)	-1(3)
N(3D)	21(3)	20(5)	23(5)	2(4)	0(3)	1(3)
N(3E)	19(5)	20(4)	25(4)	-2(4)	4(3)	-1(4)
N(3F)	21(5)	31(5)	31(4)	-3(4)	-6(3)	-5(4)
N(3S)	28(5)	30(5)	34(7)	7(5)	5(4)	-3(4)
N(4A)	17(3)	19(4)	21(3)	4(4)	-1(3)	1(3)

Table D.3.3 continued…

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(4B)	17(3)	18(4)	19(3)	-5(3)	1(2)	4(3)
N(4C)	24(3)	30(4)	18(3)	-9(4)	-4(3)	5(4)
N(4D)	21(3)	22(4)	23(3)	6(4)	-3(3)	4(3)
N(4E)	25(3)	18(4)	18(4)	-1(4)	1(3)	0(3)
N(4F)	25(3)	24(4)	22(4)	-4(4)	-4(3)	3(3)
N(4S)	28(6)	27(5)	44(8)	6(6)	0(5)	2(4)
N(5A)	20(3)	21(5)	25(3)	1(4)	2(3)	-4(4)
N(5B)	17(4)	18(4)	23(4)	-4(4)	-1(3)	4(3)
N(5C)	23(3)	36(6)	27(4)	-3(5)	2(3)	1(4)
N(5E)	37(3)	23(5)	32(4)	0(4)	-10(3)	4(4)
N(5F)	30(3)	22(4)	25(4)	-8(4)	3(3)	0(4)
N(5S)	31(7)	48(7)	47(10)	-2(6)	6(6)	-6(6)
N(6A)	22(3)	21(4)	16(3)	-3(4)	-4(3)	6(4)
N(6B)	19(3)	22(4)	24(5)	0(4)	1(3)	3(4)
N(6C)	29(3)	19(4)	25(4)	-3(4)	-2(3)	1(4)
N(6E)	25(3)	27(5)	44(4)	-2(5)	-13(3)	-4(4)
N(6F)	23(3)	20(5)	30(4)	-2(4)	5(3)	0(4)
N(6S)	39(7)	63(8)	26(7)	-2(6)	-4(5)	1(6)
N(41)	26(3)	27(5)	46(4)	5(5)	-14(3)	3(4)
N(42)	41(3)	14(4)	33(4)	-1(4)	-14(3)	-1(4)
C(1A)	20(3)	13(4)	22(4)	-1(4)	-1(2)	6(4)
C(1B)	19(4)	17(4)	22(3)	-3(4)	1(3)	0(4)
C(1C)	28(3)	14(4)	20(4)	3(4)	-3(3)	-2(4)
C(1D)	30(3)	25(4)	24(4)	5(4)	-4(3)	-3(4)
C(1E)	20(4)	22(4)	28(3)	-5(4)	-2(3)	2(4)
C(1F)	23(4)	32(5)	25(3)	2(4)	0(3)	0(4)
C(1S)	30(5)	28(5)	36(7)	-6(5)	-8(4)	3(5)
C(2A)	25(4)	24(4)	23(4)	-2(4)	-4(3)	2(4)
C(2B)	18(3)	29(4)	25(4)	-1(4)	0(3)	5(4)
C(2C)	34(4)	9(4)	19(4)	0(4)	-2(3)	1(4)
C(2D)	37(4)	21(4)	22(4)	5(4)	-5(3)	8(4)
C(2E)	20(3)	33(5)	32(4)	-1(4)	-1(3)	1(4)
C(2F)	24(4)	46(5)	29(4)	2(4)	-4(3)	1(4)
C(2S)	40(8)	41(8)	44(9)	-3(8)	2(6)	4(6)
C(3A)	24(3)	20(4)	26(3)	-1(4)	-9(3)	0(4)
C(3B)	22(3)	22(4)	23(3)	0(4)	-3(3)	3(4)

Table D.3.3 continued…

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(3C)	33(4)	6(4)	19(4)	0(4)	-6(3)	0(4)
C(3D)	35(4)	18(4)	21(3)	6(4)	1(3)	6(4)
C(3E)	22(3)	37(5)	28(4)	-4(4)	0(3)	-6(4)
C(3F)	27(4)	46(5)	28(4)	0(4)	-5(3)	-3(4)
C(3S)	24(5)	32(6)	34(7)	3(5)	-12(5)	-3(5)
C(4A)	20(3)	17(4)	27(3)	1(4)	-7(3)	-2(4)
C(4B)	22(3)	17(4)	18(3)	-4(4)	-1(3)	0(4)
C(4C)	21(3)	15(3)	20(3)	0(2)	-2(2)	-6(2)
C(4D)	28(3)	16(4)	20(4)	2(4)	3(3)	2(4)
C(4E)	21(3)	28(4)	22(3)	-3(4)	2(3)	0(4)
C(4F)	27(3)	39(5)	20(4)	0(4)	-6(3)	-2(4)
C(4S)	35(7)	33(7)	22(8)	-1(6)	-7(5)	-4(6)
C(5A)	17(4)	18(5)	34(4)	-1(5)	-6(3)	-5(4)
C(5B)	25(3)	13(5)	18(5)	3(4)	0(3)	1(4)
C(5C)	16(6)	31(6)	34(4)	2(5)	-11(4)	-5(4)
C(5D)	22(4)	40(6)	24(4)	0(5)	6(4)	7(5)
C(5E)	24(3)	13(5)	22(5)	4(4)	2(3)	-3(4)
C(5F)	32(4)	38(6)	18(5)	1(5)	-2(3)	3(5)
C(5S)	17(5)	29(6)	36(7)	3(5)	-3(4)	6(5)
C(6A)	27(6)	25(5)	37(5)	-2(4)	2(4)	-4(4)
C(6B)	25(4)	29(5)	25(6)	-1(5)	6(3)	0(4)
C(6C)	23(5)	37(6)	33(5)	7(4)	-5(4)	3(5)
C(6D)	13(5)	26(5)	28(4)	-1(4)	3(3)	0(4)
C(6E)	25(4)	24(5)	16(6)	2(4)	-11(4)	3(3)
C(6F)	31(4)	43(6)	38(7)	5(5)	7(5)	6(4)
C(6S)	27(7)	38(7)	63(11)	-7(7)	15(6)	4(6)
C(7A)	31(5)	17(5)	37(6)	4(4)	2(4)	2(4)
C(7B)	26(4)	23(5)	34(6)	-6(4)	3(4)	1(3)
C(7C)	24(5)	23(5)	33(5)	4(3)	1(4)	5(4)
C(7D)	15(5)	28(5)	25(4)	-1(3)	-6(4)	-2(4)
C(7E)	27(5)	31(5)	18(5)	1(4)	-9(4)	-2(4)
C(7F)	33(5)	35(6)	43(5)	0(5)	2(5)	5(4)
C(7S)	23(5)	25(5)	29(6)	2(5)	-8(4)	1(5)
C(8A)	25(4)	21(5)	36(6)	-1(4)	11(4)	-1(3)
C(8B)	19(5)	24(5)	35(6)	-1(4)	9(4)	-4(4)
C(8C)	28(6)	24(5)	26(5)	2(4)	13(5)	6(4)

Table D.3.3 continued…

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(8D)	23(5)	34(5)	21(5)	0(4)	-5(4)	-1(4)
C(8E)	20(5)	26(5)	22(4)	3(3)	-5(4)	4(4)
C(8F)	44(6)	38(6)	40(5)	-4(4)	0(5)	9(5)
C(8S)	35(7)	53(9)	42(9)	8(7)	6(6)	-5(7)
C(9A)	27(4)	20(5)	31(6)	2(5)	4(4)	-8(4)
C(9B)	16(5)	22(5)	31(5)	-2(4)	0(4)	-6(4)
C(9C)	29(6)	36(6)	29(6)	0(5)	-1(5)	-3(4)
C(9D)	26(4)	26(5)	22(6)	-2(4)	-1(4)	-2(3)
C(9E)	22(5)	27(5)	23(4)	4(4)	4(3)	-7(4)
C(9F)	29(6)	36(6)	43(5)	-5(5)	3(4)	2(5)
C(9S)	29(6)	37(6)	37(8)	5(6)	0(5)	1(5)
C(10A)	28(3)	26(5)	22(5)	5(5)	-1(3)	-3(5)
C(10B)	17(4)	21(5)	30(3)	-2(5)	-3(3)	-2(4)
C(10C)	31(4)	36(6)	20(5)	-4(5)	0(4)	-1(5)
C(10D)	27(3)	32(6)	22(5)	-4(5)	4(3)	3(5)
C(10E)	19(4)	18(5)	24(4)	-3(4)	6(3)	3(4)
C(10F)	23(4)	14(5)	29(4)	-13(5)	-11(3)	3(4)
C(10S)	22(7)	43(8)	62(13)	5(7)	3(7)	0(6)
C(11A)	26(3)	21(4)	21(3)	4(4)	-2(3)	0(4)
C(11B)	21(3)	16(4)	26(3)	4(4)	-5(3)	-2(4)
C(11C)	23(3)	30(5)	18(3)	-3(4)	-7(3)	-2(4)
C(11D)	23(3)	25(4)	25(3)	5(4)	6(3)	2(4)
C(11E)	26(3)	21(4)	22(4)	-2(4)	3(3)	0(4)
C(11F)	29(3)	18(4)	26(4)	-1(4)	-9(3)	2(4)
C(11S)	39(6)	54(7)	31(7)	5(6)	2(5)	-3(6)
C(12A)	28(4)	29(5)	23(4)	3(4)	-6(3)	-3(4)
C(12B)	22(3)	16(4)	26(3)	-1(4)	-6(3)	0(4)
C(12C)	25(4)	31(5)	23(4)	2(4)	-7(3)	0(4)
C(12D)	25(3)	33(5)	32(4)	-3(4)	7(3)	1(4)
C(12E)	33(4)	21(4)	22(4)	-1(4)	2(3)	-3(4)
C(12F)	36(4)	23(4)	26(4)	-3(4)	-8(3)	8(4)
C(12S)	31(8)	48(8)	59(11)	25(8)	7(6)	2(6)
C(13A)	19(4)	27(5)	25(4)	-1(4)	-3(3)	2(4)
C(13B)	26(4)	21(4)	21(3)	4(4)	-4(3)	-6(4)
C(13C)	23(4)	36(5)	26(4)	6(4)	-3(3)	0(4)
C(13D)	22(4)	33(5)	34(4)	1(4)	2(3)	5(4)

Table D.3.3 continued…

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(13E)	34(4)	28(5)	22(4)	0(4)	-4(3)	-1(4)
C(13F)	38(4)	10(4)	25(4)	-1(4)	-3(3)	8(4)
C(14A)	16(4)	22(4)	20(3)	-3(4)	-1(2)	1(4)
C(14B)	20(3)	18(4)	19(4)	5(4)	-1(2)	-1(4)
C(14C)	24(4)	24(4)	23(3)	0(4)	-1(3)	-1(4)
C(14D)	19(4)	27(4)	30(3)	3(4)	-2(3)	5(4)
C(14E)	29(3)	18(4)	23(4)	-4(4)	-2(3)	4(4)
C(14F)	29(3)	20(4)	25(4)	-2(4)	-1(3)	5(4)
C(15A)	20(3)	8(5)	19(3)	-1(4)	-1(2)	-3(4)
C(15B)	20(3)	11(5)	22(4)	5(4)	-1(3)	3(4)
C(15C)	23(3)	18(5)	24(3)	1(5)	1(3)	2(4)
C(15D)	25(3)	25(6)	33(3)	-4(5)	-6(3)	-7(5)
C(15E)	31(3)	18(5)	29(4)	7(5)	-7(3)	-12(5)
C(15F)	28(3)	17(5)	24(4)	-4(5)	2(2)	-3(4)
C(16A)	22(3)	19(5)	18(3)	3(5)	-2(2)	2(4)
C(16B)	19(4)	16(5)	21(3)	-4(5)	1(3)	-1(4)
C(16C)	28(3)	15(5)	25(4)	-5(5)	0(3)	-7(4)
C(16D)	32(3)	15(5)	28(4)	2(5)	-8(3)	9(4)
C(16E)	22(3)	18(5)	30(3)	-6(5)	-7(3)	-4(4)
C(16F)	23(3)	25(6)	26(3)	2(5)	3(3)	0(4)
C(17A)	19(3)	19(4)	26(3)	1(4)	2(2)	3(4)
C(17B)	21(3)	13(3)	19(3)	-2(2)	0(2)	0(2)
C(17C)	25(3)	26(5)	26(4)	1(4)	2(3)	3(4)
C(17D)	34(4)	39(5)	48(4)	4(5)	-18(3)	0(4)
C(17E)	38(3)	28(5)	42(4)	-2(4)	-17(3)	-3(4)
C(17F)	31(3)	19(4)	32(4)	-1(4)	6(3)	-1(4)
C(18A)	19(3)	20(4)	24(4)	5(4)	2(3)	1(4)
C(18B)	30(4)	22(4)	21(5)	-2(4)	-1(4)	3(4)
C(18C)	24(3)	28(5)	35(4)	-4(4)	3(3)	5(4)
C(18D)	35(4)	51(5)	55(5)	1(5)	-22(4)	2(5)
C(18E)	45(4)	31(5)	43(4)	1(5)	-19(4)	4(4)
C(18F)	34(4)	21(4)	32(4)	3(4)	6(3)	-3(4)
C(19A)	24(4)	16(4)	25(4)	-1(4)	4(3)	4(4)
C(19B)	31(4)	18(4)	26(4)	4(4)	0(3)	6(4)
C(19C)	26(4)	34(5)	37(4)	-2(4)	6(3)	1(4)
C(19D)	42(5)	48(5)	58(5)	-2(5)	-26(3)	5(5)

Table D.3.3 continued…

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(19E)	45(4)	30(5)	50(4)	-1(5)	-24(4)	8(4)
C(19F)	35(4)	28(5)	38(4)	-1(5)	11(3)	0(4)
C(20A)	28(4)	15(4)	26(4)	-3(4)	2(3)	0(4)
C(20B)	27(4)	16(4)	28(4)	0(4)	2(3)	4(4)
C(20C)	32(4)	32(5)	34(4)	2(4)	5(3)	7(4)
C(20D)	48(4)	50(5)	52(5)	-6(5)	-27(4)	11(5)
C(20E)	37(4)	30(5)	54(5)	-2(5)	-22(3)	6(4)
C(20F)	28(4)	30(5)	41(5)	1(4)	11(3)	1(4)
C(21A)	27(4)	21(4)	25(4)	-4(4)	1(3)	4(4)
C(21B)	21(4)	12(4)	27(4)	0(4)	-1(4)	-2(4)
C(21C)	33(4)	35(5)	26(4)	1(4)	1(3)	0(4)
C(21D)	49(4)	46(5)	45(4)	-7(5)	-22(4)	3(5)
C(21E)	32(3)	33(5)	51(4)	-7(5)	-19(3)	6(4)
C(21F)	28(3)	22(4)	37(4)	0(4)	7(3)	0(4)
C(22A)	24(3)	17(4)	27(3)	-10(4)	2(3)	5(4)
C(22B)	17(3)	16(3)	19(3)	-3(2)	1(2)	3(2)
C(22C)	30(3)	28(5)	26(4)	6(4)	0(3)	6(4)
C(22D)	40(3)	38(5)	44(4)	-1(5)	-19(3)	3(4)
C(22E)	31(3)	24(5)	45(4)	-4(5)	-15(3)	3(4)
C(22F)	27(3)	20(4)	31(4)	-2(4)	7(3)	3(4)

Table D.3.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [Au(L3)](PF_6).

	x	y	z	U(eq)
H(2A)	5643	2097	6840	29
H(2B)	5806	6795	6717	29
H(2C)	9412	3193	6267	25
H(2D)	9361	7314	5159	32
H(2E)	9068	3059	8295	34
H(2F)	8922	7748	9603	40
H(2SA)	5740	829	9247	62
H(2SB)	5939	1452	9508	62
H(2SC)	5785	3118	9320	62
H(3A)	5091	1477	6956	28
H(3B)	6018	7020	6241	27
H(3C)	9976	3121	6213	23
H(3D)	9911	7189	5233	30
H(3E)	8807	3764	7862	35
H(3F)	8627	7362	10051	40
H(4SA)	6234	8410	8595	45
H(4SB)	6411	7497	8852	45
H(4SC)	6267	6063	8625	45
H(5A)	4808	830	7495	28
H(5B)	6643	7461	6058	22
H(5C)	10357	2502	5736	32
H(5D)	10261	7534	5750	35
H(5E)	8133	4298	7747	24
H(5F)	7966	6723	10130	35
H(6AA)	4957	-736	8137	36
H(6AB)	4680	-276	7934	36
H(6BA)	7298	9106	6137	32
H(6BB)	7163	7188	5990	32
H(6CA)	10450	875	5140	37
H(6CB)	10601	2613	5316	37
H(6DA)	10331	9272	6319	27
H(6DB)	10444	7253	6181	27
H(6EA)	7641	5206	7761	26
H(6EB)	7484	5423	8055	26

Table D.3.3 continued…

	x	y	z	U(eq)
H(6FA)	7359	4702	9817	45
H(6FB)	7493	5373	10106	45
H(6SA)	8408	9454	7388	64
H(6SB)	8540	7630	7560	64
H(6SC)	8601	9848	7660	64
H(7AA)	4640	2924	8098	34
H(7AB)	4618	1416	8349	34
H(7BA)	7575	5738	6131	33
H(7BB)	7399	5557	6416	33
H(7CA)	10592	4269	4936	32
H(7CB)	10241	4647	5008	32
H(7DA)	10021	5847	6504	27
H(7DB)	10370	5946	6594	27
H(7EA)	7184	3325	7787	30
H(7EB)	7471	1947	7720	30
H(7FA)	7255	8362	10078	44
H(7FB)	7009	6660	10029	44
H(8AA)	4908	3852	8504	33
H(8AB)	5095	4028	8225	33
H(8BA)	7870	6805	6534	31
H(8BB)	7871	8337	6284	31
H(8CA)	10222	3478	4566	31
H(8CB)	10480	1863	4620	31
H(8DA)	10298	8641	6852	31
H(8DB)	10016	7231	6921	31
H(8EA)	7132	597	8059	27
H(8EB)	7480	669	8151	27
H(8FA)	6892	8965	9706	49
H(8FB)	7241	9372	9634	49
H(8SA)	8852	3911	6958	65
H(8SB)	9009	5489	7157	65
H(8SC)	9041	3173	7219	65
H(9AA)	5310	2301	8655	31
H(9AB)	5172	424	8498	31
H(9BA)	7789	9992	6709	28
H(9BB)	7514	10360	6502	28

Table D.3.3 continued…

	x	y	z	U(eq)
H(9CA)	10016	325	4558	38
H(9CB)	10139	-97	4859	38
H(9DA)	9838	10425	6881	29
H(9DB)	9995	10679	6588	29
H(9EA)	7139	3917	8317	29
H(9EB)	7040	1863	8454	29
H(9FA)	7034	5587	9502	43
H(9FB)	6890	7343	9324	43
H(10A)	5824	2070	8586	30
H(10B)	7678	8926	7137	27
H(10C)	9516	1476	4532	35
H(10D)	9335	9449	6886	32
H(10E)	7242	2156	8891	24
H(10F)	7119	7215	8916	27
H(10G)	6081	2879	5798	63
H(10H)	6203	1035	5971	63
H(10I)	6265	3242	6076	63
H(12A)	6464	2757	8403	32
H(12B)	7388	8247	7680	26
H(12C)	8866	2174	4609	32
H(12D)	8675	8567	6779	36
H(12E)	7596	2004	9400	30
H(12F)	7500	7867	8432	34
H(12G)	6558	7538	5115	69
H(12H)	6759	8300	5368	69
H(12I)	6680	5999	5339	69
H(13A)	6680	2710	7934	28
H(13B)	6840	7662	7800	27
H(13C)	8577	2748	5041	34
H(13D)	8425	7789	6337	36
H(13E)	8170	2228	9480	34
H(13F)	8068	8063	8377	29
H(18A)	7115	3261	7261	25
H(18B)	6057	7342	8104	29
H(18C)	8003	2157	5630	35
H(18D)	7899	7233	5710	56

Table D.3.3 continued…

	x	y	z	U(eq)
H(18E)	9000	2538	9702	48
H(18F)	8918	8308	8196	35
H(19A)	7296	3401	6813	26
H(19B)	5538	6699	8191	30
H(19C)	7761	2407	6047	39
H(19D)	7700	7037	5254	59
H(19E)	9545	2517	9708	50
H(19F)	9434	8249	8191	40
H(20A)	6945	2750	6449	28
H(20B)	5196	6293	7824	28
H(20C)	8026	2905	6443	39
H(20D)	8013	7186	4887	60
H(20E)	9830	2668	9310	48
H(20F)	9724	7825	8600	39
H(21A)	6443	2262	6536	29
H(21B)	5353	6358	7378	24
H(21C)	8564	3191	6441	38
H(21D)	8516	7588	4920	56
H(21E)	9592	2851	8906	46
H(21F)	9468	7582	9017	35

Table D.3.4: Torsion angles [°] for [Au(L3)](PF_6).

N(4A)-Au(1)-N(1A)-C(1A)	-2.1(13)
N(2A)-Au(1)-N(1A)-C(1A)	-179.3(13)
N(4A)-Au(1)-N(1A)-C(4A)	-177.6(8)
N(2A)-Au(1)-N(1A)-C(4A)	5.1(7)
N(4B)-Au(2)-N(1B)-C(1B)	0.7(13)
N(2B)-Au(2)-N(1B)-C(1B)	178.3(13)
N(4B)-Au(2)-N(1B)-C(4B)	177.3(8)
N(2B)-Au(2)-N(1B)-C(4B)	-5.1(8)
N(4C)-Au(3)-N(1C)-C(4C)	-179.2(8)
N(2C)-Au(3)-N(1C)-C(4C)	-1.6(8)
N(4C)-Au(3)-N(1C)-C(1C)	2.7(13)
N(2C)-Au(3)-N(1C)-C(1C)	-179.7(13)
N(4D)-Au(4)-N(1D)-C(4D)	-178.1(8)
N(2D)-Au(4)-N(1D)-C(4D)	-2.6(8)
N(4D)-Au(4)-N(1D)-C(1D)	9.3(14)
N(2D)-Au(4)-N(1D)-C(1D)	-175.2(15)
N(4E)-Au(5)-N(1E)-C(1E)	5.3(14)
N(2E)-Au(5)-N(1E)-C(1E)	-177.3(14)
N(4E)-Au(5)-N(1E)-C(4E)	177.0(9)
N(2E)-Au(5)-N(1E)-C(4E)	-5.6(9)
N(2F)-Au(6)-N(1F)-C(1F)	171.8(16)
N(4F)-Au(6)-N(1F)-C(1F)	-6.7(16)
N(2F)-Au(6)-N(1F)-C(4F)	-0.4(10)
N(4F)-Au(6)-N(1F)-C(4F)	-179.0(10)
N(1A)-Au(1)-N(2A)-C(5A)	-4.2(9)
N(3A)-Au(1)-N(2A)-C(5A)	173.3(9)
N(1A)-Au(1)-N(2A)-C(6A)	168.1(10)
N(3A)-Au(1)-N(2A)-C(6A)	-14.4(10)
N(1B)-Au(2)-N(2B)-C(5B)	3.0(8)
N(3B)-Au(2)-N(2B)-C(5B)	-173.5(8)
N(1B)-Au(2)-N(2B)-C(6B)	-171.0(11)
N(3B)-Au(2)-N(2B)-C(6B)	12.5(11)
N(1C)-Au(3)-N(2C)-C(5C)	2.0(9)
N(3C)-Au(3)-N(2C)-C(5C)	-176.9(9)
N(1C)-Au(3)-N(2C)-C(6C)	-174.0(11)
N(3C)-Au(3)-N(2C)-C(6C)	7.1(11)

Table D.3.4 continued…

N(1D)-Au(4)-N(2D)-C(5D)	3.1(10)
N(3D)-Au(4)-N(2D)-C(5D)	-173.2(10)
N(1D)-Au(4)-N(2D)-C(6D)	-173.0(11)
N(3D)-Au(4)-N(2D)-C(6D)	10.8(11)
N(1E)-Au(5)-N(2E)-C(5E)	2.4(8)
N(3E)-Au(5)-N(2E)-C(5E)	-173.4(8)
N(1E)-Au(5)-N(2E)-C(6E)	-165.8(10)
N(3E)-Au(5)-N(2E)-C(6E)	18.4(10)
N(1F)-Au(6)-N(2F)-C(5F)	3.4(10)
N(3F)-Au(6)-N(2F)-C(5F)	-172.4(10)
N(1F)-Au(6)-N(2F)-C(6F)	-167.4(13)
N(3F)-Au(6)-N(2F)-C(6F)	16.9(13)
N(4A)-Au(1)-N(3A)-C(10A)	-1.8(10)
N(2A)-Au(1)-N(3A)-C(10A)	175.5(9)
N(4A)-Au(1)-N(3A)-C(9A)	171.1(11)
N(2A)-Au(1)-N(3A)-C(9A)	-11.5(11)
N(4B)-Au(2)-N(3B)-C(10B)	4.8(9)
N(2B)-Au(2)-N(3B)-C(10B)	-172.8(9)
N(4B)-Au(2)-N(3B)-C(9B)	-167.8(10)
N(2B)-Au(2)-N(3B)-C(9B)	14.6(10)
N(4C)-Au(3)-N(3C)-C(10C)	3.2(10)
N(2C)-Au(3)-N(3C)-C(10C)	-174.4(10)
N(4C)-Au(3)-N(3C)-C(9C)	-164.7(11)
N(2C)-Au(3)-N(3C)-C(9C)	17.7(11)
N(4D)-Au(4)-N(3D)-C(10D)	4.0(9)
N(2D)-Au(4)-N(3D)-C(10D)	-171.6(9)
N(4D)-Au(4)-N(3D)-C(9D)	-168.3(10)
N(2D)-Au(4)-N(3D)-C(9D)	16.1(10)
N(4E)-Au(5)-N(3E)-C(10E)	1.6(9)
N(2E)-Au(5)-N(3E)-C(10E)	-175.8(8)
N(4E)-Au(5)-N(3E)-C(9E)	-170.5(10)
N(2E)-Au(5)-N(3E)-C(9E)	12.1(10)
N(2F)-Au(6)-N(3F)-C(10F)	-177.4(9)
N(4F)-Au(6)-N(3F)-C(10F)	1.1(9)
N(2F)-Au(6)-N(3F)-C(9F)	7.2(13)
N(4F)-Au(6)-N(3F)-C(9F)	-174.2(12)
N(1A)-Au(1)-N(4A)-C(14A)	1.2(14)

Table D.3.4 continued…

N(3A)-Au(1)-N(4A)-C(14A)	-176.3(14)
N(1A)-Au(1)-N(4A)-C(11A)	-179.4(8)
N(3A)-Au(1)-N(4A)-C(11A)	3.1(9)
N(1B)-Au(2)-N(4B)-C(14B)	2.7(14)
N(3B)-Au(2)-N(4B)-C(14B)	179.1(14)
N(1B)-Au(2)-N(4B)-C(11B)	176.8(8)
N(3B)-Au(2)-N(4B)-C(11B)	-6.8(8)
N(1C)-Au(3)-N(4C)-C(11C)	172.6(9)
N(3C)-Au(3)-N(4C)-C(11C)	-8.6(9)
N(1C)-Au(3)-N(4C)-C(14C)	3.0(14)
N(3C)-Au(3)-N(4C)-C(14C)	-178.3(14)
N(1D)-Au(4)-N(4D)-C(14D)	10.4(14)
N(3D)-Au(4)-N(4D)-C(14D)	-173.4(14)
N(1D)-Au(4)-N(4D)-C(11D)	176.5(8)
N(3D)-Au(4)-N(4D)-C(11D)	-7.3(8)
N(1E)-Au(5)-N(4E)-C(14E)	10.3(14)
N(3E)-Au(5)-N(4E)-C(14E)	-173.9(14)
N(1E)-Au(5)-N(4E)-C(11E)	179.9(8)
N(3E)-Au(5)-N(4E)-C(11E)	-4.3(8)
N(1F)-Au(6)-N(4F)-C(14F)	2.4(15)
N(3F)-Au(6)-N(4F)-C(14F)	178.1(15)
N(1F)-Au(6)-N(4F)-C(11F)	-177.4(8)
N(3F)-Au(6)-N(4F)-C(11F)	-1.7(8)
C(4A)-N(1A)-C(1A)-C(2A)	1.7(13)
Au(1)-N(1A)-C(1A)-C(2A)	-173.9(9)
C(4A)-N(1A)-C(1A)-C(16A)	-178.2(12)
C(4B)-N(1B)-C(1B)-C(2B)	1.4(13)
Au(2)-N(1B)-C(1B)-C(2B)	178.2(10)
C(4B)-N(1B)-C(1B)-C(16B)	-178.2(12)
Au(2)-N(1B)-C(1B)-C(16B)	-1(2)
C(4C)-N(1C)-C(1C)-C(2C)	0.3(13)
Au(3)-N(1C)-C(1C)-C(2C)	178.5(9)
C(4C)-N(1C)-C(1C)-C(16C)	-177.2(12)
Au(3)-N(1C)-C(1C)-C(16C)	1(2)
C(4D)-N(1D)-C(1D)-C(2D)	-0.8(14)
Au(4)-N(1D)-C(1D)-C(2D)	172.0(10)
C(4D)-N(1D)-C(1D)-C(16D)	174.6(12)

Table D.3.4 continued…

Au(4)-N(1D)-C(1D)-C(16D)	-13(2)
C(4E)-N(1E)-C(1E)-C(16E)	173.8(13)
Au(5)-N(1E)-C(1E)-C(16E)	-14(2)
C(4E)-N(1E)-C(1E)-C(2E)	1.3(15)
Au(5)-N(1E)-C(1E)-C(2E)	173.1(11)
C(4F)-N(1F)-C(1F)-C(2F)	-6.5(16)
Au(6)-N(1F)-C(1F)-C(2F)	-178.8(12)
C(4F)-N(1F)-C(1F)-C(16F)	174.1(13)
Au(6)-N(1F)-C(1F)-C(16F)	2(2)
N(1A)-C(1A)-C(2A)-C(3A)	-1.7(14)
C(16A)-C(1A)-C(2A)-C(3A)	178.1(11)
N(1B)-C(1B)-C(2B)-C(3B)	-0.6(15)
C(16B)-C(1B)-C(2B)-C(3B)	179.1(11)
N(1C)-C(1C)-C(2C)-C(3C)	0.8(13)
C(16C)-C(1C)-C(2C)-C(3C)	178.7(11)
N(1D)-C(1D)-C(2D)-C(3D)	0.1(15)
C(16D)-C(1D)-C(2D)-C(3D)	-175.5(12)
N(1E)-C(1E)-C(2E)-C(3E)	0.2(16)
C(16E)-C(1E)-C(2E)-C(3E)	-173.3(12)
N(1F)-C(1F)-C(2F)-C(3F)	3.2(17)
C(16F)-C(1F)-C(2F)-C(3F)	-177.3(13)
C(1A)-C(2A)-C(3A)-C(4A)	1.1(14)
C(1B)-C(2B)-C(3B)-C(4B)	-0.5(15)
C(1C)-C(2C)-C(3C)-C(4C)	-1.6(13)
C(1D)-C(2D)-C(3D)-C(4D)	0.6(14)
C(1E)-C(2E)-C(3E)-C(4E)	-1.7(16)
C(1F)-C(2F)-C(3F)-C(4F)	1.4(17)
C(1A)-N(1A)-C(4A)-C(5A)	177.5(11)
Au(1)-N(1A)-C(4A)-C(5A)	-5.5(13)
C(1A)-N(1A)-C(4A)-C(3A)	-1.0(13)
Au(1)-N(1A)-C(4A)-C(3A)	176.0(8)
C(2A)-C(3A)-C(4A)-C(5A)	-178.2(14)
C(2A)-C(3A)-C(4A)-N(1A)	-0.1(13)
C(2B)-C(3B)-C(4B)-C(5B)	173.4(14)
C(2B)-C(3B)-C(4B)-N(1B)	1.4(14)
C(1B)-N(1B)-C(4B)-C(5B)	-175.7(10)
Au(2)-N(1B)-C(4B)-C(5B)	6.6(12)

Table D.3.4 continued…

C(1B)-N(1B)-C(4B)-C(3B)	-1.7(13)
Au(2)-N(1B)-C(4B)-C(3B)	-179.5(8)
C(2C)-C(3C)-C(4C)-N(1C)	1.8(13)
C(2C)-C(3C)-C(4C)-C(5C)	-179.4(13)
C(1C)-N(1C)-C(4C)-C(3C)	-1.4(13)
Au(3)-N(1C)-C(4C)-C(3C)	179.9(8)
C(1C)-N(1C)-C(4C)-C(5C)	179.7(11)
Au(3)-N(1C)-C(4C)-C(5C)	1.0(13)
C(1D)-N(1D)-C(4D)-C(3D)	1.2(14)
Au(4)-N(1D)-C(4D)-C(3D)	-173.8(8)
C(1D)-N(1D)-C(4D)-C(5D)	176.8(11)
Au(4)-N(1D)-C(4D)-C(5D)	1.8(14)
C(2D)-C(3D)-C(4D)-N(1D)	-1.1(14)
C(2D)-C(3D)-C(4D)-C(5D)	-175.9(13)
C(1E)-N(1E)-C(4E)-C(3E)	-2.4(15)
Au(5)-N(1E)-C(4E)-C(3E)	-176.6(9)
C(1E)-N(1E)-C(4E)-C(5E)	-177.8(11)
Au(5)-N(1E)-C(4E)-C(5E)	8.0(14)
C(2E)-C(3E)-C(4E)-N(1E)	2.5(16)
C(2E)-C(3E)-C(4E)-C(5E)	176.5(15)
C(1F)-N(1F)-C(4F)-C(5F)	-177.4(13)
Au(6)-N(1F)-C(4F)-C(5F)	-2.5(17)
C(1F)-N(1F)-C(4F)-C(3F)	7.5(17)
Au(6)-N(1F)-C(4F)-C(3F)	-177.5(11)
C(2F)-C(3F)-C(4F)-N(1F)	-5.3(18)
C(2F)-C(3F)-C(4F)-C(5F)	-179.3(17)
C(6A)-N(2A)-C(5A)-C(4A)	-170.2(11)
Au(1)-N(2A)-C(5A)-C(4A)	2.3(15)
N(1A)-C(4A)-C(5A)-N(2A)	2.2(17)
C(3A)-C(4A)-C(5A)-N(2A)	-179.8(13)
C(6B)-N(2B)-C(5B)-C(4B)	174.3(11)
Au(2)-N(2B)-C(5B)-C(4B)	-0.1(13)
C(3B)-C(4B)-C(5B)-N(2B)	-175.8(14)
N(1B)-C(4B)-C(5B)-N(2B)	-4.3(16)
C(6C)-N(2C)-C(5C)-C(4C)	174.0(12)
Au(3)-N(2C)-C(5C)-C(4C)	-2.1(15)
C(3C)-C(4C)-C(5C)-N(2C)	-177.8(13)

Table D.3.4 continued…

N(1C)-C(4C)-C(5C)-N(2C)	0.9(18)
C(6D)-N(2D)-C(5D)-C(4D)	173.5(11)
Au(4)-N(2D)-C(5D)-C(4D)	-2.9(16)
N(1D)-C(4D)-C(5D)-N(2D)	0.8(18)
C(3D)-C(4D)-C(5D)-N(2D)	175.2(13)
C(6E)-N(2E)-C(5E)-C(4E)	170.3(11)
Au(5)-N(2E)-C(5E)-C(4E)	1.3(14)
N(1E)-C(4E)-C(5E)-N(2E)	-6.4(17)
C(3E)-C(4E)-C(5E)-N(2E)	179.9(15)
C(6F)-N(2F)-C(5F)-C(4F)	166.2(13)
Au(6)-N(2F)-C(5F)-C(4F)	-5.6(17)
N(1F)-C(4F)-C(5F)-N(2F)	5(2)
C(3F)-C(4F)-C(5F)-N(2F)	179.1(16)
C(5A)-N(2A)-C(6A)-C(7A)	-112.2(15)
Au(1)-N(2A)-C(6A)-C(7A)	76.3(14)
C(5B)-N(2B)-C(6B)-C(7B)	-134.8(12)
Au(2)-N(2B)-C(6B)-C(7B)	38.6(16)
C(5C)-N(2C)-C(6C)-C(7C)	-130.2(15)
Au(3)-N(2C)-C(6C)-C(7C)	45.2(17)
C(5D)-N(2D)-C(6D)-C(7D)	-137.5(13)
Au(4)-N(2D)-C(6D)-C(7D)	38.4(15)
C(5E)-N(2E)-C(6E)-C(7E)	111.7(14)
Au(5)-N(2E)-C(6E)-C(7E)	-80.8(13)
C(5F)-N(2F)-C(6F)-C(7F)	112.4(18)
Au(6)-N(2F)-C(6F)-C(7F)	-77.1(19)
N(2A)-C(6A)-C(7A)-C(8A)	-56.3(18)
N(2B)-C(6B)-C(7B)-C(8B)	-98.7(15)
N(2C)-C(6C)-C(7C)-C(8C)	-99.4(15)
N(2D)-C(6D)-C(7D)-C(8D)	-98.4(13)
N(2E)-C(6E)-C(7E)-C(8E)	54.8(16)
N(2F)-C(6F)-C(7F)-C(8F)	54(2)
C(6A)-C(7A)-C(8A)-C(9A)	-42.8(19)
C(6B)-C(7B)-C(8B)-C(9B)	44.3(18)
C(6C)-C(7C)-C(8C)-C(9C)	40.8(18)
C(6D)-C(7D)-C(8D)-C(9D)	44.7(16)
C(6E)-C(7E)-C(8E)-C(9E)	47.2(17)
C(6F)-C(7F)-C(8F)-C(9F)	42(2)

Table D.3.4 continued…

C(10A)-N(3A)-C(9A)-C(8A)	133.0(13)
Au(1)-N(3A)-C(9A)-C(8A)	-39.5(15)
C(7A)-C(8A)-C(9A)-N(3A)	99.0(14)
C(10B)-N(3B)-C(9B)-C(8B)	110.6(14)
Au(2)-N(3B)-C(9B)-C(8B)	-77.3(14)
C(7B)-C(8B)-C(9B)-N(3B)	54.5(17)
C(10C)-N(3C)-C(9C)-C(8C)	112.9(17)
Au(3)-N(3C)-C(9C)-C(8C)	-80.6(16)
C(7C)-C(8C)-C(9C)-N(3C)	58.9(18)
C(10D)-N(3D)-C(9D)-C(8D)	110.4(15)
Au(4)-N(3D)-C(9D)-C(8D)	-78.0(14)
C(7D)-C(8D)-C(9D)-N(3D)	54.1(16)
C(10E)-N(3E)-C(9E)-C(8E)	-135.4(13)
Au(5)-N(3E)-C(9E)-C(8E)	35.8(14)
C(7E)-C(8E)-C(9E)-N(3E)	-99.7(13)
C(10F)-N(3F)-C(9F)-C(8F)	-132.4(14)
Au(6)-N(3F)-C(9F)-C(8F)	42.7(18)
C(7F)-C(8F)-C(9F)-N(3F)	-97.6(18)
C(9A)-N(3A)-C(10A)-C(11A)	-173.4(12)
Au(1)-N(3A)-C(10A)-C(11A)	0.1(16)
C(9B)-N(3B)-C(10B)-C(11B)	171.4(11)
Au(2)-N(3B)-C(10B)-C(11B)	-1.6(14)
C(9C)-N(3C)-C(10C)-C(11C)	170.9(13)
Au(3)-N(3C)-C(10C)-C(11C)	3.1(18)
C(9D)-N(3D)-C(10D)-C(11D)	173.0(11)
Au(4)-N(3D)-C(10D)-C(11D)	0.4(15)
C(9E)-N(3E)-C(10E)-C(11E)	173.9(11)
Au(5)-N(3E)-C(10E)-C(11E)	1.5(14)
C(9F)-N(3F)-C(10F)-C(11F)	175.6(11)
Au(6)-N(3F)-C(10F)-C(11F)	-0.3(14)
C(14A)-N(4A)-C(11A)-C(12A)	1.7(14)
Au(1)-N(4A)-C(11A)-C(12A)	-177.9(9)
C(14A)-N(4A)-C(11A)-C(10A)	175.7(11)
Au(1)-N(4A)-C(11A)-C(10A)	-4.0(14)
N(3A)-C(10A)-C(11A)-N(4A)	2.6(19)
N(3A)-C(10A)-C(11A)-C(12A)	174.7(14)
C(14B)-N(4B)-C(11B)-C(12B)	0.2(13)

Table D.3.4 continued…

Au(2)-N(4B)-C(11B)-C(12B)	-175.9(8)
C(14B)-N(4B)-C(11B)-C(10B)	-175.9(11)
Au(2)-N(4B)-C(11B)-C(10B)	8.1(13)
N(3B)-C(10B)-C(11B)-C(12B)	-178.9(13)
N(3B)-C(10B)-C(11B)-N(4B)	-4.4(17)
N(3C)-C(10C)-C(11C)-C(12C)	-175.5(16)
N(3C)-C(10C)-C(11C)-N(4C)	-11(2)
C(14C)-N(4C)-C(11C)-C(12C)	-5.6(15)
Au(3)-N(4C)-C(11C)-C(12C)	-178.4(9)
C(14C)-N(4C)-C(11C)-C(10C)	-174.6(12)
Au(3)-N(4C)-C(11C)-C(10C)	12.6(15)
N(3D)-C(10D)-C(11D)-N(4D)	-7.0(18)
N(3D)-C(10D)-C(11D)-C(12D)	175.9(15)
C(14D)-N(4D)-C(11D)-C(10D)	-179.6(11)
Au(4)-N(4D)-C(11D)-C(10D)	9.8(14)
C(14D)-N(4D)-C(11D)-C(12D)	-1.7(14)
Au(4)-N(4D)-C(11D)-C(12D)	-172.3(9)
C(14E)-N(4E)-C(11E)-C(12E)	-1.9(14)
Au(5)-N(4E)-C(11E)-C(12E)	-174.8(9)
C(14E)-N(4E)-C(11E)-C(10E)	179.2(10)
Au(5)-N(4E)-C(11E)-C(10E)	6.3(13)
N(3E)-C(10E)-C(11E)-C(12E)	176.1(15)
N(3E)-C(10E)-C(11E)-N(4E)	-5.4(17)
C(14F)-N(4F)-C(11F)-C(12F)	-1.9(14)
Au(6)-N(4F)-C(11F)-C(12F)	178.0(9)
C(14F)-N(4F)-C(11F)-C(10F)	-177.8(10)
Au(6)-N(4F)-C(11F)-C(10F)	2.1(13)
N(3F)-C(10F)-C(11F)-C(12F)	-175.7(14)
N(3F)-C(10F)-C(11F)-N(4F)	-1.2(16)
N(4A)-C(11A)-C(12A)-C(13A)	-4.7(15)
C(10A)-C(11A)-C(12A)-C(13A)	-177.0(15)
N(4B)-C(11B)-C(12B)-C(13B)	0.5(13)
C(10B)-C(11B)-C(12B)-C(13B)	175.4(14)
C(10C)-C(11C)-C(12C)-C(13C)	171.1(17)
N(4C)-C(11C)-C(12C)-C(13C)	5.8(16)
C(10D)-C(11D)-C(12D)-C(13D)	178.5(16)
N(4D)-C(11D)-C(12D)-C(13D)	1.3(15)

Table D.3.4 continued…

N(4E)-C(11E)-C(12E)-C(13E)	1.3(15)
C(10E)-C(11E)-C(12E)-C(13E)	179.9(15)
N(4F)-C(11F)-C(12F)-C(13F)	2.8(15)
C(10F)-C(11F)-C(12F)-C(13F)	177.6(13)
C(11A)-C(12A)-C(13A)-C(14A)	5.8(15)
C(11B)-C(12B)-C(13B)-C(14B)	-1.0(14)
C(11C)-C(12C)-C(13C)-C(14C)	-3.9(16)
C(11D)-C(12D)-C(13D)-C(14D)	-0.4(17)
C(11E)-C(12E)-C(13E)-C(14E)	-0.3(15)
C(11F)-C(12F)-C(13F)-C(14F)	-2.6(14)
C(11A)-N(4A)-C(14A)-C(13A)	1.9(14)
Au(1)-N(4A)-C(14A)-C(13A)	-178.7(10)
C(11A)-N(4A)-C(14A)-C(15A)	177.0(12)
Au(1)-N(4A)-C(14A)-C(15A)	-4(2)
C(12A)-C(13A)-C(14A)-N(4A)	-4.9(15)
C(12A)-C(13A)-C(14A)-C(15A)	179.6(11)
C(11B)-N(4B)-C(14B)-C(13B)	-0.8(13)
Au(2)-N(4B)-C(14B)-C(13B)	173.4(10)
C(11B)-N(4B)-C(14B)-C(15B)	179.9(11)
Au(2)-N(4B)-C(14B)-C(15B)	-6(2)
C(12B)-C(13B)-C(14B)-N(4B)	1.1(14)
C(12B)-C(13B)-C(14B)-C(15B)	-179.5(10)
C(11C)-N(4C)-C(14C)-C(13C)	3.2(15)
Au(3)-N(4C)-C(14C)-C(13C)	173.1(11)
C(11C)-N(4C)-C(14C)-C(15C)	178.1(13)
Au(3)-N(4C)-C(14C)-C(15C)	-12(2)
C(12C)-C(13C)-C(14C)-N(4C)	0.5(15)
C(12C)-C(13C)-C(14C)-C(15C)	-174.9(11)
C(12D)-C(13D)-C(14D)-N(4D)	-0.7(16)
C(12D)-C(13D)-C(14D)-C(15D)	-173.7(13)
C(11D)-N(4D)-C(14D)-C(13D)	1.4(14)
Au(4)-N(4D)-C(14D)-C(13D)	167.7(11)
C(11D)-N(4D)-C(14D)-C(15D)	174.2(13)
Au(4)-N(4D)-C(14D)-C(15D)	-19(2)
C(11E)-N(4E)-C(14E)-C(13E)	1.7(14)
Au(5)-N(4E)-C(14E)-C(13E)	171.5(10)
C(11E)-N(4E)-C(14E)-C(15E)	176.5(12)

Table D.3.4 continued…

Au(5)-N(4E)-C(14E)-C(15E)	-14(2)
C(12E)-C(13E)-C(14E)-N(4E)	-0.9(14)
C(12E)-C(13E)-C(14E)-C(15E)	-176.2(11)
C(11F)-N(4F)-C(14F)-C(13F)	0.3(14)
Au(6)-N(4F)-C(14F)-C(13F)	-179.5(10)
C(11F)-N(4F)-C(14F)-C(15F)	-176.6(12)
Au(6)-N(4F)-C(14F)-C(15F)	4(2)
C(12F)-C(13F)-C(14F)-N(4F)	1.4(14)
C(12F)-C(13F)-C(14F)-C(15F)	178.4(11)
C(17A)-N(5A)-C(15A)-C(14A)	179.5(11)
C(17A)-N(5A)-C(15A)-C(16A)	-1.3(16)
N(4A)-C(14A)-C(15A)-N(5A)	-177.9(12)
C(13A)-C(14A)-C(15A)-N(5A)	-3.4(16)
N(4A)-C(14A)-C(15A)-C(16A)	3(2)
C(13A)-C(14A)-C(15A)-C(16A)	177.6(12)
C(17B)-N(5B)-C(15B)-C(16B)	1.2(16)
C(17B)-N(5B)-C(15B)-C(14B)	-177.7(10)
N(4B)-C(14B)-C(15B)-N(5B)	-175.2(12)
C(13B)-C(14B)-C(15B)-N(5B)	5.6(15)
N(4B)-C(14B)-C(15B)-C(16B)	6(2)
C(13B)-C(14B)-C(15B)-C(16B)	-173.1(12)
C(17C)-N(5C)-C(15C)-C(16C)	0.1(18)
C(17C)-N(5C)-C(15C)-C(14C)	179.4(11)
N(4C)-C(14C)-C(15C)-N(5C)	-166.5(13)
C(13C)-C(14C)-C(15C)-N(5C)	7.8(17)
N(4C)-C(14C)-C(15C)-C(16C)	13(2)
C(13C)-C(14C)-C(15C)-C(16C)	-173.1(13)
C(17D)-N(41)-C(15D)-C(16D)	-1.6(19)
C(17D)-N(41)-C(15D)-C(14D)	178.4(12)
C(13D)-C(14D)-C(15D)-N(41)	-0.8(19)
N(4D)-C(14D)-C(15D)-N(41)	-172.3(12)
C(13D)-C(14D)-C(15D)-C(16D)	179.2(14)
N(4D)-C(14D)-C(15D)-C(16D)	8(2)
C(17E)-N(5E)-C(15E)-C(14E)	178.6(12)
C(17E)-N(5E)-C(15E)-C(16E)	-4.0(19)
N(4E)-C(14E)-C(15E)-N(5E)	-179.4(12)
C(13E)-C(14E)-C(15E)-N(5E)	-5.1(17)

Table D.3.4 continued…

N(4E)-C(14E)-C(15E)-C(16E)	4(2)
C(13E)-C(14E)-C(15E)-C(16E)	177.8(13)
C(17F)-N(5F)-C(15F)-C(16F)	0.7(19)
C(17F)-N(5F)-C(15F)-C(14F)	-178.6(11)
N(4F)-C(14F)-C(15F)-N(5F)	175.7(12)
C(13F)-C(14F)-C(15F)-N(5F)	-0.8(17)
N(4F)-C(14F)-C(15F)-C(16F)	-3(2)
C(13F)-C(14F)-C(15F)-C(16F)	-179.9(13)
C(22A)-N(6A)-C(16A)-C(15A)	-1.8(18)
C(22A)-N(6A)-C(16A)-C(1A)	177.9(10)
N(5A)-C(15A)-C(16A)-N(6A)	2.5(17)
C(14A)-C(15A)-C(16A)-N(6A)	-178.5(12)
N(5A)-C(15A)-C(16A)-C(1A)	-177.1(11)
C(14A)-C(15A)-C(16A)-C(1A)	2(2)
N(1A)-C(1A)-C(16A)-N(6A)	173.6(12)
C(2A)-C(1A)-C(16A)-N(6A)	-6.2(16)
N(1A)-C(1A)-C(16A)-C(15A)	-7(2)
C(2A)-C(1A)-C(16A)-C(15A)	173.5(12)
C(22B)-N(6B)-C(16B)-C(15B)	-0.4(18)
C(22B)-N(6B)-C(16B)-C(1B)	-178.5(11)
N(5B)-C(15B)-C(16B)-N(6B)	-0.2(17)
C(14B)-C(15B)-C(16B)-N(6B)	178.3(11)
N(5B)-C(15B)-C(16B)-C(1B)	177.4(12)
C(14B)-C(15B)-C(16B)-C(1B)	-4(2)
C(2B)-C(1B)-C(16B)-N(6B)	0.1(17)
N(1B)-C(1B)-C(16B)-N(6B)	179.8(12)
C(2B)-C(1B)-C(16B)-C(15B)	-177.6(13)
N(1B)-C(1B)-C(16B)-C(15B)	2(2)
C(22C)-N(6C)-C(16C)-C(15C)	1.6(18)
C(22C)-N(6C)-C(16C)-C(1C)	-178.1(11)
N(5C)-C(15C)-C(16C)-N(6C)	-3.5(18)
C(14C)-C(15C)-C(16C)-N(6C)	177.4(12)
N(5C)-C(15C)-C(16C)-C(1C)	176.1(12)
C(14C)-C(15C)-C(16C)-C(1C)	-3(2)
N(1C)-C(1C)-C(16C)-N(6C)	175.4(12)
C(2C)-C(1C)-C(16C)-N(6C)	-1.8(16)
N(1C)-C(1C)-C(16C)-C(15C)	-4(2)

Table D.3.4 continued…

C(2C)-C(1C)-C(16C)-C(15C)	178.5(12)
C(22D)-N(42)-C(16D)-C(15D)	-4.2(17)
C(22D)-N(42)-C(16D)-C(1D)	177.3(11)
N(41)-C(15D)-C(16D)-N(42)	6.8(19)
C(14D)-C(15D)-C(16D)-N(42)	-173.2(13)
N(41)-C(15D)-C(16D)-C(1D)	-175.2(13)
C(14D)-C(15D)-C(16D)-C(1D)	5(3)
N(1D)-C(1D)-C(16D)-N(42)	177.8(13)
C(2D)-C(1D)-C(16D)-N(42)	-7.7(18)
N(1D)-C(1D)-C(16D)-C(15D)	0(2)
C(2D)-C(1D)-C(16D)-C(15D)	174.1(13)
C(22E)-N(6E)-C(16E)-C(1E)	178.1(12)
C(22E)-N(6E)-C(16E)-C(15E)	-2.8(19)
N(1E)-C(1E)-C(16E)-N(6E)	-172.3(13)
C(2E)-C(1E)-C(16E)-N(6E)	-0.6(18)
N(1E)-C(1E)-C(16E)-C(15E)	9(2)
C(2E)-C(1E)-C(16E)-C(15E)	-179.6(13)
N(5E)-C(15E)-C(16E)-N(6E)	4.2(18)
C(14E)-C(15E)-C(16E)-N(6E)	-179.1(13)
N(5E)-C(15E)-C(16E)-C(1E)	-176.8(13)
C(14E)-C(15E)-C(16E)-C(1E)	0(2)
C(22F)-N(6F)-C(16F)-C(15F)	0.8(18)
C(22F)-N(6F)-C(16F)-C(1F)	-177.1(11)
N(5F)-C(15F)-C(16F)-N(6F)	-1.2(18)
C(14F)-C(15F)-C(16F)-N(6F)	177.9(12)
N(5F)-C(15F)-C(16F)-C(1F)	176.2(13)
C(14F)-C(15F)-C(16F)-C(1F)	-5(2)
N(1F)-C(1F)-C(16F)-N(6F)	-175.2(13)
C(2F)-C(1F)-C(16F)-N(6F)	5.4(17)
N(1F)-C(1F)-C(16F)-C(15F)	7(2)
C(2F)-C(1F)-C(16F)-C(15F)	-172.2(14)
C(15A)-N(5A)-C(17A)-C(18A)	179.6(11)
C(15A)-N(5A)-C(17A)-C(22A)	-0.6(18)
C(15B)-N(5B)-C(17B)-C(22B)	-1.6(16)
C(15B)-N(5B)-C(17B)-C(18B)	179.5(11)
C(15C)-N(5C)-C(17C)-C(22C)	4.9(19)
C(15C)-N(5C)-C(17C)-C(18C)	-179.9(12)

Table D.3.4 continued…

C(15D)-N(41)-C(17D)-C(22D)	-6(2)
C(15D)-N(41)-C(17D)-C(18D)	-179.2(13)
C(15E)-N(5E)-C(17E)-C(18E)	178.7(14)
C(15E)-N(5E)-C(17E)-C(22E)	2.3(19)
C(15F)-N(5F)-C(17F)-C(18F)	-179.4(12)
C(15F)-N(5F)-C(17F)-C(22F)	0.2(19)
N(5A)-C(17A)-C(18A)-C(19A)	-179.9(11)
C(22A)-C(17A)-C(18A)-C(19A)	0.3(18)
N(5B)-C(17B)-C(18B)-C(19B)	-179.1(11)
C(22B)-C(17B)-C(18B)-C(19B)	2.0(18)
N(5C)-C(17C)-C(18C)-C(19C)	-176.0(13)
C(22C)-C(17C)-C(18C)-C(19C)	-1(2)
C(22D)-C(17D)-C(18D)-C(19D)	4(2)
N(41)-C(17D)-C(18D)-C(19D)	177.4(14)
N(5E)-C(17E)-C(18E)-C(19E)	-179.6(13)
C(22E)-C(17E)-C(18E)-C(19E)	-3(2)
N(5F)-C(17F)-C(18F)-C(19F)	-178.5(13)
C(22F)-C(17F)-C(18F)-C(19F)	2(2)
C(17A)-C(18A)-C(19A)-C(20A)	-2.1(17)
C(17B)-C(18B)-C(19B)-C(20B)	-1.9(18)
C(17C)-C(18C)-C(19C)-C(20C)	0(2)
C(17D)-C(18D)-C(19D)-C(20D)	-2(2)
C(17E)-C(18E)-C(19E)-C(20E)	2(2)
C(17F)-C(18F)-C(19F)-C(20F)	0(2)
C(18A)-C(19A)-C(20A)-C(21A)	2.6(17)
C(18B)-C(19B)-C(20B)-C(21B)	1.3(19)
C(18C)-C(19C)-C(20C)-C(21C)	0(2)
C(18D)-C(19D)-C(20D)-C(21D)	-1(3)
C(18E)-C(19E)-C(20E)-C(21E)	0(2)
C(18F)-C(19F)-C(20F)-C(21F)	-1(2)
C(19A)-C(20A)-C(21A)-C(22A)	-1.2(19)
C(19B)-C(20B)-C(21B)-C(22B)	-0.7(18)
C(19C)-C(20C)-C(21C)-C(22C)	0(2)
C(19D)-C(20D)-C(21D)-C(22D)	2(3)
C(19E)-C(20E)-C(21E)-C(22E)	-1(2)
C(19F)-C(20F)-C(21F)-C(22F)	1(2)
C(16A)-N(6A)-C(22A)-C(17A)	-0.2(17)

Table D.3.4 continued…

C(16A)-N(6A)-C(22A)-C(21A)	179.9(12)
N(5A)-C(17A)-C(22A)-N(6A)	1.4(18)
C(18A)-C(17A)-C(22A)-N(6A)	-178.8(11)
N(5A)-C(17A)-C(22A)-C(21A)	-178.7(11)
C(18A)-C(17A)-C(22A)-C(21A)	1.2(18)
C(20A)-C(21A)-C(22A)-N(6A)	179.2(11)
C(20A)-C(21A)-C(22A)-C(17A)	-0.7(18)
C(16B)-N(6B)-C(22B)-C(17B)	0.0(18)
C(16B)-N(6B)-C(22B)-C(21B)	-178.7(11)
N(5B)-C(17B)-C(22B)-N(6B)	1.0(17)
C(18B)-C(17B)-C(22B)-N(6B)	179.9(11)
N(5B)-C(17B)-C(22B)-C(21B)	179.7(10)
C(18B)-C(17B)-C(22B)-C(21B)	-1.4(17)
C(20B)-C(21B)-C(22B)-N(6B)	179.4(11)
C(20B)-C(21B)-C(22B)-C(17B)	0.7(17)
C(16C)-N(6C)-C(22C)-C(17C)	4(2)
C(16C)-N(6C)-C(22C)-C(21C)	-179.3(12)
N(5C)-C(17C)-C(22C)-N(6C)	-7(2)
C(18C)-C(17C)-C(22C)-N(6C)	177.6(13)
N(5C)-C(17C)-C(22C)-C(21C)	176.0(13)
C(18C)-C(17C)-C(22C)-C(21C)	1(2)
C(20C)-C(21C)-C(22C)-N(6C)	-177.3(13)
C(20C)-C(21C)-C(22C)-C(17C)	0(2)
N(41)-C(17D)-C(22D)-N(42)	9(2)
C(18D)-C(17D)-C(22D)-N(42)	-178.2(14)
N(41)-C(17D)-C(22D)-C(21D)	-176.5(14)
C(18D)-C(17D)-C(22D)-C(21D)	-4(2)
C(16D)-N(42)-C(22D)-C(17D)	-3(2)
C(16D)-N(42)-C(22D)-C(21D)	-178.2(12)
C(20D)-C(21D)-C(22D)-C(17D)	1(2)
C(20D)-C(21D)-C(22D)-N(42)	175.6(14)
C(16E)-N(6E)-C(22E)-C(21E)	-178.5(13)
C(16E)-N(6E)-C(22E)-C(17E)	1(2)
C(20E)-C(21E)-C(22E)-N(6E)	179.8(14)
C(20E)-C(21E)-C(22E)-C(17E)	0(2)
N(5E)-C(17E)-C(22E)-N(6E)	-1(2)
C(18E)-C(17E)-C(22E)-N(6E)	-177.5(13)

Table D.3.4 continued…

N(5E)-C(17E)-C(22E)-C(21E)	179.0(13)
C(18E)-C(17E)-C(22E)-C(21E)	2(2)
C(16F)-N(6F)-C(22F)-C(21F)	-178.9(12)
C(16F)-N(6F)-C(22F)-C(17F)	0.1(19)
C(20F)-C(21F)-C(22F)-N(6F)	179.5(12)
C(20F)-C(21F)-C(22F)-C(17F)	0.5(19)
N(5F)-C(17F)-C(22F)-N(6F)	-0.7(19)
C(18F)-C(17F)-C(22F)-N(6F)	178.9(12)
N(5F)-C(17F)-C(22F)-C(21F)	178.4(12)
C(18F)-C(17F)-C(22F)-C(21F)	-2.0(19)

D.4: Full crystallographic Data Tables of [Au(L10)](AuCl$_4$)

Table D.4.1: Bond lengths [Å] and angles [°] for [Au(L10)](AuCl$_4$).

C(10)-C(11)	1.354(12)
C(10)-C(9)	1.434(10)
C(10)-H(10)	0.9500
C(11)-C(11)#1	1.409(16)
C(11)-H(11)	0.9500
Au(1)-N(1)#1	1.988(6)
Au(1)-N(1)	1.988(6)
Au(1)-N(2)#1	2.059(6)
Au(1)-N(2)	2.059(6)
N(3)-C(8)	1.335(9)
N(3)-C(9)	1.346(10)
N(2)-C(3)	1.297(10)
N(2)-C(2)	1.471(9)
C-C(2)	1.515(11)
C-H(0A)	0.9800
C-H(0B)	0.9800
C-H(0C)	0.9800
C(3)-C(4)	1.400(11)
N(1)-C(4)	1.370(9)
N(1)-C(7)	1.371(10)
C(6)-C(5)	1.386(11)
C(6)-C(7)	1.410(11)
C(6)-H(6)	0.9500
C(8)-C(8)#1	1.435(14)
C(8)-C(7)	1.468(10)
C(4)-C(5)	1.392(10)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(5)-H(5)	0.9500
C(9)-C(9)#1	1.417(16)
Au(2)-Cl(1)#1	2.272(2)
Au(2)-Cl(1)	2.271(2)
Au(2)-Cl(2)	2.287(2)
Au(2)-Cl(2)#1	2.287(2)

Table D.4.1 continued…

C(11)-C(10)-C(9)	118.1(8)
C(11)-C(10)-H(10)	120.9
C(9)-C(10)-H(10)	120.9
C(10)-C(11)-C(11)#1	122.0(5)
C(10)-C(11)-H(11)	119.0
C(11)#1-C(11)-H(11)	119.0
N(1)#1-Au(1)-N(1)	95.8(3)
N(1)#1-Au(1)-N(2)#1	81.5(2)
N(1)-Au(1)-N(2)#1	176.7(2)
N(1)#1-Au(1)-N(2)	176.7(2)
N(1)-Au(1)-N(2)	81.5(3)
N(2)#1-Au(1)-N(2)	101.2(3)
C(8)-N(3)-C(9)	119.6(7)
C(3)-N(2)-C(2)	121.3(6)
C(3)-N(2)-Au(1)	110.9(5)
C(2)-N(2)-Au(1)	127.7(5)
C(2)-C-H(0A)	109.5
C(2)-C-H(0B)	109.5
H(0A)-C-H(0B)	109.5
C(2)-C-H(0C)	109.5
H(0A)-C-H(0C)	109.5
H(0B)-C-H(0C)	109.5
N(2)-C(3)-C(4)	119.2(7)
C(4)-N(1)-C(7)	107.6(6)
C(4)-N(1)-Au(1)	111.9(5)
C(7)-N(1)-Au(1)	140.3(5)
C(5)-C(6)-C(7)	108.8(7)
C(5)-C(6)-H(6)	125.6
C(7)-C(6)-H(6)	125.6
N(3)-C(8)-C(8)#1	120.0(4)
N(3)-C(8)-C(7)	109.5(6)
C(8)#1-C(8)-C(7)	130.5(4)
N(1)-C(7)-C(6)	107.6(6)
N(1)-C(7)-C(8)	130.6(7)
C(6)-C(7)-C(8)	121.8(7)
N(1)-C(4)-C(5)	110.6(7)
N(1)-C(4)-C(3)	116.4(7)

Table D.4.1

C(5)-C(4)-C(3)	133.1(7)
N(2)-C(2)-C	114.1(7)
N(2)-C(2)-H(2A)	108.7
C-C(2)-H(2A)	108.7
N(2)-C(2)-H(2B)	108.7
C-C(2)-H(2B)	108.7
H(2A)-C(2)-H(2B)	107.6
C(6)-C(5)-C(4)	105.5(7)
C(6)-C(5)-H(5)	127.3
C(4)-C(5)-H(5)	127.3
N(3)-C(9)-C(9)#1	120.2(4)
N(3)-C(9)-C(10)	119.9(7)
C(9)#1-C(9)-C(10)	119.8(5)
Cl(1)#1-Au(2)-Cl(1)	88.62(11)
Cl(1)#1-Au(2)-Cl(2)	175.84(8)
Cl(1)-Au(2)-Cl(2)	90.10(8)
Cl(1)#1-Au(2)-Cl(2)#1	90.10(8)
Cl(1)-Au(2)-Cl(2)#1	175.84(8)
Cl(2)-Au(2)-Cl(2)#1	91.45(12)

Table D.4.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for [Au(L10)]($AuCl_4$). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(10)	20(4)	19(4)	17(4)	0(3)	-2(3)	-5(3)
C(11)	21(4)	8(3)	25(4)	2(3)	6(3)	-7(3)
Au(1)	11(1)	6(1)	13(1)	0	3(1)	0
N(3)	12(3)	12(3)	12(3)	1(2)	1(2)	-1(2)
N(2)	15(3)	11(3)	19(3)	0(2)	6(2)	1(2)
C	22(4)	16(4)	19(4)	-1(3)	3(3)	4(3)
C(3)	16(3)	14(4)	19(4)	0(3)	4(3)	2(3)
N(1)	13(3)	12(3)	17(3)	-1(2)	5(2)	4(2)
C(6)	21(4)	14(4)	26(4)	0(3)	7(3)	-1(3)
C(8)	14(3)	3(3)	20(4)	-3(2)	3(3)	-2(2)
C(7)	15(3)	12(4)	21(4)	-2(3)	4(3)	-2(3)
C(4)	13(3)	16(4)	18(4)	-1(3)	7(3)	2(3)
C(2)	20(4)	10(3)	14(4)	-2(3)	2(3)	1(3)
C(5)	23(4)	13(4)	33(5)	3(3)	17(3)	-2(3)
C(9)	21(4)	8(3)	12(3)	0(2)	-2(3)	-3(3)
Au(2)	13(1)	9(1)	18(1)	0	5(1)	0
Cl(1)	36(1)	16(1)	21(1)	4(1)	-1(1)	0(1)
Cl(2)	30(1)	18(1)	32(1)	-10(1)	14(1)	-5(1)

Table D.4.3: Hydrogen coordinates ($x\ 10^4$) and isotropic displacement parameters ($Å^2 x\ 10^3$) for [Au(L10)]($AuCl_4$).

	x	**y**	**z**	**U(eq)**
H(10)	1784	6493	932	24
H(11)	873	7124	1726	22
H(0A)	2501	3069	204	29
H(0B)	2661	2701	1577	29
H(0C)	3637	3127	1948	29
H(6)	2987	5330	725	24
H(2A)	555	3111	1496	18
H(2B)	1675	3156	3254	18
H(5)	4134	4615	403	26

Table D.4.4: Torsion angles [°] for [Au(L10)]($AuCl_4$).

C(9)-C(10)-C(11)-C(11)#1	0.1(14)
N(1)-Au(1)-N(2)-C(3)	-1.6(5)
N(2)#1-Au(1)-N(2)-C(3)	176.5(6)
N(1)-Au(1)-N(2)-C(2)	175.2(6)
N(2)#1-Au(1)-N(2)-C(2)	-6.7(5)
C(2)-N(2)-C(3)-C(4)	-176.3(7)
Au(1)-N(2)-C(3)-C(4)	0.7(9)
N(1)#1-Au(1)-N(1)-C(4)	-179.8(6)
N(2)-Au(1)-N(1)-C(4)	2.2(5)
N(1)#1-Au(1)-N(1)-C(7)	-6.2(7)
N(2)-Au(1)-N(1)-C(7)	175.7(9)
C(9)-N(3)-C(8)-C(8)#1	5.5(12)
C(9)-N(3)-C(8)-C(7)	-172.3(6)
C(4)-N(1)-C(7)-C(6)	-0.1(9)
Au(1)-N(1)-C(7)-C(6)	-173.9(6)
C(4)-N(1)-C(7)-C(8)	-178.1(8)
Au(1)-N(1)-C(7)-C(8)	8.1(14)
C(5)-C(6)-C(7)-N(1)	-0.8(10)
C(5)-C(6)-C(7)-C(8)	177.4(7)
N(3)-C(8)-C(7)-N(1)	-177.4(8)
C(8)#1-C(8)-C(7)-N(1)	5.1(16)
N(3)-C(8)-C(7)-C(6)	4.8(10)
C(8)#1-C(8)-C(7)-C(6)	-172.6(10)
C(7)-N(1)-C(4)-C(5)	1.0(9)
Au(1)-N(1)-C(4)-C(5)	176.7(6)
C(7)-N(1)-C(4)-C(3)	-178.2(7)
Au(1)-N(1)-C(4)-C(3)	-2.5(8)
N(2)-C(3)-C(4)-N(1)	1.2(11)
N(2)-C(3)-C(4)-C(5)	-177.8(9)
C(3)-N(2)-C(2)-C	-7.7(10)
Au(1)-N(2)-C(2)-C	175.8(5)
C(7)-C(6)-C(5)-C(4)	1.4(10)
N(1)-C(4)-C(5)-C(6)	-1.5(10)
C(3)-C(4)-C(5)-C(6)	177.5(8)
C(8)-N(3)-C(9)-C(9)#1	-0.7(12)
C(8)-N(3)-C(9)-C(10)	178.4(7)

Table D.4.4 continued

C(11)-C(10)-C(9)-N(3)	-179.1(7)
C(11)-C(10)-C(9)-C(9)#1	0.0(13)

D.5: Full crystallographic Data Tables of [Au(L12)](PF_6)

Table D.5.1: Bond lengths [Å] and angles [°] for [Au(L12)](PF_6)

Au(01)-N(4)	1.979(6)
Au(01)-N(1)	2.008(4)
Au(01)-N(3)	2.041(4)
Au(01)-N(2)	2.044(5)
P-F(3)	1.556(5)
P-F(2)	1.587(4)
P-F(5)	1.593(4)
P-F(6)	1.595(5)
P-F(4)	1.599(5)
P-F(1)	1.607(4)
N(3)-C(10)	1.325(7)
N(3)-C(9)	1.462(7)
N(4)-C(14)	1.362(8)
N(4)-C(11)	1.387(7)
N(1)-C(1)	1.340(7)
N(1)-C(4)	1.384(7)
C(3)-C(4)	1.390(8)
C(3)-C(2)	1.427(8)
C(3)-H(3)	0.9500
C(10)-C(11)	1.398(9)
C(10)-H(10)	0.9500
C(2)-C(1)	1.403(8)
C(2)-H(2)	0.9500
C(12)-C(13)	1.398(9)
C(12)-C(11)	1.404(8)
C(12)-H(12)	0.9500
C(14)-C(13)	1.396(8)
C(14)-H(14)	0.9500
C(8)-C(9)	1.518(8)
C(8)-C(7)	1.534(8)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(7)-C(6)	1.523(8)
C(7)-H(7A)	0.9900

Table D.5.1 continued…

C(7)-H(7B)	0.9900
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(6)-N(2)	1.481(7)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
N(2)-C(5)	1.299(7)
C(1)-H(1)	0.9500
C(4)-C(5)	1.414(8)
C(13)-H(13)	0.9500
C(5)-H(5)	0.9500
N(4)-Au(01)-N(1)	99.84(19)
N(4)-Au(01)-N(3)	80.68(19)
N(1)-Au(01)-N(3)	175.92(18)
N(4)-Au(01)-N(2)	178.14(18)
N(1)-Au(01)-N(2)	80.84(19)
N(3)-Au(01)-N(2)	98.77(18)
F(3)-P-F(2)	91.6(4)
F(3)-P-F(5)	90.6(4)
F(2)-P-F(5)	177.6(3)
F(3)-P-F(6)	178.2(4)
F(2)-P-F(6)	89.8(3)
F(5)-P-F(6)	88.0(3)
F(3)-P-F(4)	91.1(4)
F(2)-P-F(4)	91.4(3)
F(5)-P-F(4)	89.7(2)
F(6)-P-F(4)	90.0(3)
F(3)-P-F(1)	89.8(3)
F(2)-P-F(1)	88.9(2)
F(5)-P-F(1)	90.1(2)
F(6)-P-F(1)	89.0(3)
F(4)-P-F(1)	179.0(3)
C(10)-N(3)-C(9)	120.7(5)
C(10)-N(3)-Au(01)	112.6(4)
C(9)-N(3)-Au(01)	125.9(4)
C(14)-N(4)-C(11)	106.8(5)

Table D.5.1 continued…

C(14)-N(4)-Au(01)	139.1(4)
C(11)-N(4)-Au(01)	113.9(4)
C(1)-N(1)-C(4)	108.0(5)
C(1)-N(1)-Au(01)	139.9(4)
C(4)-N(1)-Au(01)	112.0(4)
C(4)-C(3)-C(2)	107.3(5)
C(4)-C(3)-H(3)	126.3
C(2)-C(3)-H(3)	126.3
N(3)-C(10)-C(11)	118.0(5)
N(3)-C(10)-H(10)	121.0
C(11)-C(10)-H(10)	121.0
C(1)-C(2)-C(3)	104.9(5)
C(1)-C(2)-H(2)	127.5
C(3)-C(2)-H(2)	127.5
C(13)-C(12)-C(11)	106.0(5)
C(13)-C(12)-H(12)	127.0
C(11)-C(12)-H(12)	127.0
N(4)-C(14)-C(13)	109.9(6)
N(4)-C(14)-H(14)	125.1
C(13)-C(14)-H(14)	125.1
C(9)-C(8)-C(7)	114.2(5)
C(9)-C(8)-H(8A)	108.7
C(7)-C(8)-H(8A)	108.7
C(9)-C(8)-H(8B)	108.7
C(7)-C(8)-H(8B)	108.7
H(8A)-C(8)-H(8B)	107.6
C(6)-C(7)-C(8)	114.8(5)
C(6)-C(7)-H(7A)	108.6
C(8)-C(7)-H(7A)	108.6
C(6)-C(7)-H(7B)	108.6
C(8)-C(7)-H(7B)	108.6
H(7A)-C(7)-H(7B)	107.5
N(3)-C(9)-C(8)	113.4(5)
N(3)-C(9)-H(9A)	108.9
C(8)-C(9)-H(9A)	108.9
N(3)-C(9)-H(9B)	108.9
C(8)-C(9)-H(9B)	108.9

Table D.5.1 continued…

H(9A)-C(9)-H(9B)	107.7
N(2)-C(6)-C(7)	111.4(5)
N(2)-C(6)-H(6A)	109.3
C(7)-C(6)-H(6A)	109.3
N(2)-C(6)-H(6B)	109.3
C(7)-C(6)-H(6B)	109.3
H(6A)-C(6)-H(6B)	108.0
C(5)-N(2)-C(6)	119.7(5)
C(5)-N(2)-Au(01)	113.3(4)
C(6)-N(2)-Au(01)	126.7(3)
N(1)-C(1)-C(2)	111.0(5)
N(1)-C(1)-H(1)	124.5
C(2)-C(1)-H(1)	124.5
N(4)-C(11)-C(10)	114.8(5)
N(4)-C(11)-C(12)	109.7(5)
C(10)-C(11)-C(12)	135.5(5)
N(1)-C(4)-C(3)	108.8(5)
N(1)-C(4)-C(5)	116.1(5)
C(3)-C(4)-C(5)	135.1(6)
C(14)-C(13)-C(12)	107.6(6)
C(14)-C(13)-H(13)	126.2
C(12)-C(13)-H(13)	126.2
N(2)-C(5)-C(4)	117.7(5)
N(2)-C(5)-H(5)	121.2
C(4)-C(5)-H(5)	121.2

Table D.5.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for [Au(L12)](PF_6). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Au(01)	20(1)	21(1)	15(1)	1(1)	3(1)	-2(1)
P	29(1)	23(1)	26(1)	-4(1)	9(1)	-1(1)
N(3)	21(2)	27(2)	14(2)	2(2)	4(2)	-4(2)
N(4)	23(2)	33(3)	17(2)	0(2)	1(2)	7(2)
N(1)	23(2)	28(2)	12(2)	1(2)	4(2)	-3(2)
F(1)	39(2)	36(2)	47(2)	-20(2)	12(2)	-7(2)
F(3)	149(6)	55(3)	41(3)	23(2)	19(4)	23(4)
F(4)	57(3)	51(3)	82(4)	-41(3)	39(3)	-28(2)
C(3)	26(3)	32(3)	20(3)	4(2)	3(2)	1(2)
C(10)	26(2)	31(3)	19(2)	8(2)	3(2)	-5(2)
F(5)	40(2)	52(3)	59(3)	-27(2)	24(2)	-10(2)
F(2)	41(2)	62(3)	98(4)	-43(3)	35(3)	-16(2)
F(6)	99(4)	73(4)	40(3)	10(3)	-10(3)	14(3)
C(2)	23(2)	23(3)	28(3)	8(2)	9(2)	6(2)
C(12)	32(3)	29(3)	32(3)	8(3)	1(2)	-6(2)
C(14)	27(3)	23(3)	36(3)	0(2)	5(2)	-2(2)
C(8)	35(3)	37(3)	17(3)	-4(2)	7(2)	-6(3)
C(7)	31(3)	32(3)	19(3)	-3(2)	2(2)	-5(2)
C(9)	25(3)	36(3)	20(3)	-3(2)	6(2)	-3(2)
C(6)	28(3)	24(3)	25(3)	-4(2)	7(2)	-2(2)
N(2)	27(2)	17(2)	15(2)	-2(2)	2(2)	-5(2)
C(1)	24(2)	27(3)	18(2)	-5(2)	4(2)	0(2)
C(11)	28(3)	27(3)	21(3)	6(2)	2(2)	-5(2)
C(4)	26(2)	25(3)	16(2)	2(2)	3(2)	-1(2)
C(13)	42(3)	22(3)	32(3)	1(2)	2(3)	-6(3)
C(5)	27(3)	21(2)	21(2)	4(2)	4(2)	0(2)

Table D.3.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [Au(L12)](PF_6).

	x	y	z	U(eq)
H(3)	5272	2646	6297	31
H(10)	10581	6054	3170	30
H(2)	5338	4852	6775	29
H(12)	10167	8611	3675	37
H(14)	7435	7513	5197	34
H(8A)	9345	2355	2577	35
H(8B)	8394	3615	2409	35
H(7A)	6594	3225	3187	33
H(7B)	6805	1922	2826	33
H(9A)	10547	3131	3664	32
H(9B)	10953	4003	3032	32
H(6A)	7151	1231	3912	30
H(6B)	8971	1727	3922	30
H(1)	6531	6140	5866	28
H(13)	8664	9349	4677	39
H(5)	6513	1640	5016	27

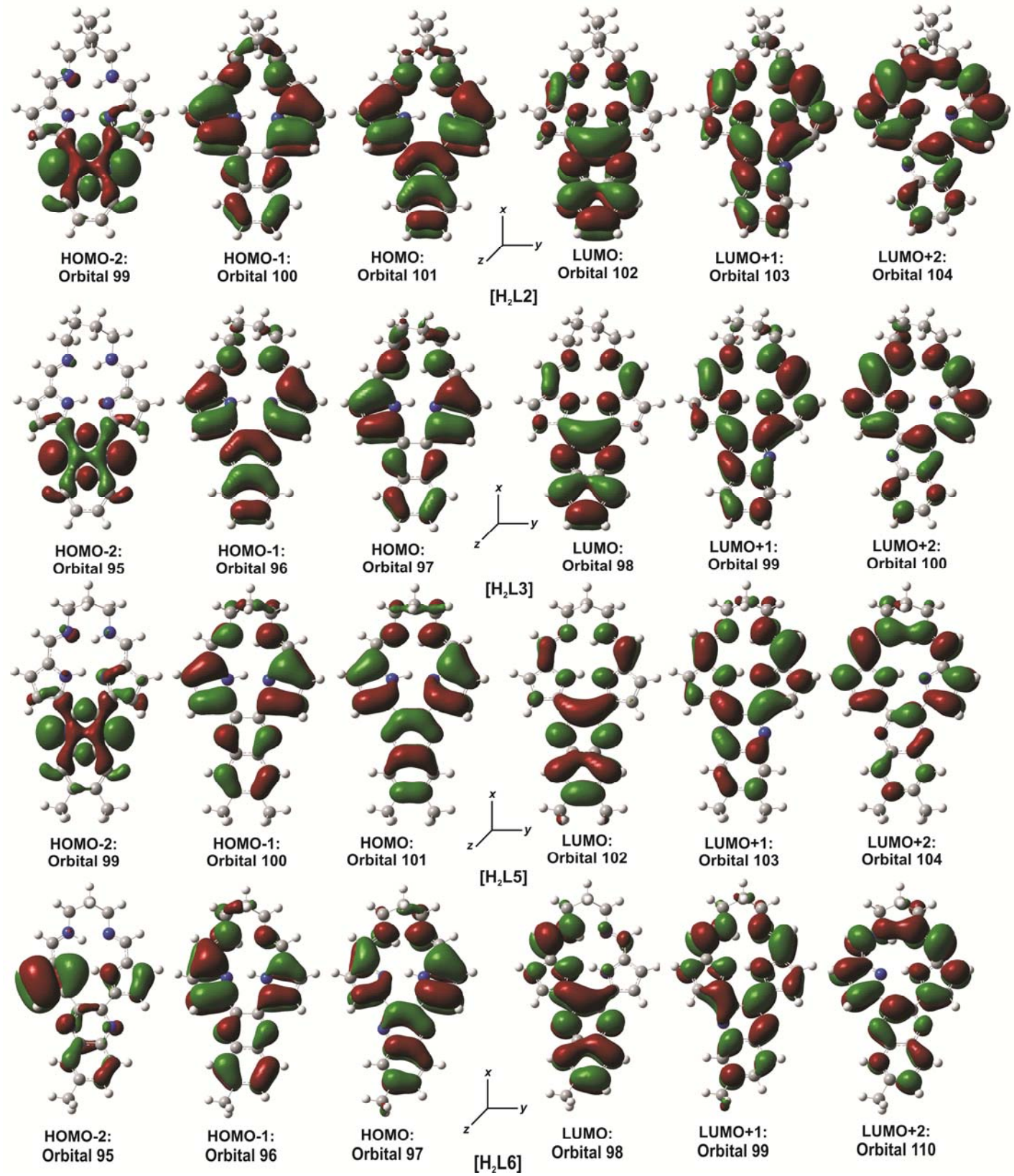
Table D.5.4: Torsion angles [°] for [Au(L12)](PF_6).

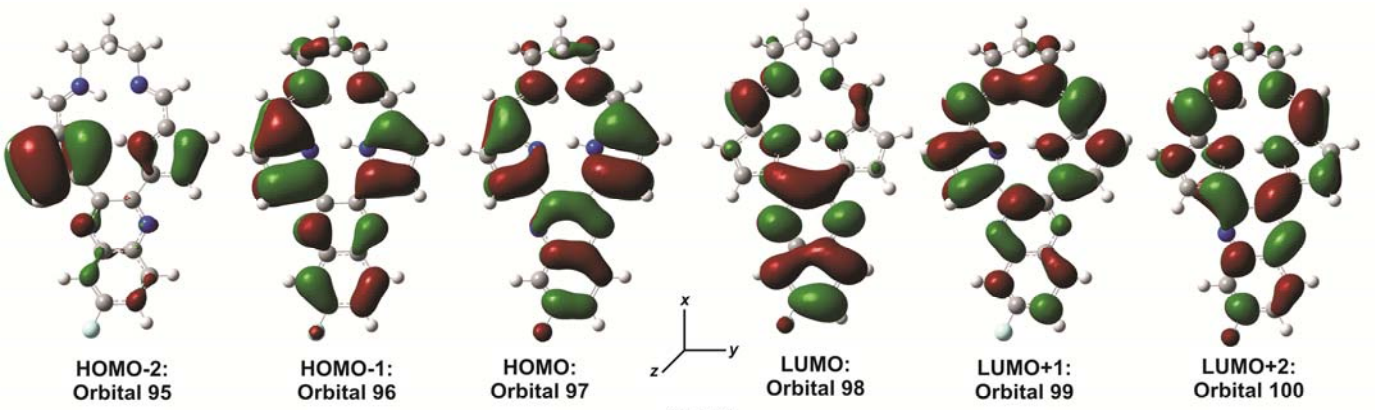
N(4)-Au(01)-N(3)-C(10)	0.6(4)
N(2)-Au(01)-N(3)-C(10)	178.8(4)
N(4)-Au(01)-N(3)-C(9)	169.7(5)
N(2)-Au(01)-N(3)-C(9)	-12.1(5)
N(1)-Au(01)-N(4)-C(14)	-7.2(7)
N(3)-Au(01)-N(4)-C(14)	176.9(6)
N(1)-Au(01)-N(4)-C(11)	177.1(4)
N(3)-Au(01)-N(4)-C(11)	1.2(4)
N(4)-Au(01)-N(1)-C(1)	-4.6(6)
N(2)-Au(01)-N(1)-C(1)	177.1(6)
N(4)-Au(01)-N(1)-C(4)	-178.6(4)
N(2)-Au(01)-N(1)-C(4)	3.2(4)
C(9)-N(3)-C(10)-C(11)	-172.1(5)
Au(01)-N(3)-C(10)-C(11)	-2.3(6)
C(4)-C(3)-C(2)-C(1)	2.0(6)
C(11)-N(4)-C(14)-C(13)	-1.2(7)
Au(01)-N(4)-C(14)-C(13)	-177.1(5)
C(9)-C(8)-C(7)-C(6)	-40.9(8)
C(10)-N(3)-C(9)-C(8)	-115.1(6)
Au(01)-N(3)-C(9)-C(8)	76.5(6)
C(7)-C(8)-C(9)-N(3)	-58.8(7)
C(8)-C(7)-C(6)-N(2)	98.9(6)
C(7)-C(6)-N(2)-C(5)	133.4(5)
C(7)-C(6)-N(2)-Au(01)	-40.3(6)
N(1)-Au(01)-N(2)-C(5)	-2.4(4)
N(3)-Au(01)-N(2)-C(5)	173.5(4)
N(1)-Au(01)-N(2)-C(6)	171.6(5)
N(3)-Au(01)-N(2)-C(6)	-12.5(5)
C(4)-N(1)-C(1)-C(2)	1.8(7)
Au(01)-N(1)-C(1)-C(2)	-172.3(5)
C(3)-C(2)-C(1)-N(1)	-2.4(7)
C(14)-N(4)-C(11)-C(10)	-179.9(5)
Au(01)-N(4)-C(11)-C(10)	-2.8(6)
C(14)-N(4)-C(11)-C(12)	1.2(7)
Au(01)-N(4)-C(11)-C(12)	178.3(4)
N(3)-C(10)-C(11)-N(4)	3.4(8)

Table D.5.4 continued…

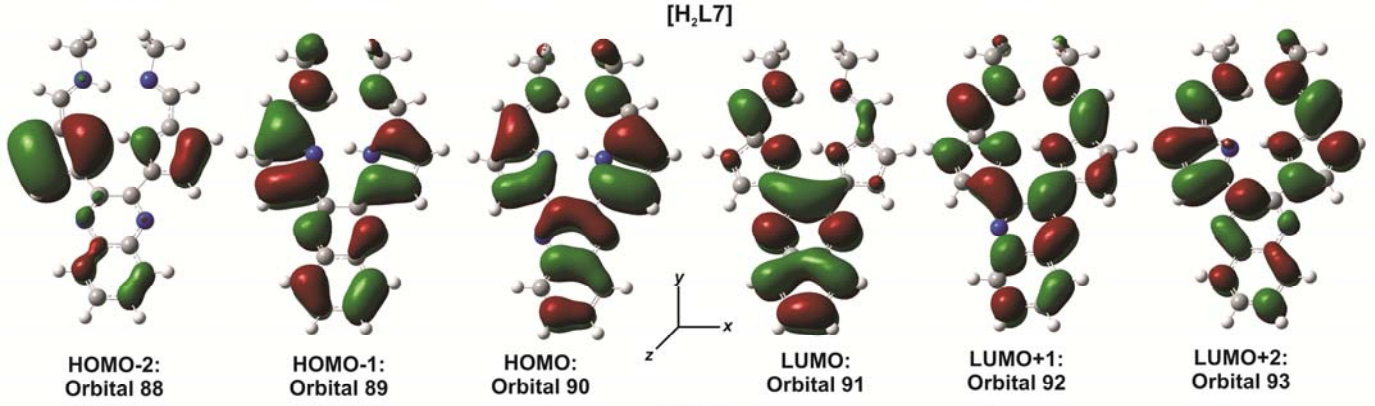
N(3)-C(10)-C(11)-C(12)	-178.0(6)
C(13)-C(12)-C(11)-N(4)	-0.7(7)
C(13)-C(12)-C(11)-C(10)	-179.3(7)
C(1)-N(1)-C(4)-C(3)	-0.4(6)
Au(01)-N(1)-C(4)-C(3)	175.5(4)
C(1)-N(1)-C(4)-C(5)	-179.5(5)
Au(01)-N(1)-C(4)-C(5)	-3.6(6)
C(2)-C(3)-C(4)-N(1)	-1.0(7)
C(2)-C(3)-C(4)-C(5)	177.8(6)
N(4)-C(14)-C(13)-C(12)	0.8(8)
C(11)-C(12)-C(13)-C(14)	0.0(7)
C(6)-N(2)-C(5)-C(4)	-173.4(5)
Au(01)-N(2)-C(5)-C(4)	1.1(7)
N(1)-C(4)-C(5)-N(2)	1.7(8)
C(3)-C(4)-C(5)-N(2)	-177.1(6)

F.1: Molecular Orbital Diagrams of Ligands

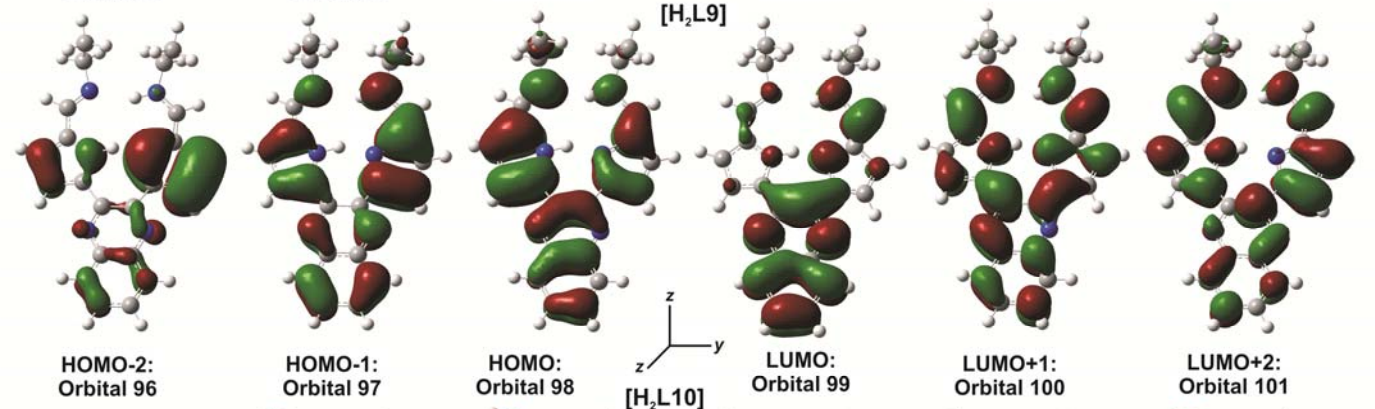




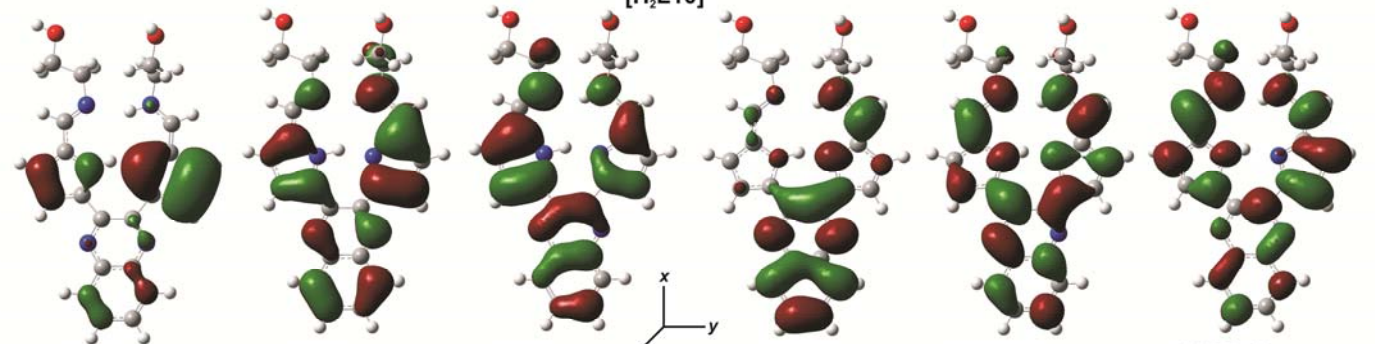
$[H_2L7]$



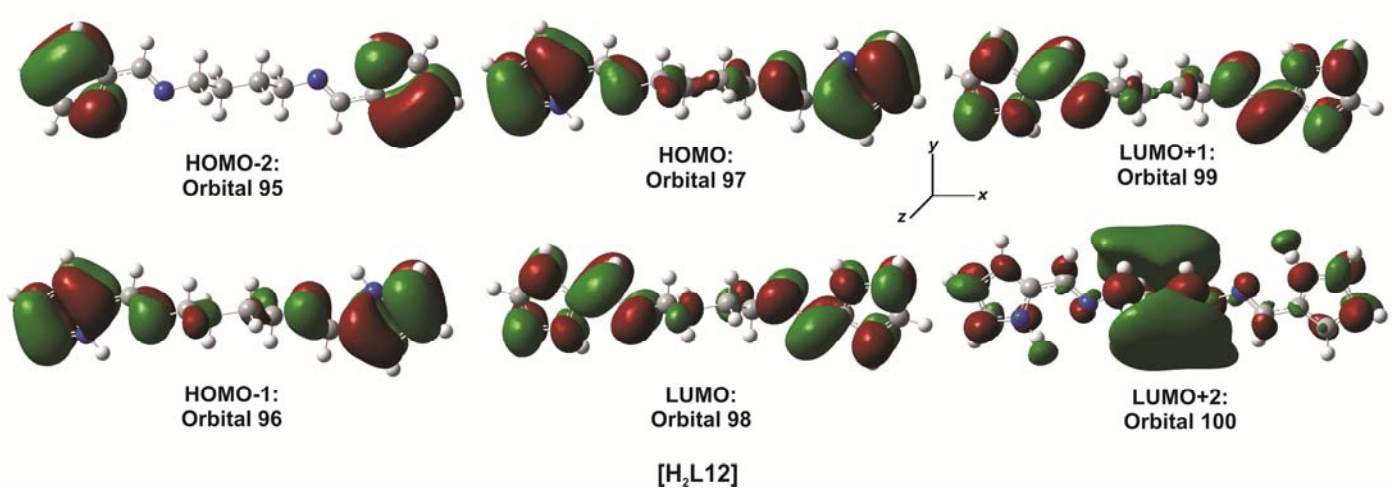
$[H_2L9]$



$[H_2L10]$

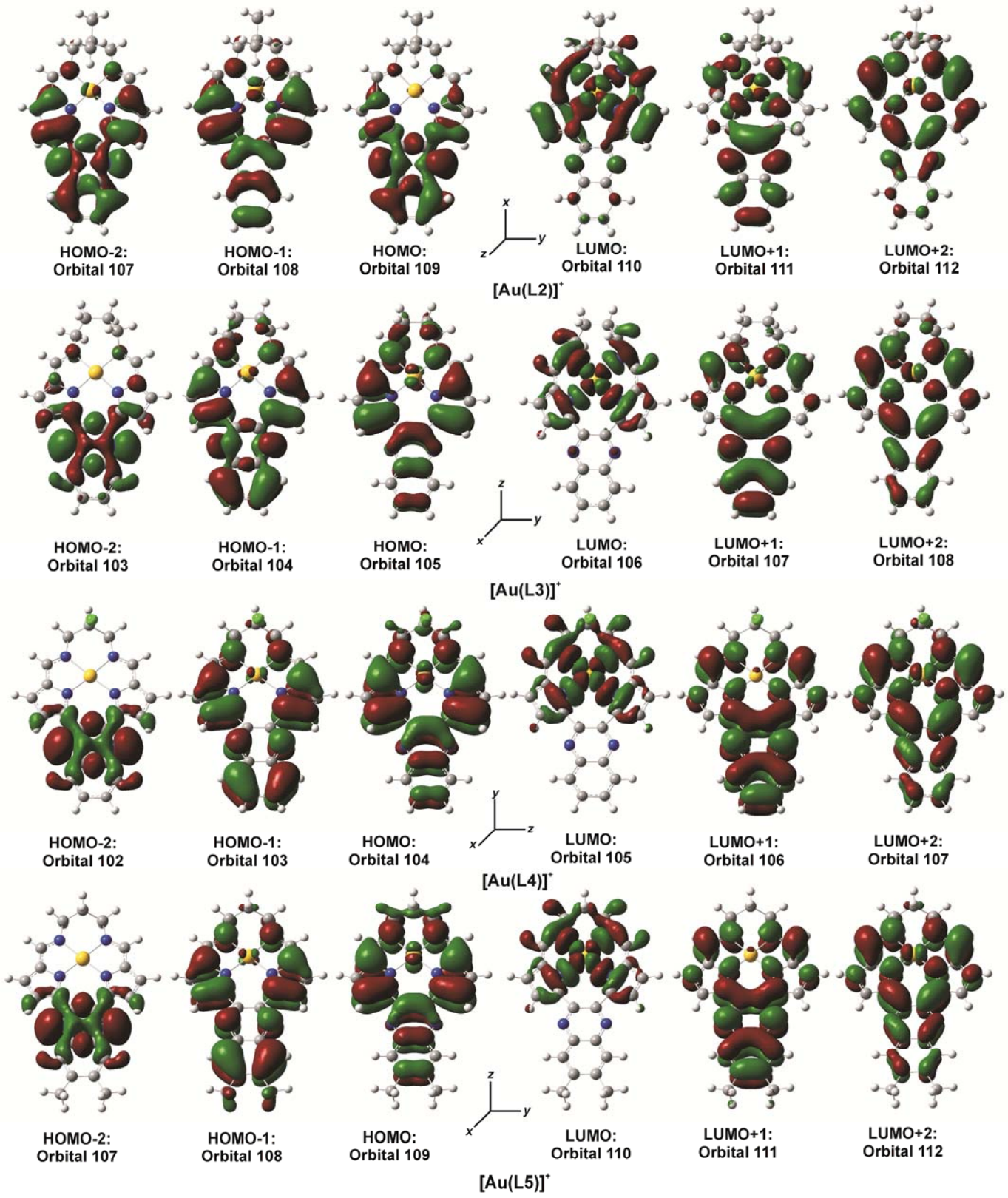


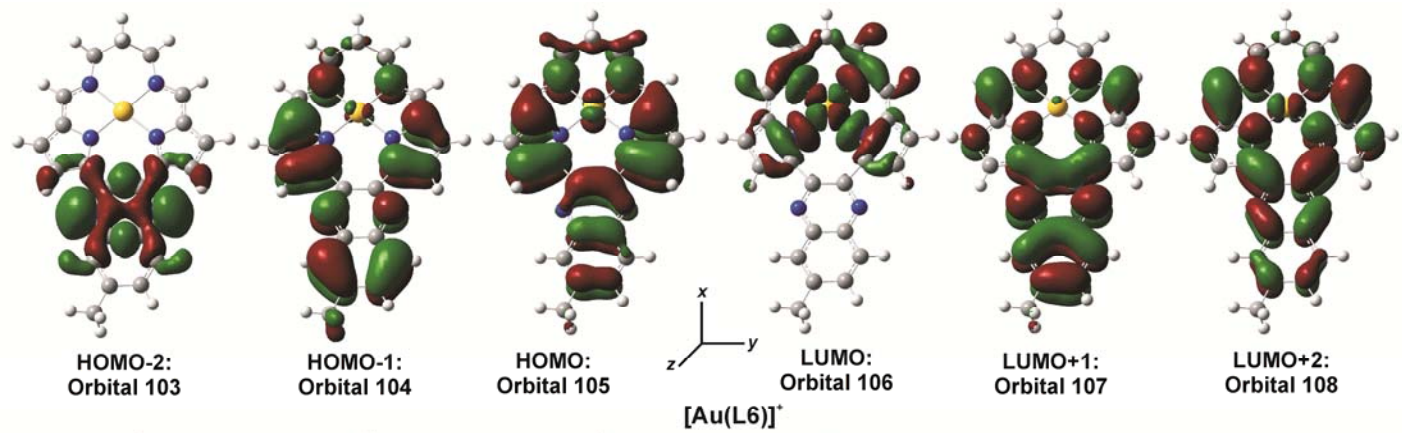
$[H_2L11]$


HOMO-2:
Orbital 95
HOMO:
Orbital 97
y
x
z
LUMO+1:
Orbital 99
HOMO-1:
Orbital 96
LUMO:
Orbital 98
LUMO+2:
Orbital 100

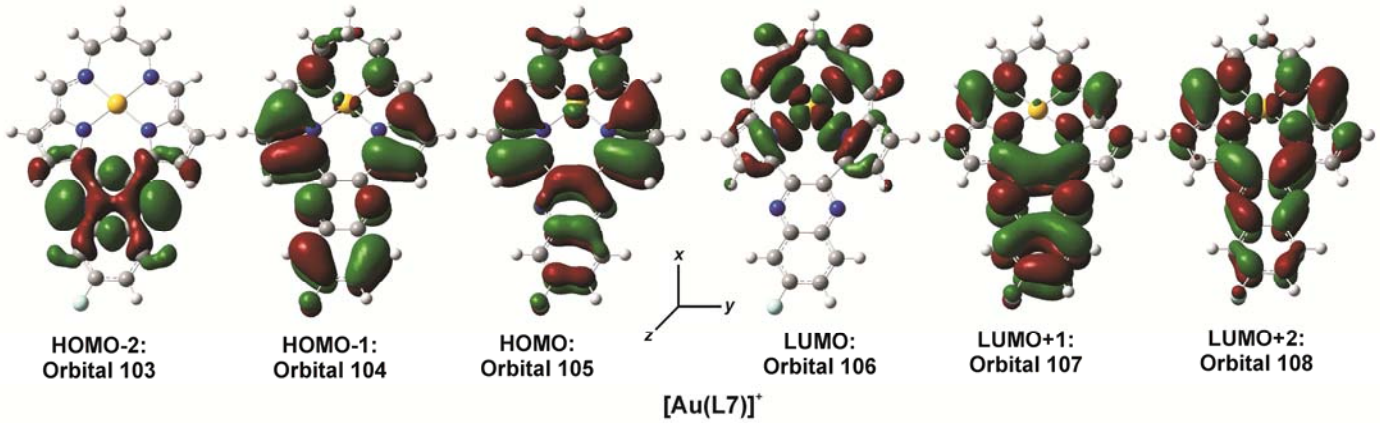
$[H_2L12]$

F.2: Molecular Orbital Diagrams of Gold(III) Complexes

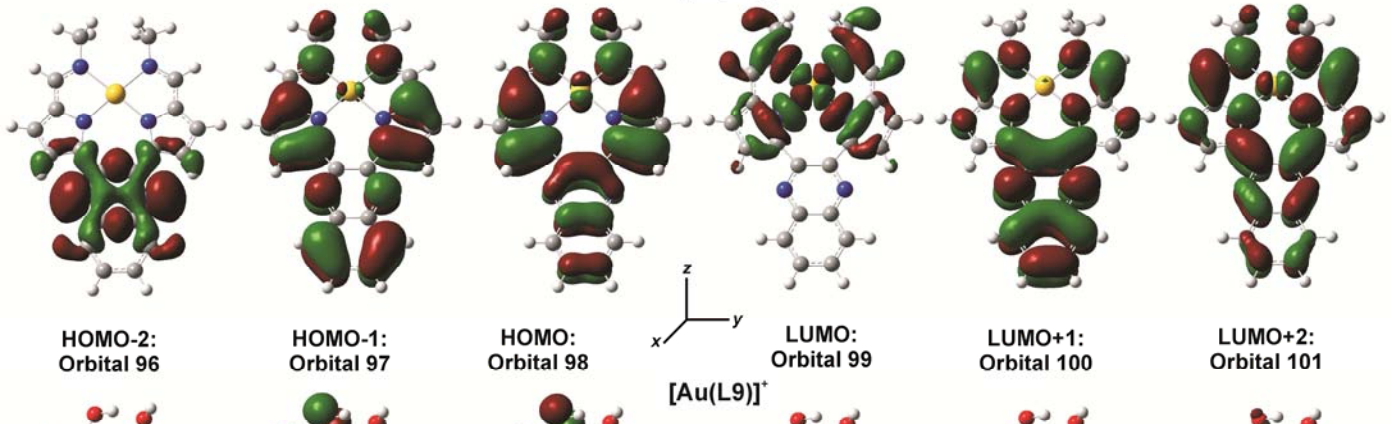




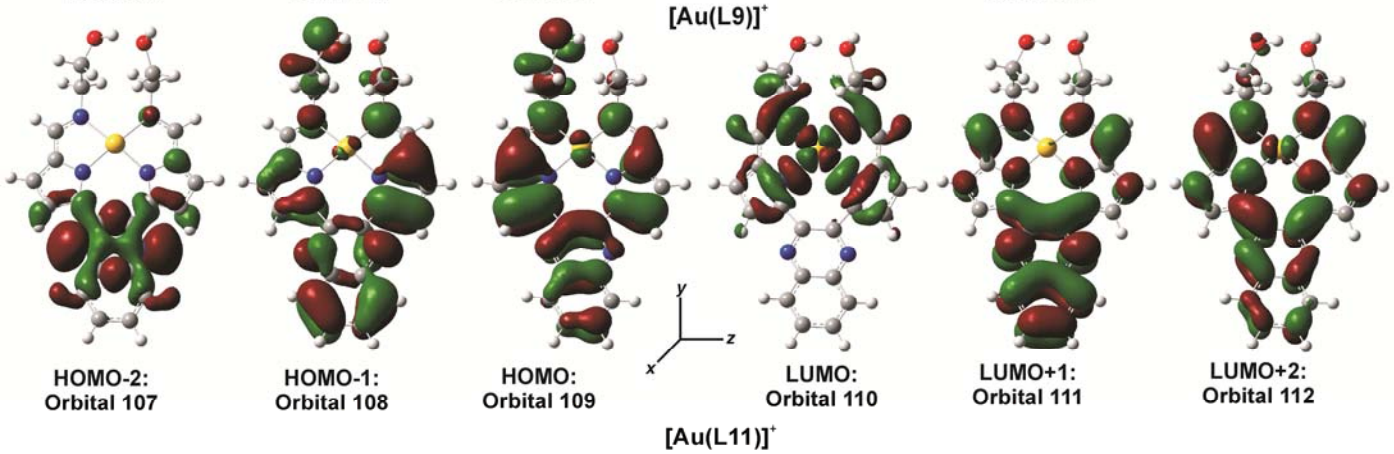
$[Au(L6)]^+$



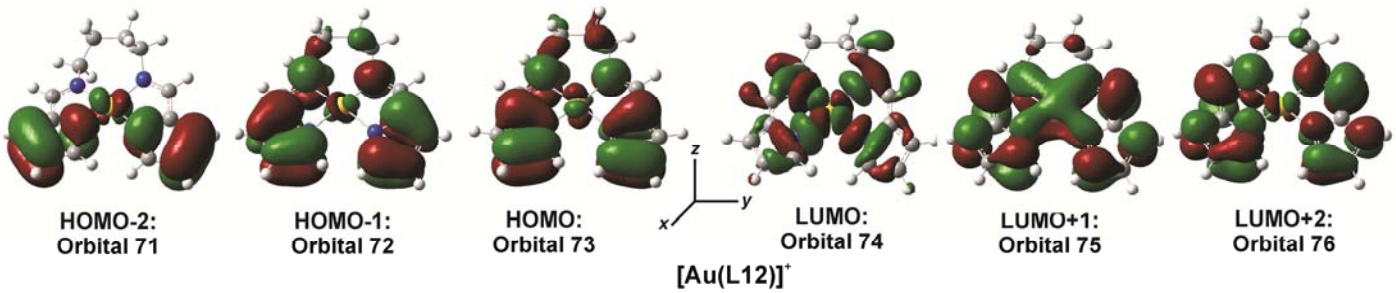
$[Au(L7)]^+$



$[Au(L9)]^+$

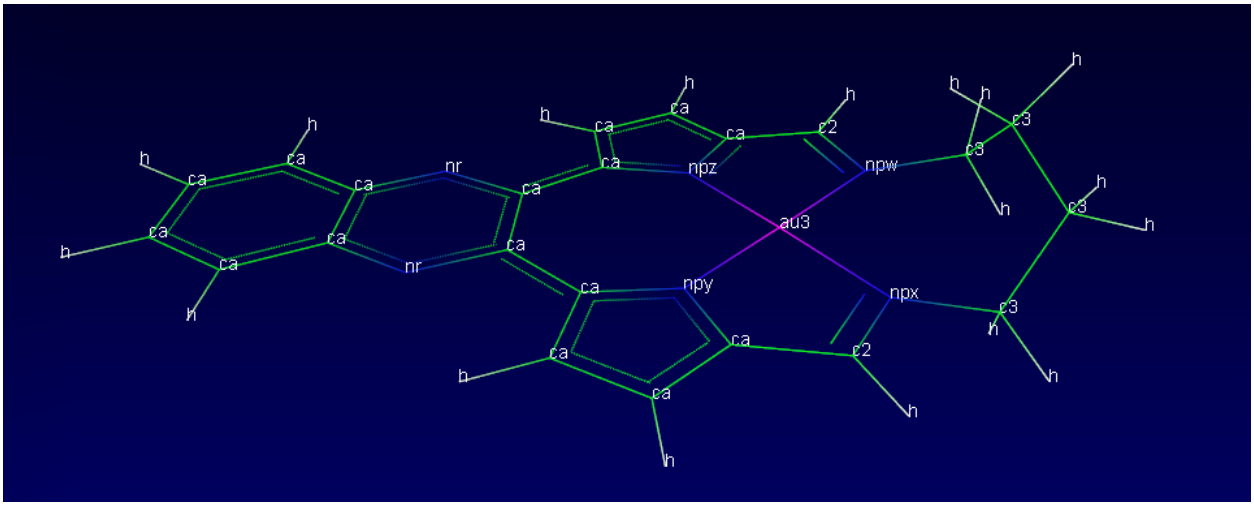


$[Au(L11)]^+$


HOMO-2:
Orbital 71
HOMO-1:
Orbital 72
HOMO:
Orbital 73
z
y
x
LUMO:
Orbital 74
LUMO+1:
Orbital 75
LUMO+2:
Orbital 76

$[Au(L12)]^+$

ATOM TYPE DEFINITIONS: MODIFIED SP4 FORCE FIELD



Four distinct nitrogen atom donors were defined for the new force field: **npw**, **npx** (the two imine nitrogen atoms in the structure of **3** above); **npy**, and **npz** (the two pyrrole nitrogen atoms). Distinct nitrogen donor atom types are mandatory to define the structurally unique *cis* and *trans* N–Au–N angles in the coordination sphere of the square planar metal ion. Key bond stretching, van der Waals, bond angle, and torsion angle terms were then added to complete the parameter set. The new parameter terms for the force field are listed below along with their standard sp4 definitions.

NEW PARAMETERS ADDED TO SP4 FORCE FIELD

```
#FF_Param SP4

; ************************************
; ****        VEGA Parameters     ****
; ****      for SP4 force field   ****
; ************************************

#Atoms

; Description:
; ~~~~~~~~~~~~
; Atom type -> Atom type
; R         -> Combining bond radius
; Theta     -> Combining angle term
; Sigma     -> VdW parameter
; Emin      -> VdW parameter
; Z         -> Effective charge
; AngleInc  -> ?
; X         -> Electronegativity
; Jaa       -> Self coulomb term
; Mass      -> Atom mass
; Charge    -> Atomic charge
; V         -> Torsion term for evaluation
; U         -> Torsion term for evaluation
; Hybrid    -> Default hybrid force (ignored if <= 0)

; Atom type  R       Theta   Sigma  Emin   Z        AngleInc  X        Jaa      Mass      Charge  V       U      Hybrid
; ================================================================================================================================
  au3        1.2800   90.00  2.912  0.013  2.43000   0.0      15.4010  30.5000   197.000   0.000   0.000  0.000    0.000
  npw        0.6400  118.00  3.660  0.069  1.71900   0.0       7.6490  11.0100   14.0067   0.000  -1.000  1.250    0.000
  npx        0.6400  118.00  3.660  0.069  1.71900   0.0       7.6490  11.0100   14.0067   0.000  -1.000  1.250    0.000
  npy        0.6380  110.00  3.660  0.069  1.90000   0.0       6.8990  11.7600   14.0067   0.000  -1.000  1.250  150.000
  npz        0.6380  110.00  3.660  0.069  1.90000   0.0       6.8990  11.7600   14.0067   0.000  -1.000  1.250  150.000
```

#Bonds

; Description:
; ~~~~~~~~~~~~
; Atom I,J   -> Bonded atoms
; Force   -> Force constant
; Length   -> Bond length

; Atom I Atom J Force Length
; ==============================
  Au3   npw   280.0 2.020
  Au3   npx   280.0 2.020
  Au3   npy   700.0 1.850
  Au3   npz   700.0 1.850

#Angles

; Description:
; ~~~~~~~~~~~~
; Atom I,J,K   -> Bonded atoms
; Force   -> Force constant
; Theta   -> Angle value

; Atom I Atom J Atom K Force Theta
; ===================================
  npw   Au3   npy   600.0   180.0
  npy   Au3   npw   600.0   180.0
  npx   Au3   npz   600.0   180.0
  npz   Au3   npx   600.0   180.0
  npw   Au3   npx   10.0   90.0
  npx   Au3   npy   10.0   90.0
  npy   Au3   npz   20.0   90.0
  npw   Au3   npz   10.0   90.0

#Torsions

; Description:
; ~~~~~~~~~~~~
; Atom I,J,K,L -> Atoms defining the torsion
; Force   -> Force constant
; N   -> Multiplicity
; Offset   -> Torsion offset

; Atom I Atom J Atom K Atom L Force N Offset
; ==
  ca   c2   npx   c3   46.0   2 180.0
  ca   c2   npw   c3   46.0   2 180.0
  c3   npx   c2   ca   46.0   2 180.0
  c3   npw   c2   ca   46.0   2 180.0
  npz   au3   npw   c2   16.0   2   0.0
  npy   au3   npz   c2   16.0   2   0.0
  npz   ca   ca   ca   16.0   2   0.0
  npy   ca   ca   ca   16.0   2   0.0
  ca   ca   ca   npy   16.0   2   0.0
  ca   ca   ca   npz   16.0   2   0.0
  npz   ca   ca   nr   56.0   2 180.0
  npy   ca   ca   nr   56.0   2 180.0
  c2   ca   ca   ca   46   2 180.0

#Hybrids

; Description:
; ~~~~~~~~~~~~
; Atom I,J,K,L -> Atoms defining the improper angle
; Force   -> Force constant
; Offset   -> Inproper offset

; Atom I Atom J Atom K Atom L Force Offset
; ==
   npw   au3   npx   c3   46.0   0.0
   npx   au3   npw   c3   46.0   0.0
   c3   npx   au3   npw   46.0   0.0
   c3   npw   au3   npx   46.0   0.0

```
#TemplateFF SP4 1.0

; ****************************
; ****  VEGA Template V4.0  ****
; ****    Force Field SP4   ****
; ****************************


; ATDL atom description:
; ~~~~~~~~~~~~~~~~~~~~~
; Element (2) - Bond order (1) - Ring indicator (1) - Aromatic indicator (1)
;
; The brackets indicates the length in characters of each field.

; Generic elements:                    Bond order:
; ~~~~~~~~~~~~~~~~~                    ~~~~~~~~~~~
; X = Any atom                         0   = Atom not bonded
; # = Heavy atom                       1-6 = Bond order
; $ = Any atom excluding C and H       9   = Any bond order
; @ = Halogen
; - = None

; Ring indicator:                      Aromatic indicator:
; ~~~~~~~~~~~~~~~                      ~~~~~~~~~~~~~~~~~~
; 0     = Don't check ring             0 = Don't check
; 2     = Not inside a ring            1 = Aromatic
; 3...7 = From 3 to 7 member ring
; 9     = Generic ring

; Logical operators:
; ~~~~~~~~~~~~~~~~~~
; to use the logical operators AND, OR and NOT (&, | and !), you must
; place the expression between square brackets at the specified position:
;
; Examples:
; [C- |  N-]900  -> the element can be carbon or nitrogen
; [X- & !Cl]900  -> all elements but not chlorine
; C-[4 | 3]00    -> sp3 or sp2 carbon
; C-4[9 & 9]0    -> sp3 carbon in a double condensed ring
; C-3[6 | 5][!1] -> sp2 carbon in 5 or 6 member ring not aromatic

; Atom types:
; ~~~~~~~~~~
; each not blank and not commented line (; is the remark indicator) must
; include at least the atom type name (max. 8 characters) and the ATDL
; description. Optionally, you can specify the bonded atoms placing them
; between round brackets.


; Type    Atm    Bonded atoms
; ========================================================================
  npw       N-300 (C-300 (N-300 N-300 N-300))
  npw       N-300 (C-300 (O-100))
  npw       N-300 (C-391)
  npw       N-300 (C-300)
  npw       N-300 (O-200 O-100 O-100)
  npw       N-300 (C-900 O-100 O-100)
  npx       N-300 (C-300 (N-300 N-300 N-300))
  npx       N-300 (C-300 (O-100))
  npx       N-300 (C-391)
  npx       N-300 (C-300)
  npx       N-300 (O-200 O-100 O-100)
  npx       N-300 (C-900 O-100 O-100)
  npy       N-300 (C-300 (N-300 N-300 N-300))
  npy       N-300 (C-300 (O-100))
  npy       N-300 (C-391)
  npy       N-300 (C-300)
  npy       N-300 (O-200 O-100 O-100)
  npy       N-300 (C-900 O-100 O-100)
  npz       N-300 (C-300 (N-300 N-300 N-300))
  npz       N-300 (C-300 (O-100))
  npz       N-300 (C-391)
  npz       N-300 (C-300)
  npz       N-300 (O-200 O-100 O-100)
  npz       N-300 (C-900 O-100 O-100)
  au3       Au900
```

FORCE FIELD VERIFICATION

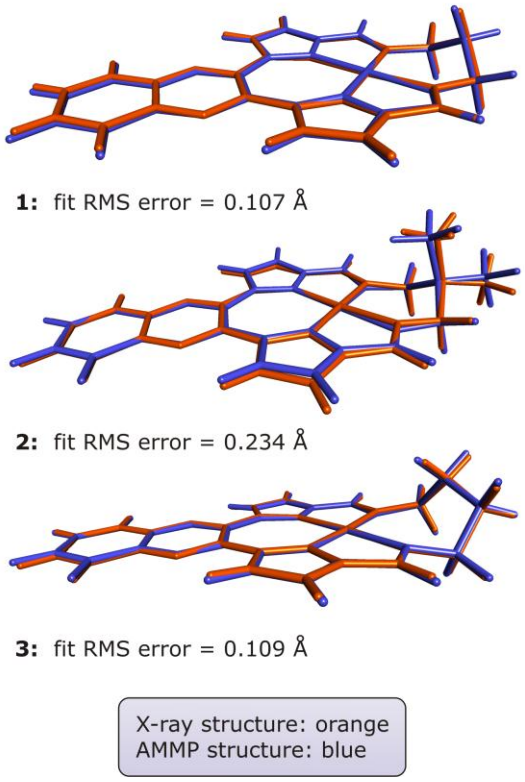


Figure 1. Non-linear least-squares fits of the AMMP-calculated and X-ray structures of cations from the experimental structures of compounds **1**–**3**. The fit root mean square (RMS) errors are shown and are determined from the fit of all atoms in each structure. The modified AMMP parameter set affords an acceptably accurate description of the structures as far as their geometric and conformational attributes are concerned.

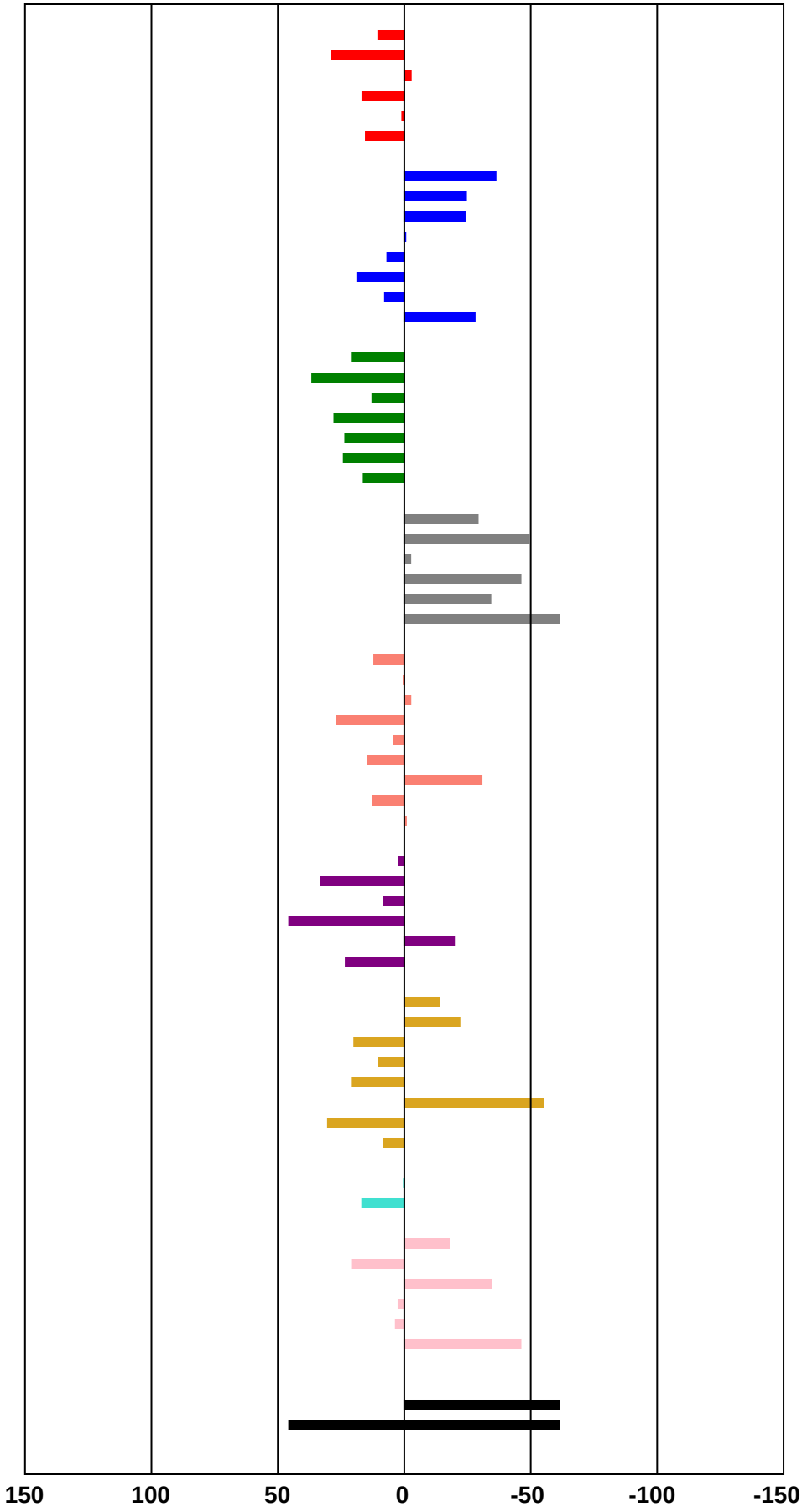
Developmental Therapeutics Program

One Dose Mean Graph

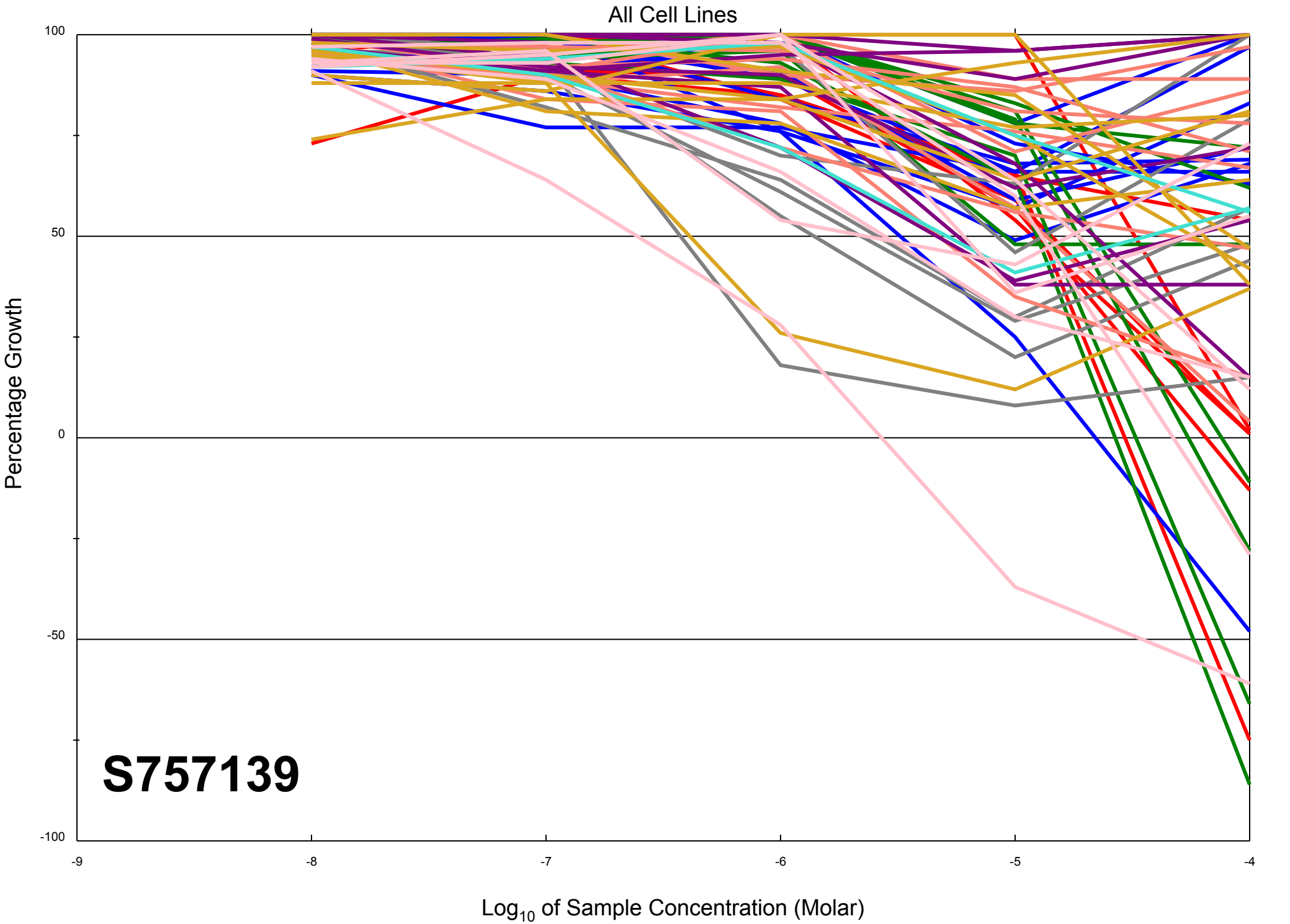
NSC: D-754844 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** Nov 15, 2010
Experiment ID: 1011OS53		**Report Date:** Dec 22, 2010

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	86.98
HL-60(TB)	105.50
K-562	74.10
MOLT-4	93.26
RPMI-8226	77.51
SR	91.90
Non-Small Cell Lung Cancer	
A549/ATCC	40.56
EKVX	52.25
HOP-62	52.77
NCI-H226	76.24
NCI-H23	83.41
NCI-H322M	95.28
NCI-H460	84.34
NCI-H522	48.82
Colon Cancer	
COLO 205	97.45
HCC-2998	113.11
HCT-116	89.32
HCT-15	104.35
HT29	100.05
KM12	100.64
SW-620	92.77
CNS Cancer	
SF-268	47.63
SF-295	27.44
SF-539	74.28
SNB-19	30.68
SNB-75	42.60
U251	15.37
Melanoma	
LOX IMVI	88.58
MALME-3M	76.94
M14	74.25
MDA-MB-435	103.39
SK-MEL-2	80.87
SK-MEL-28	91.02
SK-MEL-5	46.11
UACC-257	88.98
UACC-62	76.02
Ovarian Cancer	
IGROV1	78.78
OVCAR-3	109.55
OVCAR-4	84.90
OVCAR-5	122.23
OVCAR-8	57.00
SK-OV-3	99.85
Renal Cancer	
786-0	62.87
A498	54.83
ACHN	96.48
CAKI-1	86.87
RXF 393	97.43
SN12C	21.60
TK-10	106.88
UO-31	84.82
Prostate Cancer	
PC-3	76.83
DU-145	93.34
Breast Cancer	
MCF7	59.05
MDA-MB-231/ATCC	97.36
HS 578T	42.19
BT-549	78.98
T-47D	80.05
MDA-MB-468	30.70
Mean	76.68
Delta	61.31
Range	106.86

Mean Growth Percent - Growth Percent



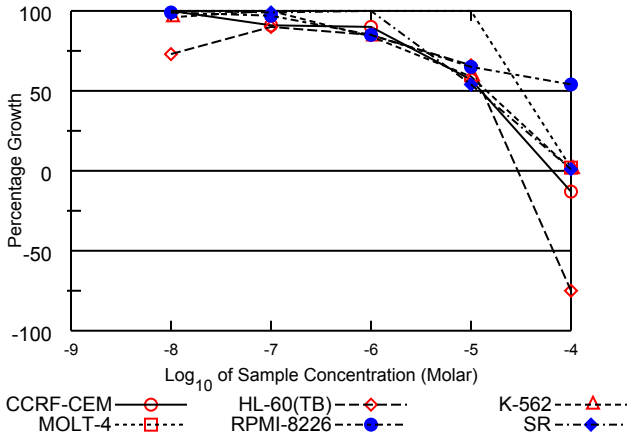
National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 757139/1	SSPL:0X1V	EXP. ID:1105NS53
	Report Date:July 14, 2011	Test Date:May 23, 2011	



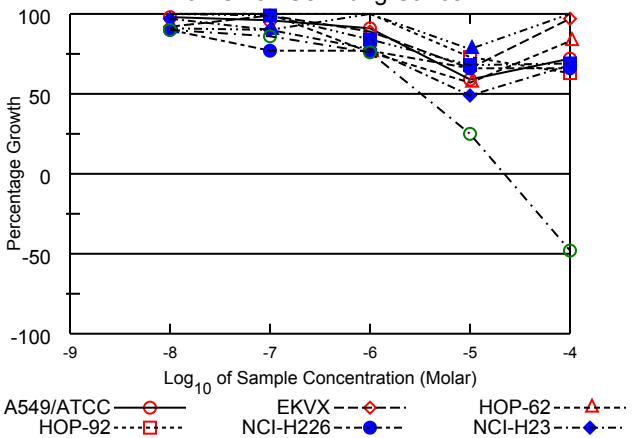
National Cancer Institute Developmental Therapeutics Program
Dose Response Curves

NSC: D - 757139 / 1	SSPL: 0X1V	EXP. ID: 1105NS53
Report Date: July 14, 2011	Test Date: May 23, 2011	

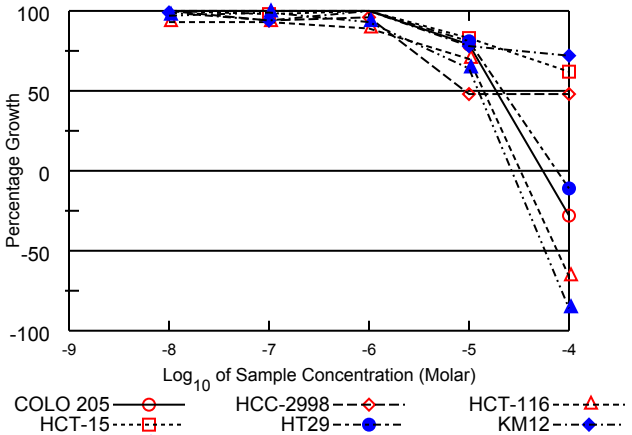
Leukemia



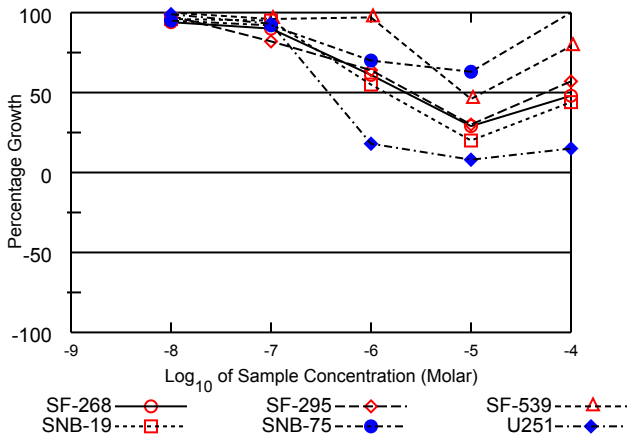
Non-Small Cell Lung Cancer



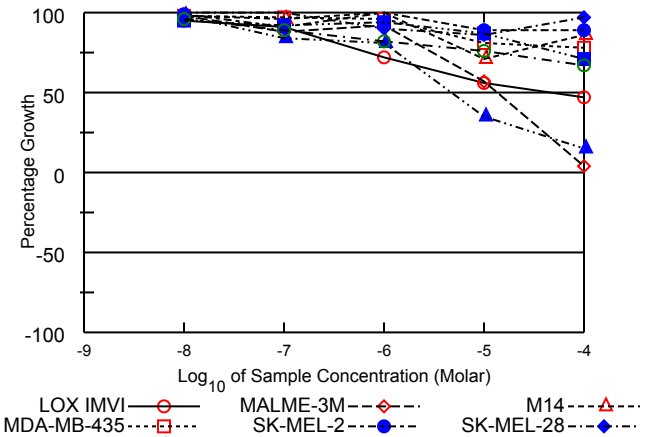
Colon Cancer



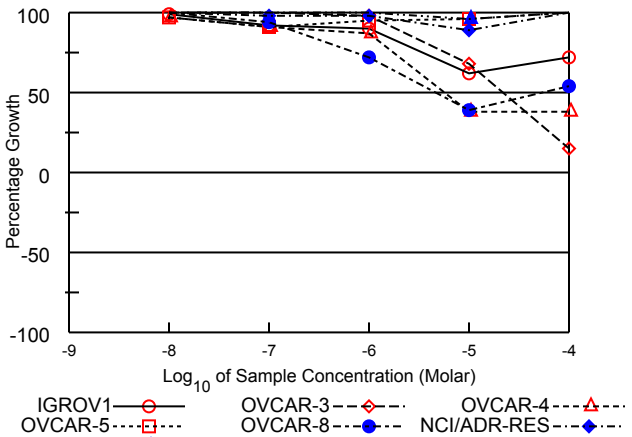
CNS Cancer



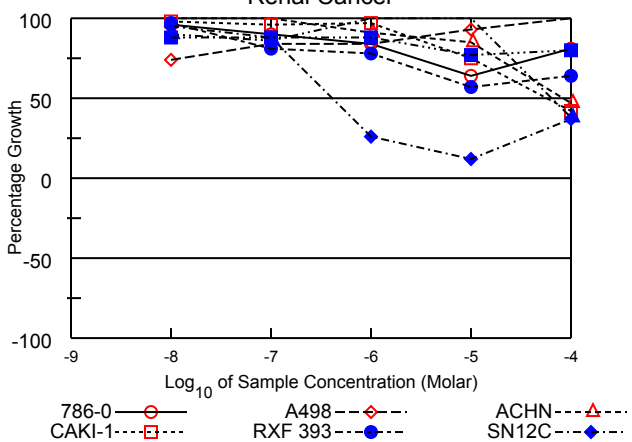
Melanoma



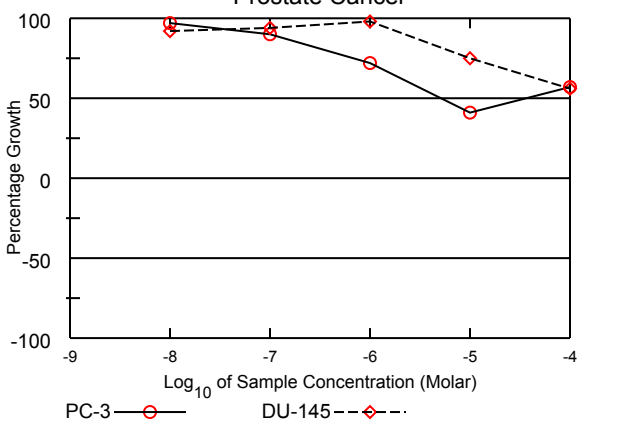
Ovarian Cancer



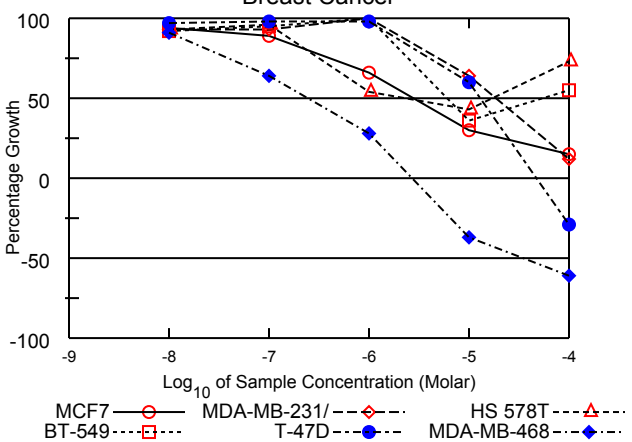
Renal Cancer



Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 757139 / 1	Experiment ID : 1105NS53	Test Type : 08	Units : Molar
Report Date : July 14, 2011	Test Date : May 23, 2011	QNS :	MC :
COMI : KA_aumacro_DM (104509)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0X1V	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.527	1.862	1.861	1.737	1.725	1.283	0.458	100	91	90	57	-13	1.24E-5	6.49E-5	> 1.00E-4
HL-60(TB)	0.594	2.436	1.933	2.248	2.157	1.806	0.150	73	90	85	66	-75	1.29E-5	2.94E-5	6.66E-5
K-562	0.249	1.772	1.708	1.777	1.525	1.147	0.258	96	100	84	59	1	1.42E-5	> 1.00E-4	> 1.00E-4
MOLT-4	0.587	1.954	1.988	1.990	2.161	1.986	0.617	102	103	115	102	2	3.33E-5	> 1.00E-4	> 1.00E-4
RPMI-8226	0.789	2.670	2.650	2.614	2.387	2.014	1.799	99	97	85	65	54	> 1.00E-4	> 1.00E-4	> 1.00E-4
SR	0.346	1.459	1.486	1.449	1.487	0.944	0.354	102	99	102	54	1	1.17E-5	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.315	1.504	1.482	1.462	1.398	1.012	1.166	98	96	91	59	72	> 1.00E-4	> 1.00E-4	> 1.00E-4
EKVX	0.746	1.702	1.629	1.688	1.594	1.375	1.671	92	99	89	66	97	> 1.00E-4	> 1.00E-4	> 1.00E-4
HOP-62	0.348	0.972	0.981	1.007	0.821	0.703	0.864	101	106	76	57	83	> 1.00E-4	> 1.00E-4	> 1.00E-4
HOP-92	1.138	1.565	1.626	1.614	1.602	1.450	1.408	114	111	109	73	63	> 1.00E-4	> 1.00E-4	> 1.00E-4
NCI-H226	0.605	1.726	1.612	1.470	1.473	1.350	1.341	90	77	77	66	66	> 1.00E-4	> 1.00E-4	> 1.00E-4
NCI-H23	0.538	1.405	1.383	1.319	1.216	0.966	1.127	97	90	78	49	68	.	> 1.00E-4	> 1.00E-4
NCI-H322M	0.821	1.549	1.483	1.479	1.555	1.386	1.604	91	90	101	78	108	> 1.00E-4	> 1.00E-4	> 1.00E-4
NCI-H460	0.226	1.845	1.953	1.823	1.586	1.331	1.336	107	99	84	68	69	> 1.00E-4	> 1.00E-4	> 1.00E-4
NCI-H522	0.593	1.559	1.463	1.421	1.324	0.839	0.309	90	86	76	25	-48	3.24E-6	2.22E-5	> 1.00E-4
Colon Cancer															
COLO 205	0.270	1.304	1.331	1.389	1.328	1.088	0.196	103	108	102	79	-28	1.88E-5	5.51E-5	> 1.00E-4
HCC-2998	0.685	1.996	2.011	1.914	1.945	1.314	1.320	101	94	96	48	48	9.06E-6	> 1.00E-4	> 1.00E-4
HCT-116	0.186	1.116	1.055	1.051	1.010	0.841	0.064	93	93	89	70	-66	1.41E-5	3.29E-5	7.68E-5
HCT-15	0.472	2.411	2.455	2.367	2.433	2.079	1.682	102	98	101	83	62	> 1.00E-4	> 1.00E-4	> 1.00E-4
HT29	0.217	1.063	1.164	1.126	1.102	0.900	0.194	112	108	105	81	-11	2.17E-5	7.62E-5	> 1.00E-4
KM12	0.439	2.274	2.258	2.164	2.265	1.870	1.757	99	94	100	78	72	> 1.00E-4	> 1.00E-4	> 1.00E-4
SW-620	0.228	1.398	1.366	1.390	1.321	0.982	0.032	97	99	93	64	-86	1.25E-5	2.68E-5	5.77E-5
CNS Cancer															
SF-268	0.469	1.633	1.568	1.512	1.179	0.805	1.023	94	90	61	29	48	2.20E-6	> 1.00E-4	> 1.00E-4
SF-295	0.640	1.964	1.941	1.721	1.484	1.039	1.400	98	82	64	30	57	.	> 1.00E-4	> 1.00E-4
SF-539	0.834	2.113	2.115	2.061	2.079	1.417	1.847	100	96	97	46	79	.	> 1.00E-4	> 1.00E-4
SNB-19	0.448	1.340	1.303	1.299	0.936	0.627	0.839	96	95	55	20	44	1.37E-6	> 1.00E-4	> 1.00E-4
SNB-75	0.603	1.236	1.207	1.183	1.048	1.002	1.255	95	92	70	63	103	> 1.00E-4	> 1.00E-4	> 1.00E-4
U251	0.254	1.262	1.249	1.189	0.437	0.334	0.403	99	93	18	8	15	3.74E-7	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.221	1.422	1.360	1.319	1.089	0.898	0.785	95	91	72	56	47	4.74E-5	> 1.00E-4	> 1.00E-4
MALME-3M	0.694	1.446	1.432	1.356	1.384	1.122	0.727	98	88	92	57	4	1.35E-5	> 1.00E-4	> 1.00E-4
M14	0.393	1.187	1.171	1.154	1.190	0.954	1.074	98	96	100	71	86	> 1.00E-4	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.445	1.974	1.945	1.922	1.913	1.678	1.633	98	97	96	81	78	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-MEL-2	0.990	1.721	1.716	1.653	1.753	1.642	1.643	99	91	104	89	89	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-MEL-28	0.516	1.473	1.498	1.494	1.377	1.343	1.440	103	102	90	86	97	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.442	2.846	2.806	2.453	2.380	1.279	0.807	98	84	81	35	15	4.66E-6	> 1.00E-4	> 1.00E-4
UACC-257	0.776	1.510	1.470	1.452	1.466	1.415	1.296	95	92	94	87	71	> 1.00E-4	> 1.00E-4	> 1.00E-4
UACC-62	0.834	2.276	2.212	2.114	2.014	1.924	1.796	96	89	82	76	67	> 1.00E-4	> 1.00E-4	> 1.00E-4
Ovarian Cancer															
IGROV1	0.523	1.707	1.691	1.608	1.585	1.259	1.380	99	92	90	62	72	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-3	0.499	1.562	1.563	1.569	1.544	1.219	0.656	100	101	98	68	15	2.16E-5	> 1.00E-4	> 1.00E-4
OVCAR-4	0.488	1.466	1.432	1.382	1.340	0.863	0.860	97	91	87	38	38	5.76E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.573	1.501	1.478	1.421	1.457	1.461	1.625	97	91	95	96	113	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-8	0.386	1.455	1.470	1.393	1.151	0.808	0.963	101	94	72	39	54	.	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.452	1.241	1.246	1.226	1.226	1.153	1.241	101	98	98	89	100	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-OV-3	0.503	1.300	1.301	1.336	1.372	1.270	1.527	100	105	109	96	128	> 1.00E-4	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.533	1.911	1.850	1.778	1.691	1.415	1.655	96	90	84	64	81	> 1.00E-4	> 1.00E-4	> 1.00E-4
A498	1.239	2.252	1.990	2.087	2.092	2.186	2.421	74	84	84	93	117	> 1.00E-4	> 1.00E-4	> 1.00E-4
ACHN	0.418	1.494	1.501	1.492	1.402	1.336	0.927	101	100	91	85	47	8.50E-5	> 1.00E-4	> 1.00E-4
CAKI-1	0.688	2.099	2.069	2.037	2.054	1.741	1.280	98	96	97	75	42	5.67E-5	> 1.00E-4	> 1.00E-4
RXF 393	0.541	1.204	1.181	1.078	1.061	0.920	0.965	97	81	78	57	64	> 1.00E-4	> 1.00E-4	> 1.00E-4
SN12C	0.583	1.813	1.749	1.660	0.909	0.736	1.034	95	88	26	12	37	4.12E-7	> 1.00E-4	> 1.00E-4
TK-10	0.657	1.203	1.150	1.129	1.251	1.303	0.865	90	86	109	118	38	7.11E-5	> 1.00E-4	> 1.00E-4
UO-31	0.566	1.649	1.524	1.523	1.524	1.401	1.431	88	88	88	77	80	> 1.00E-4	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.488	1.263	1.238	1.188	1.050	0.803	0.929	97	90	72	41	57	.	> 1.00E-4	> 1.00E-4
DU-145	0.300	1.459	1.367	1.395	1.440	1.170	0.954	92	94	98	75	56	> 1.00E-4	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.335	1.886	1.789	1.711	1.354	0.799	0.561	94	89	66	30	15	2.75E-6	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.577	1.336	1.282	1.281	1.360	1.066	0.668	93	93	103	64	12	1.89E-5	> 1.00E-4	> 1.00E-4
HS 578T	0.733	1.466	1.414	1.434	1.130	1.046	1.265	93	96	54	43	73	.	> 1.00E-4	> 1.00E-4
BT-549	0.750	1.504	1.443	1.463	1.536	1.023	1.163	92	95	104	36	55	.	> 1.00E-4	> 1.00E-4
T-47D	0.672	1.510	1.487	1.495	1.497	1.173	0.479	97	98	98	60	-29	1.29E-5	4.73E-5	> 1.00E-4
MDA-MB-468	0.587	1.381	1.308	1.095	0.813	0.369	0.231	91	64	28	-37	-61	2.48E-7	2.71E-6	3.50E-5

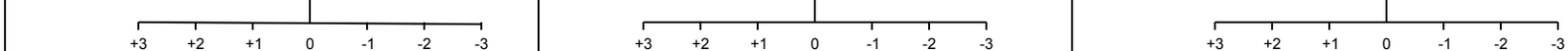
National Cancer Institute Developmental Therapeutics Program

Mean Graphs

NSC : D - 757139/1 | Units :Molar | SSPL :0X1V | EXP. ID :1105NS53

Report Date :July 14, 2011 | Test Date :May 23, 2011

Panel/Cell Line	Log_{10}GI50	GI50	Log_{10}TGI	TGI	Log_{10}LC50	LC50
Leukemia						
CCRF-CEM	-4.91		-4.19		> -4.00	
HL-60(TB)	-4.89		-4.53		-4.18	
K-562	-4.85		> -4.00		> -4.00	
MOLT-4	-4.48		> -4.00		> -4.00	
RPMI-8226	> -4.00		> -4.00		> -4.00	
SR	-4.93		> -4.00		> -4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	> -4.00		> -4.00		> -4.00	
EKVX	> -4.00		> -4.00		> -4.00	
HOP-62	> -4.00		> -4.00		> -4.00	
HOP-92	> -4.00		> -4.00		> -4.00	
NCI-H226	> -4.00		> -4.00		> -4.00	
NCI-H23			> -4.00		> -4.00	
NCI-H322M	> -4.00		> -4.00		> -4.00	
NCI-H460	> -4.00		> -4.00		> -4.00	
NCI-H522	-5.49		-4.65		> -4.00	
Colon Cancer						
COLO 205	-4.73		-4.26		> -4.00	
HCC-2998	-5.04		> -4.00		> -4.00	
HCT-116	-4.85		-4.48		-4.11	
HCT-15	> -4.00		> -4.00		> -4.00	
HT29	-4.66		-4.12		> -4.00	
KM12	> -4.00		> -4.00		> -4.00	
SW-620	-4.90		-4.57		-4.24	
CNS Cancer						
SF-268	-5.66		> -4.00		> -4.00	
SF-295			> -4.00		> -4.00	
SF-539			> -4.00		> -4.00	
SNB-19	-5.86		> -4.00		> -4.00	
SNB-75	> -4.00		> -4.00		> -4.00	
U251	-6.43		> -4.00		> -4.00	
Melanoma						
LOX IMVI	-4.32		> -4.00		> -4.00	
MALME-3M	-4.87		> -4.00		> -4.00	
M14	> -4.00		> -4.00		> -4.00	
MDA-MB-435	> -4.00		> -4.00		> -4.00	
SK-MEL-2	> -4.00		> -4.00		> -4.00	
SK-MEL-28	> -4.00		> -4.00		> -4.00	
SK-MEL-5	-5.33		> -4.00		> -4.00	
UACC-257	> -4.00		> -4.00		> -4.00	
UACC-62	> -4.00		> -4.00		> -4.00	
Ovarian Cancer						
IGROV1	> -4.00		> -4.00		> -4.00	
OVCAR-3	-4.67		> -4.00		> -4.00	
OVCAR-4	-5.24		> -4.00		> -4.00	
OVCAR-5	> -4.00		> -4.00		> -4.00	
OVCAR-8			> -4.00		> -4.00	
NCI/ADR-RES	> -4.00		> -4.00		> -4.00	
SK-OV-3	> -4.00		> -4.00		> -4.00	
Renal Cancer						
786-0	> -4.00		> -4.00		> -4.00	
A498	> -4.00		> -4.00		> -4.00	
ACHN	-4.07		> -4.00		> -4.00	
CAKI-1	-4.25		> -4.00		> -4.00	
RXF 393	> -4.00		> -4.00		> -4.00	
SN12C	-6.39		> -4.00		> -4.00	
TK-10	-4.15		> -4.00		> -4.00	
UO-31	> -4.00		> -4.00		> -4.00	
Prostate Cancer						
PC-3			> -4.00		> -4.00	
DU-145	> -4.00		> -4.00		> -4.00	
Breast Cancer						
MCF7	-5.56		> -4.00		> -4.00	
MDA-MB-231/ATCC	-4.72		> -4.00		> -4.00	
HS 578T			> -4.00		> -4.00	
BT-549			> -4.00		> -4.00	
T-47D	-4.89		-4.33		> -4.00	
MDA-MB-468	-6.61		-5.57		-4.46	
_MID	-4.54		-4.08		-4.02	
Delta	2.07		1.49		0.44	
Range	2.61		1.57		0.46	



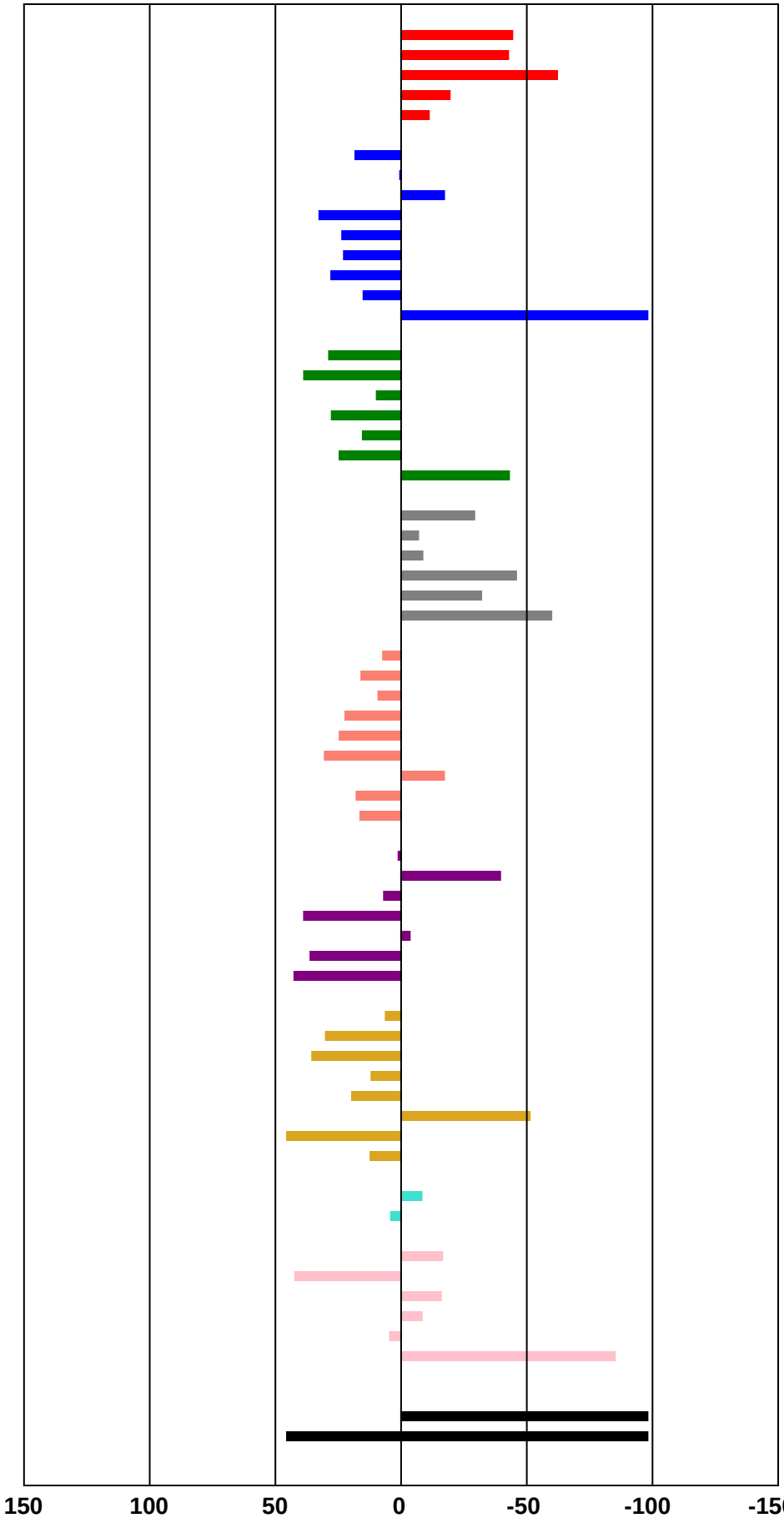
Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-757139 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** Apr 11, 2011
Experiment ID: 1104OS33		**Report Date:** May 10, 2011

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	28.30
HL-60(TB)	29.96
K-562	10.49
MOLT-4	53.22
RPMI-8226	61.51
Non-Small Cell Lung Cancer	
A549/ATCC	90.82
EKVX	72.99
HOP-62	55.44
HOP-92	105.12
NCI-H226	96.05
NCI-H23	95.35
NCI-H322M	100.40
NCI-H460	87.56
NCI-H522	-25.45
Colon Cancer	
COLO 205	101.27
HCC-2998	111.20
HCT-116	82.29
HCT-15	100.19
HT29	87.83
KM12	97.10
SW-620	29.61
CNS Cancer	
SF-268	43.43
SF-295	65.77
SF-539	64.06
SNB-19	26.81
SNB-75	40.68
U251	12.79
Melanoma	
LOX IMVI	79.78
MALME-3M	88.42
M14	81.65
MDA-MB-435	94.79
SK-MEL-2	97.04
SK-MEL-28	102.97
SK-MEL-5	55.48
UACC-257	90.35
UACC-62	88.83
Ovarian Cancer	
IGROV1	73.63
OVCAR-3	33.14
OVCAR-4	79.41
OVCAR-5	111.23
OVCAR-8	69.11
NCI/ADR-RES	108.67
SK-OV-3	115.06
Renal Cancer	
786-0	78.73
A498	102.55
ACHN	107.98
CAKI-1	84.40
RXF 393	92.13
SN12C	21.40
TK-10	117.98
UO-31	84.78
Prostate Cancer	
PC-3	64.43
DU-145	76.64
Breast Cancer	
MCF7	56.17
MDA-MB-231/ATCC	114.74
HS 578T	56.72
BT-549	64.32
T-47D	77.04
MDA-MB-468	-12.46
Mean	72.58
Delta	98.03
Range	143.43

Mean Growth Percent - Growth Percent



Nontumored Animal Toxicity Assay for S758065

Report generated on 25-Oct-2012

EXPERIMENT: AAZ-607 / 0 / 8B	**TUMOR:** NO CELLS	**HOST:** Athymic Nudes	**IMPLANT DATE:** 03-APR-2012
MEMO NO:	**SOURCE/LINE:** 0	**SOURCE:** APA	**STAGING DATE:** 03-APR-2012
BOOK NO:	**IMPLANT SITE:** 0	**SEX:** F	**EVALUATION DATE:** 20-APR-2012

TREATMENT

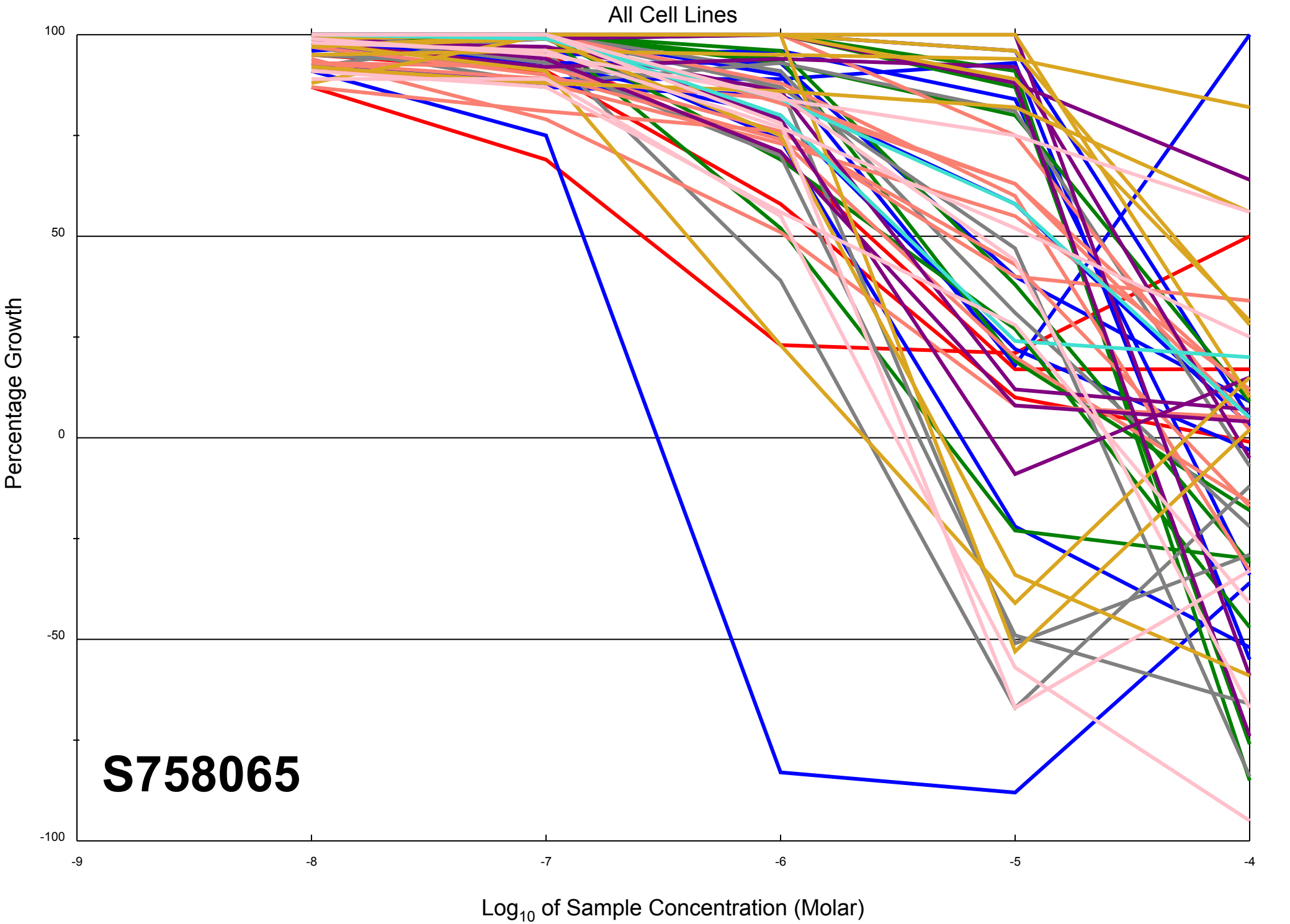
Grp	NSC	Dose/Units	Rt.	Schedule	Death Days	Surv/Total Day 17
4	D-S758065	100.00 mg/kg/dose	IP	QD X 1, Day 0	--	1/1
5	D-S758065	200.00 mg/kg/dose	IP	QD X 1, Day 0	--	1/1
6	D-S758065	400.00 mg/kg/dose	IP	QD X 1, Day 0	--	1/1

VEHICLES

Grp	4	->	NSC # S758065 / 2 (Dose = 100.00)	: in 100% DMSO	(Smooth suspension - homogeneous)	200.0 mg/ml	Inj. Vol.: 0.5 ul/gm body wt
Grp	5	->	NSC # S758065 / 2 (Dose = 200.00)	: in 100% DMSO	(Smooth suspension - homogeneous)	200.0 mg/ml	Inj. Vol.: 1 ul/gm body wt
Grp	6	->	NSC # S758065 / 2 (Dose = 400.00)	: in 100% DMSO	(Smooth suspension - homogeneous)	200.0 mg/ml	Inj. Vol.: 2 ul/gm body wt

NOTE: All treatment was administered according to exact body weight.

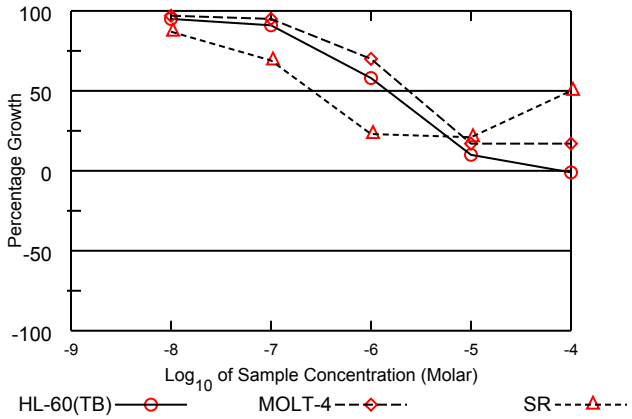
National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 758065/1	SSPL:0X1V	EXP. ID:1106NS66
	Report Date:August 22, 2011	Test Date:June 20, 2011	



National Cancer Institute Developmental Therapeutics Program
Dose Response Curves

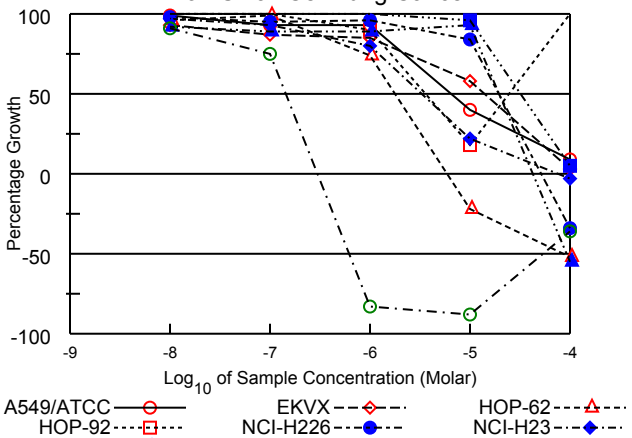
NSC: D - 758065 / 1	SSPL: 0X1V	EXP. ID: 1106NS66
Report Date: August 22, 2011	Test Date: June 20, 2011	

Leukemia



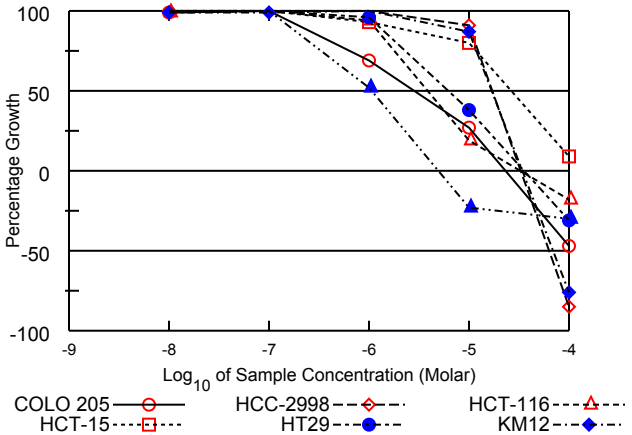
HL-60(TB) MOLT-4 SR

Non-Small Cell Lung Cancer



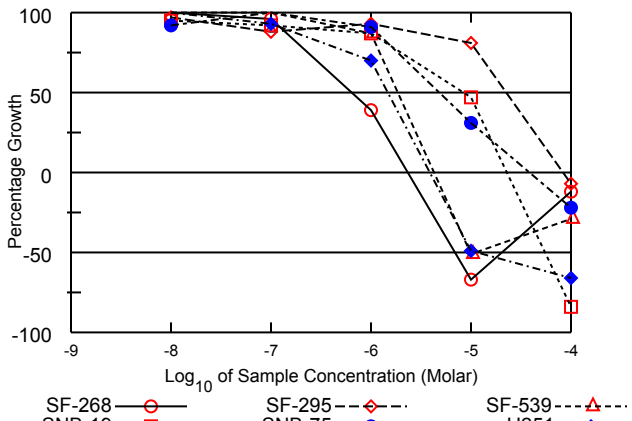
A549/ATCC EKVX HOP-62
HOP-92 NCI-H226 NCI-H23
NCI-H322M NCI-H460 NCI-H522

Colon Cancer



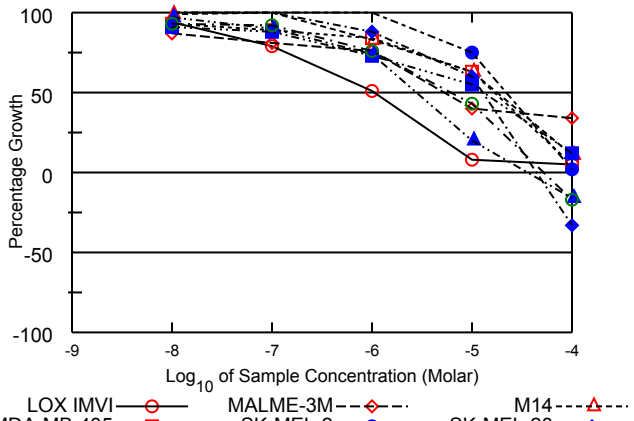
COLO 205 HCC-2998 HCT-116
HCT-15 HT29 KM12
SW-620

CNS Cancer



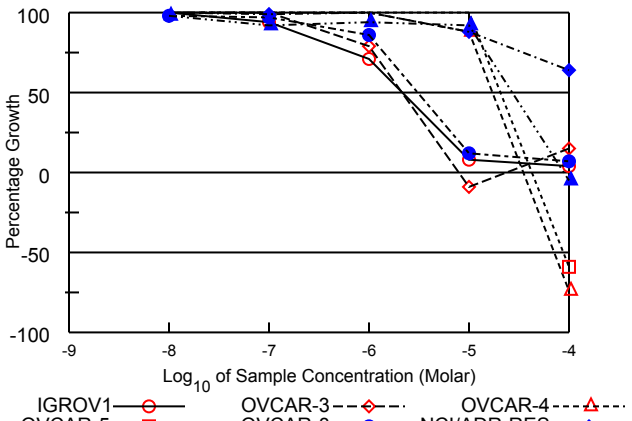
SF-268 SF-295 SF-539
SNB-19 SNB-75 U251

Melanoma



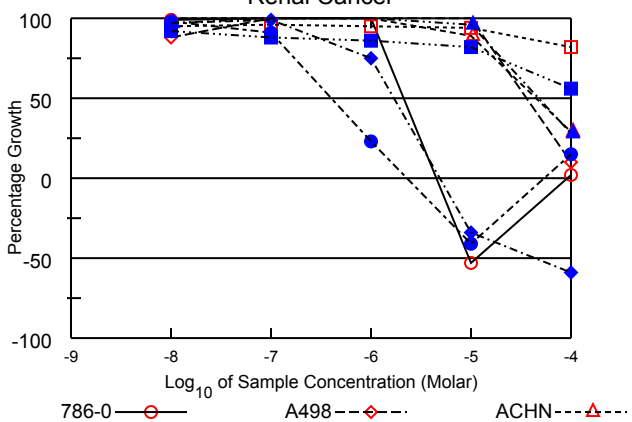
LOX IMVI MALME-3M M14
MDA-MB-435 SK-MEL-2 SK-MEL-28
SK-MEL-5 UACC-257 UACC-62

Ovarian Cancer



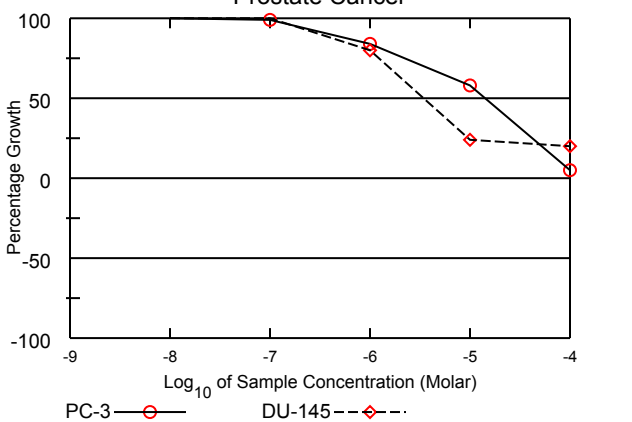
IGROV1 OVCAR-3 OVCAR-4
OVCAR-5 OVCAR-8 NCI/ADR-RES
SK-OV-3

Renal Cancer



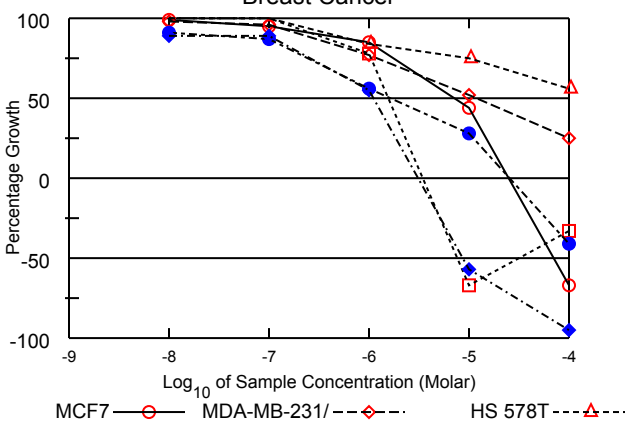
786-0 A498 ACHN
CAKI-1 RXF 393 SN12C
TK-10 UO-31

Prostate Cancer



PC-3 DU-145

Breast Cancer



MCF7 MDA-MB-231/ HS 578T
BT-549 T-47D MDA-MB-468

National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 758065 / 1	Experiment ID : 1106NS66	Test Type : 08	Units : Molar
Report Date : August 22, 2011	Test Date : June 20, 2011	QNS :	MC :
COMI : KA_aumacro_Bu (104506)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0X1V	

		Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth						
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
HL-60(TB)	0.836	2.606	2.522	2.441	1.863	1.022	0.829	95	91	58	10	-1	1.47E-6	8.34E-5	> 1.00E-4
MOLT-4	0.495	1.918	1.874	1.840	1.486	0.740	0.732	97	95	70	17	17	2.37E-6	> 1.00E-4	> 1.00E-4
SR	0.409	1.631	1.467	1.256	0.694	0.665	1.015	87	69	23	21	50	2.63E-7	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.264	1.356	1.340	1.276	1.282	0.704	0.368	99	93	93	40	9	6.56E-6	> 1.00E-4	> 1.00E-4
EKVX	0.774	1.796	1.724	1.668	1.646	1.368	0.808	93	87	85	58	3	1.40E-5	> 1.00E-4	> 1.00E-4
HOP-62	0.479	1.352	1.314	1.346	1.128	0.373	0.228	96	99	74	-22	-52	1.79E-6	5.90E-6	8.33E-5
HOP-92	1.062	1.466	1.485	1.544	1.424	1.135	1.547	105	119	90	18	120	.	> 1.00E-4	> 1.00E-4
NCI-H226	0.558	1.397	1.379	1.358	1.360	1.262	0.370	98	95	96	84	-34	1.94E-5	5.17E-5	> 1.00E-4
NCI-H23	0.486	1.683	1.651	1.597	1.448	0.752	0.472	97	93	80	22	-3	3.32E-6	7.61E-5	> 1.00E-4
NCI-H322M	0.705	1.658	1.584	1.555	1.550	1.596	0.317	92	89	89	93	-55	1.96E-5	4.26E-5	9.24E-5
NCI-H460	0.246	2.456	2.561	2.548	2.510	2.371	0.352	105	104	102	96	5	3.20E-5	> 1.00E-4	> 1.00E-4
NCI-H522	0.526	1.226	1.165	1.051	0.088	0.061	0.336	91	75	-83	-88	-36	1.44E-7	2.98E-7	.
Colon Cancer															
COLO 205	0.240	1.223	1.217	1.233	0.920	0.501	0.128	99	101	69	27	-47	2.81E-6	2.30E-5	> 1.00E-4
HCC-2998	0.539	2.060	2.041	2.074	2.104	1.922	0.083	99	101	103	91	-85	1.71E-5	3.30E-5	6.35E-5
HCT-116	0.226	1.682	1.662	1.752	1.596	0.504	0.185	99	105	94	19	-18	3.87E-6	3.26E-5	> 1.00E-4
HCT-15	0.301	1.768	1.807	1.771	1.670	1.472	0.434	103	100	93	80	9	2.64E-5	> 1.00E-4	> 1.00E-4
HT29	0.175	1.057	1.096	1.077	1.018	0.509	0.120	104	102	96	38	-31	6.15E-6	3.52E-5	> 1.00E-4
KM12	0.441	2.286	2.270	2.263	2.287	2.047	0.108	99	99	100	87	-76	1.69E-5	3.43E-5	6.96E-5
SW-620	0.199	1.316	1.331	1.349	0.776	0.154	0.139	101	103	52	-23	-30	1.05E-6	4.93E-6	> 1.00E-4
CNS Cancer															
SF-268	0.360	1.219	1.217	1.182	0.695	0.120	0.316	100	96	39	-67	-12	6.40E-7	2.34E-6	.
SF-295	0.860	2.538	2.488	2.340	2.426	2.215	0.804	97	88	93	81	-7	2.25E-5	8.42E-5	> 1.00E-4
SF-539	0.572	1.568	1.601	1.619	1.438	0.282	0.409	103	105	87	-51	-29	1.86E-6	4.28E-6	.
SNB-19	0.503	1.623	1.565	1.538	1.482	1.034	0.082	95	92	87	47	-84	8.59E-6	2.30E-5	5.52E-5
SNB-75	0.771	1.308	1.266	1.313	1.259	0.939	0.603	92	101	91	31	-22	4.83E-6	3.88E-5	> 1.00E-4
U251	0.239	1.059	1.061	1.005	0.811	0.122	0.082	100	93	70	-49	-66	1.47E-6	3.86E-6	1.12E-5
Melanoma															
LOX IMVI	0.214	1.433	1.361	1.173	0.841	0.316	0.276	94	79	51	8	5	1.08E-6	> 1.00E-4	> 1.00E-4
MALME-3M	0.626	0.971	0.926	0.904	0.888	0.763	0.742	87	81	76	40	34	5.21E-6	> 1.00E-4	> 1.00E-4
M14	0.405	1.611	1.602	1.612	1.406	1.167	0.539	99	100	83	63	11	1.79E-5	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.416	1.930	1.830	1.765	1.684	1.373	0.490	93	89	84	63	5	1.68E-5	> 1.00E-4	> 1.00E-4
SK-MEL-2	0.883	1.734	1.761	1.864	1.806	1.521	0.901	103	115	108	75	2	2.20E-5	> 1.00E-4	> 1.00E-4
SK-MEL-28	0.484	1.212	1.254	1.245	1.126	0.919	0.326	106	105	88	60	-33	1.28E-5	4.43E-5	> 1.00E-4
SK-MEL-5	0.517	2.162	2.107	2.003	1.743	0.851	0.433	97	90	74	20	-16	2.83E-6	3.59E-5	> 1.00E-4
UACC-257	0.628	1.368	1.301	1.276	1.172	1.039	0.718	91	88	73	55	12	1.34E-5	> 1.00E-4	> 1.00E-4
UACC-62	0.701	2.434	2.321	2.302	2.016	1.446	0.585	93	92	76	43	-17	6.12E-6	5.27E-5	> 1.00E-4
Ovarian Cancer															
IGROV1	0.425	1.419	1.459	1.359	1.130	0.506	0.466	104	94	71	8	4	2.15E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.455	1.439	1.468	1.516	1.236	0.413	0.601	103	108	79	-9	15	2.14E-6	.	> 1.00E-4
OVCAR-4	0.677	1.608	1.652	1.645	1.637	1.493	0.174	105	104	103	88	-74	1.71E-5	3.47E-5	7.07E-5
OVCAR-5	0.487	1.147	1.156	1.176	1.183	1.196	0.200	101	104	105	107	-59	2.21E-5	4.42E-5	8.83E-5
OVCAR-8	0.321	1.343	1.327	1.315	1.205	0.439	0.394	98	97	86	12	7	3.07E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.467	1.533	1.552	1.521	1.545	1.407	1.144	102	99	101	88	64	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-OV-3	0.485	1.210	1.192	1.150	1.166	1.154	0.459	98	92	94	92	-5	2.71E-5	8.79E-5	> 1.00E-4
Renal Cancer															
786-0	0.595	1.899	1.890	1.912	1.934	0.283	0.623	99	101	103	-53	2	2.18E-6	.	.
A498	1.041	1.973	1.862	2.033	2.056	2.011	1.133	88	106	109	104	10	3.75E-5	> 1.00E-4	> 1.00E-4
ACHN	0.410	1.559	1.605	1.631	1.632	1.429	0.744	104	106	106	89	29	4.45E-5	> 1.00E-4	> 1.00E-4
CAKI-1	0.760	2.212	2.135	2.148	2.138	2.129	1.956	95	96	95	94	82	> 1.00E-4	> 1.00E-4	> 1.00E-4
RXF 393	0.282	0.710	0.700	0.671	0.381	0.165	0.348	98	91	23	-41	15	4.01E-7	.	> 1.00E-4
SN12C	0.524	1.899	1.861	1.886	1.560	0.345	0.214	97	99	75	-34	-59	1.70E-6	4.87E-6	4.26E-5
TK-10	0.583	1.338	1.314	1.344	1.352	1.306	0.793	97	101	102	96	28	4.72E-5	> 1.00E-4	> 1.00E-4
UO-31	0.535	1.452	1.382	1.340	1.325	1.284	1.045	92	88	86	82	56	> 1.00E-4	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.493	1.624	1.634	1.610	1.448	1.144	0.555	101	99	84	58	5	1.40E-5	> 1.00E-4	> 1.00E-4
DU-145	0.410	1.583	1.657	1.644	1.344	0.692	0.640	106	105	80	24	20	3.40E-6	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.549	2.101	2.080	2.029	1.863	1.234	0.181	99	95	85	44	-67	7.16E-6	2.49E-5	7.03E-5
MDA-MB-231/ATCC	0.465	1.113	1.100	1.089	0.961	0.802	0.627	98	96	77	52	25	1.19E-5	> 1.00E-4	> 1.00E-4
HS 578T	0.722	1.501	1.520	1.499	1.373	1.305	1.161	102	100	84	75	56	> 1.00E-4	> 1.00E-4	> 1.00E-4
BT-549	0.750	1.519	1.579	1.604	1.347	0.249	0.504	108	111	78	-67	-33	1.55E-6	3.45E-6	.
T-47D	0.518	1.189	1.128	1.103	0.892	0.707	0.306	91	87	56	28	-41	1.61E-6	2.55E-5	> 1.00E-4
MDA-MB-468	0.569	1.438	1.338	1.341	1.048	0.247	0.029	89	89	55	-57	-95	1.11E-6	3.11E-6	8.73E-6

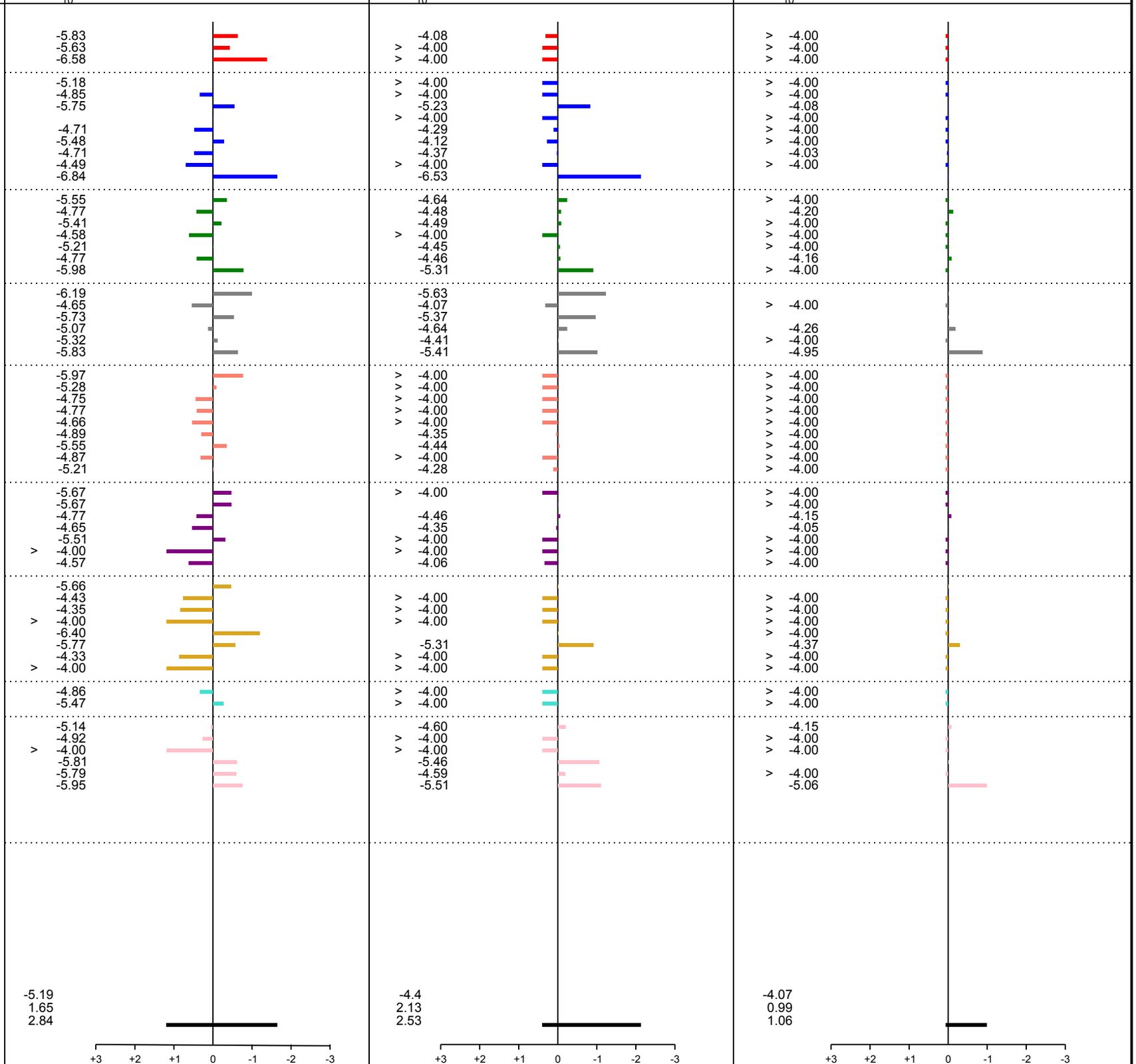
National Cancer Institute Developmental Therapeutics Program

Mean Graphs

NSC : D - 758065/1 | Units :Molar | SSPL :0X1V | EXP. ID :1106NS66

Report Date :August 22, 2011 | Test Date :June 20, 2011

Panel/Cell Line	Log_{10}GI50	Log_{10}TGI	Log_{10}LC50
Leukemia			
HL-60(TB)	-5.83	-4.08	> -4.00
MOLT-4	-5.63	> -4.00	> -4.00
SR	-6.58	> -4.00	> -4.00
Non-Small Cell Lung Cancer			
A549/ATCC	-5.18	> -4.00	> -4.00
EKVX	-4.85	> -4.00	> -4.00
HOP-62	-5.75	-5.23	-4.08
HOP-92		> -4.00	> -4.00
NCI-H226	-4.71	-4.29	> -4.00
NCI-H23	-5.48	-4.12	> -4.00
NCI-H322M	-4.71	-4.37	-4.03
NCI-H460	-4.49	> -4.00	> -4.00
NCI-H522	-6.84	-6.53	
Colon Cancer			
COLO 205	-5.55	-4.64	> -4.00
HCC-2998	-4.77	-4.48	-4.20
HCT-116	-5.41	-4.49	> -4.00
HCT-15	-4.58	> -4.00	> -4.00
HT29	-5.21	-4.45	> -4.00
KM12	-4.77	-4.46	-4.16
SW-620	-5.98	-5.31	> -4.00
CNS Cancer			
SF-268	-6.19	-5.63	
SF-295	-4.65	-4.07	> -4.00
SF-539	-5.73	-5.37	
SNB-19	-5.07	-4.64	-4.26
SNB-75	-5.32	-4.41	> -4.00
U251	-5.83	-5.41	-4.95
Melanoma			
LOX IMVI	-5.97	> -4.00	> -4.00
MALME-3M	-5.28	> -4.00	> -4.00
M14	-4.75	> -4.00	> -4.00
MDA-MB-435	-4.77	> -4.00	> -4.00
SK-MEL-2	-4.66	> -4.00	> -4.00
SK-MEL-28	-4.89	-4.35	> -4.00
SK-MEL-5	-5.55	-4.44	> -4.00
UACC-257	-4.87	> -4.00	> -4.00
UACC-62	-5.21	-4.28	> -4.00
Ovarian Cancer			
IGROV1	-5.67	> -4.00	> -4.00
OVCAR-3	-5.67		> -4.00
OVCAR-4	-4.77	-4.46	-4.15
OVCAR-5	-4.65	-4.35	-4.05
OVCAR-8	-5.51	> -4.00	> -4.00
NCI/ADR-RES	> -4.00	> -4.00	> -4.00
SK-OV-3	-4.57	-4.06	> -4.00
Renal Cancer			
786-0	-5.66		
A498	-4.43	> -4.00	> -4.00
ACHN	-4.35	> -4.00	> -4.00
CAKI-1	> -4.00	> -4.00	> -4.00
RXF 393	-6.40		> -4.00
SN12C	-5.77	-5.31	-4.37
TK-10	-4.33	> -4.00	> -4.00
UO-31	> -4.00	> -4.00	> -4.00
Prostate Cancer			
PC-3	-4.86	> -4.00	> -4.00
DU-145	-5.47	> -4.00	> -4.00
Breast Cancer			
MCF7	-5.14	-4.60	-4.15
MDA-MB-231/ATCC	-4.92	> -4.00	> -4.00
HS 578T	> -4.00	> -4.00	> -4.00
BT-549	-5.81	-5.46	
T-47D	-5.79	-4.59	> -4.00
MDA-MB-468	-5.95	-5.51	-5.06
_MID	-5.19	-4.4	-4.07
Delta	1.65	2.13	0.99
Range	2.84	2.53	1.06



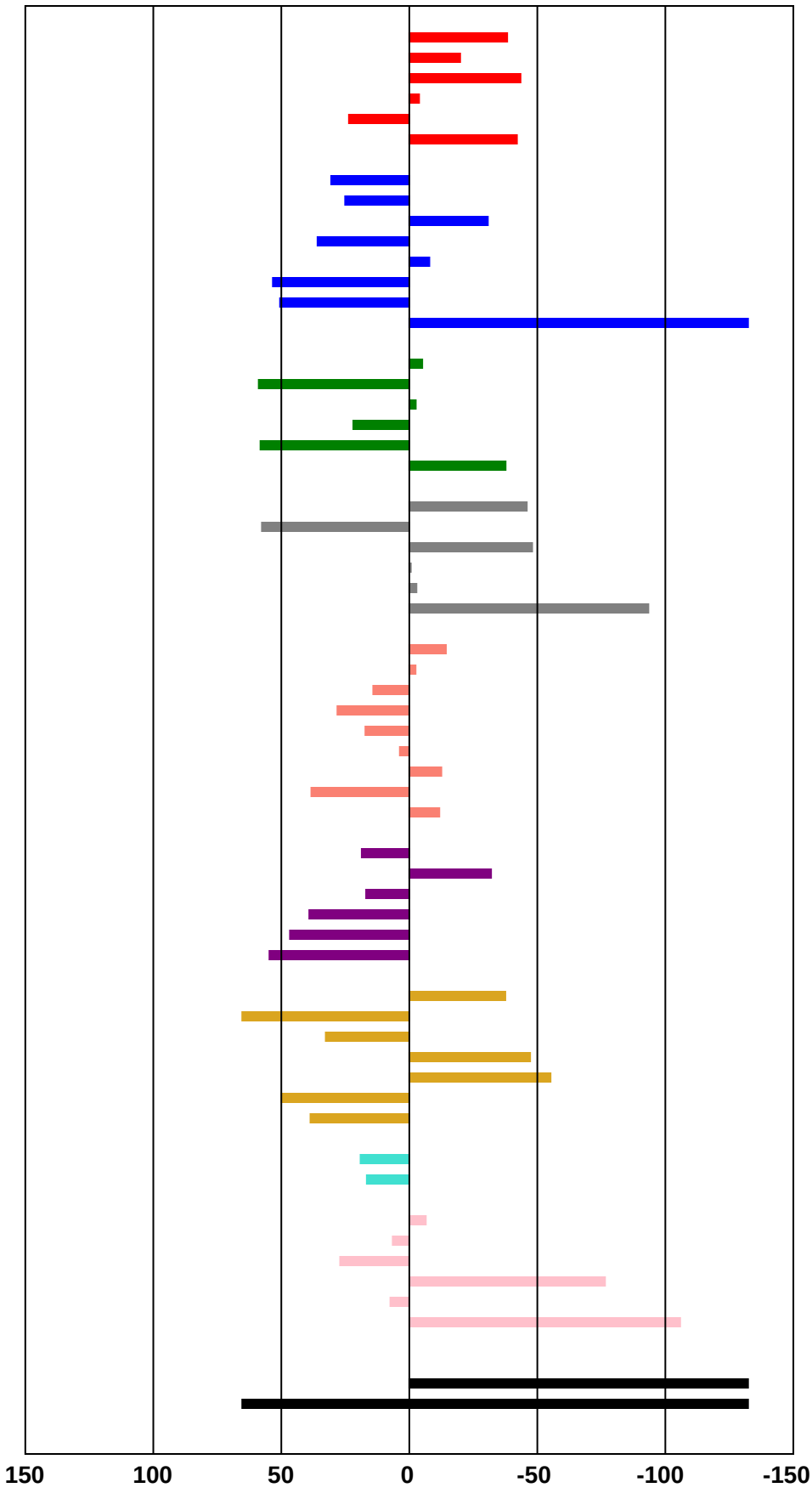
Developmental Therapeutics Program

One Dose Mean Graph

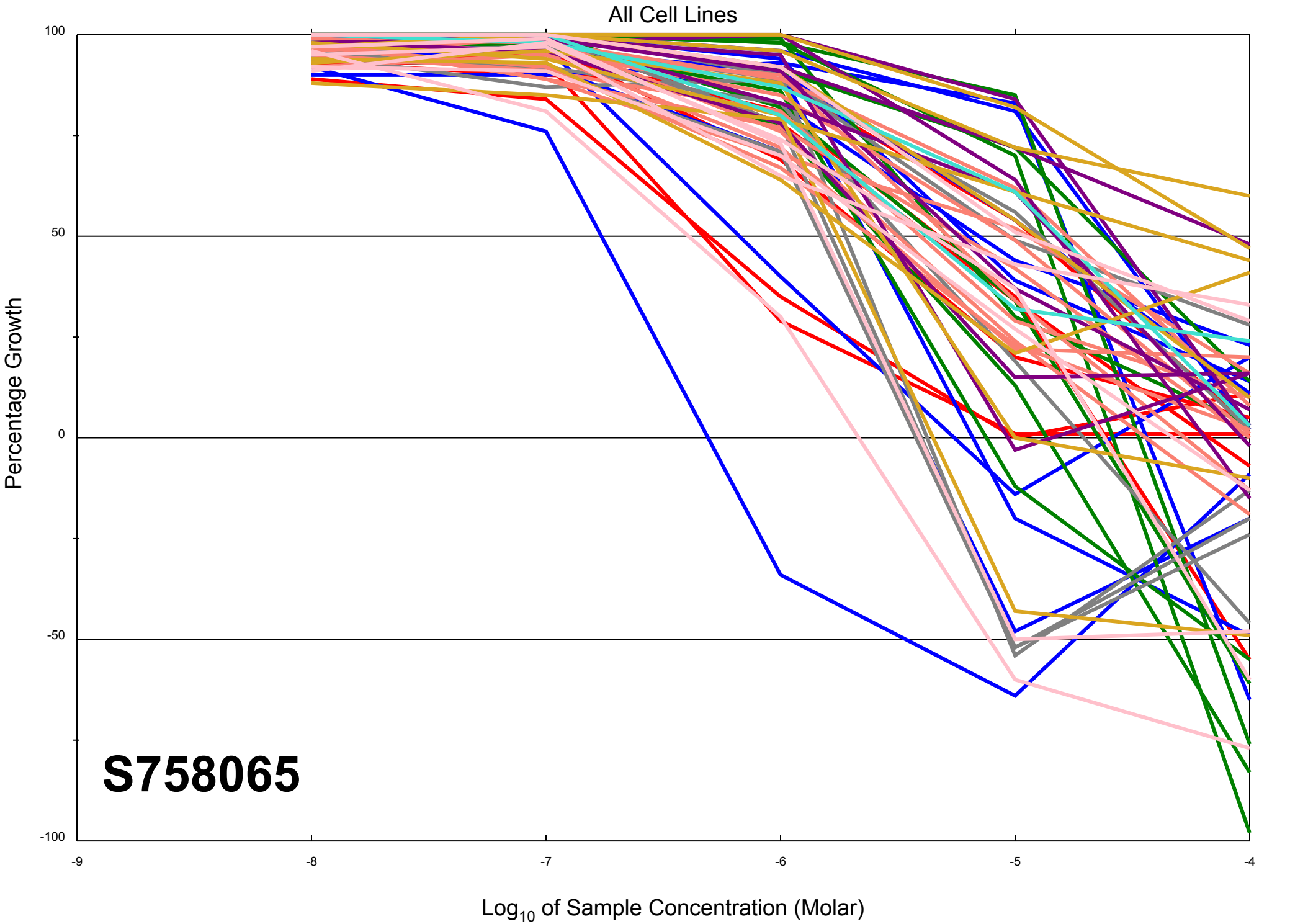
NSC: D-758065 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** May 02, 2011
Experiment ID: 1105OS43		**Report Date:** Jun 01, 2011

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	9.71
HL-60(TB)	28.09
K-562	4.51
MOLT-4	44.13
RPMI-8226	71.52
SR	5.91
Non-Small Cell Lung Cancer	
A549/ATCC	78.45
EKVX	73.00
HOP-62	17.27
HOP-92	83.78
NCI-H23	40.12
NCI-H322M	101.22
NCI-H460	98.43
NCI-H522	-84.36
Colon Cancer	
COLO 205	42.89
HCC-2998	106.75
HCT-116	45.43
HCT-15	69.81
KM12	106.07
SW-620	10.34
CNS Cancer	
SF-268	2.06
SF-295	105.50
SF-539	-0.04
SNB-19	47.36
SNB-75	45.16
U251	-45.44
Melanoma	
LOX IMVI	33.65
MALME-3M	45.51
M14	62.03
MDA-MB-435	76.02
SK-MEL-2	65.09
SK-MEL-28	51.64
SK-MEL-5	35.43
UACC-257	86.20
UACC-62	36.22
Ovarian Cancer	
IGROV1	66.51
OVCAR-3	16.01
OVCAR-4	64.81
OVCAR-8	87.01
NCI/ADR-RES	94.55
SK-OV-3	102.57
Renal Cancer	
786-0	10.44
A498	113.19
CAKI-1	80.57
RXF 393	0.75
SN12C	-7.22
TK-10	97.85
UO-31	86.55
Prostate Cancer	
PC-3	66.98
DU-145	64.54
Breast Cancer	
MCF7	41.50
MDA-MB-231/ATCC	54.41
HS 578T	74.95
BT-549	-28.50
T-47D	55.33
MDA-MB-468	-57.85
Mean	47.94
Delta	132.30
Range	197.55

Mean Growth Percent - Growth Percent



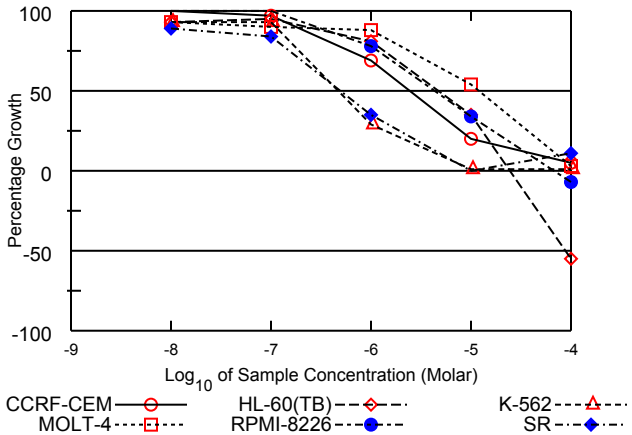
National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 758065/1	SSPL:0X1V	EXP. ID:1108RS14
	Report Date:October 25, 2011	Test Date:August 29, 2011	



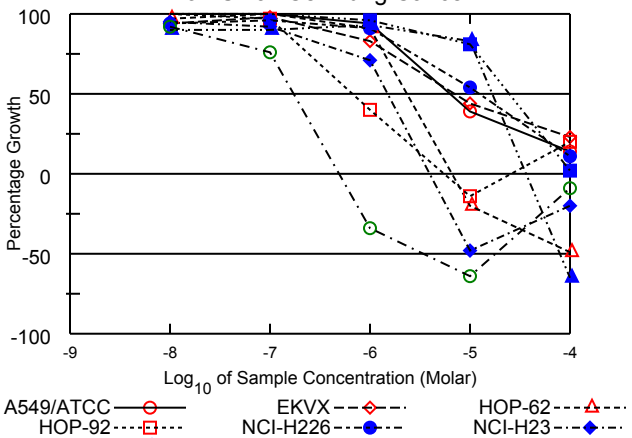
National Cancer Institute Developmental Therapeutics Program
Dose Response Curves

NSC: D - 758065 / 1	SSPL: 0X1V	EXP. ID: 1108RS14
Report Date: October 25, 2011	Test Date: August 29, 2011	

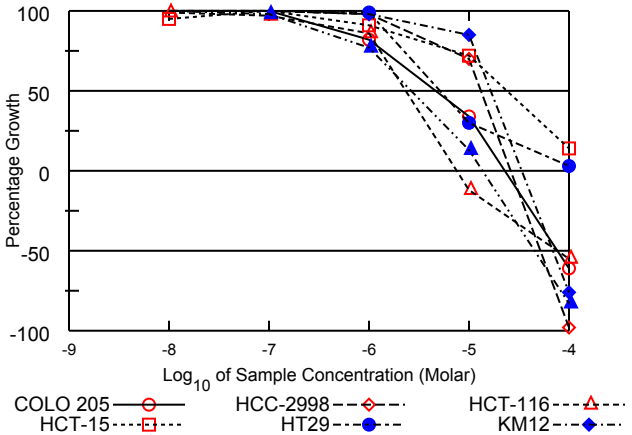
Leukemia



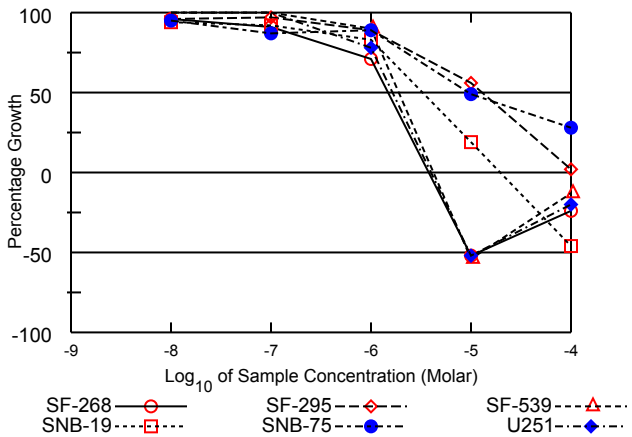
Non-Small Cell Lung Cancer



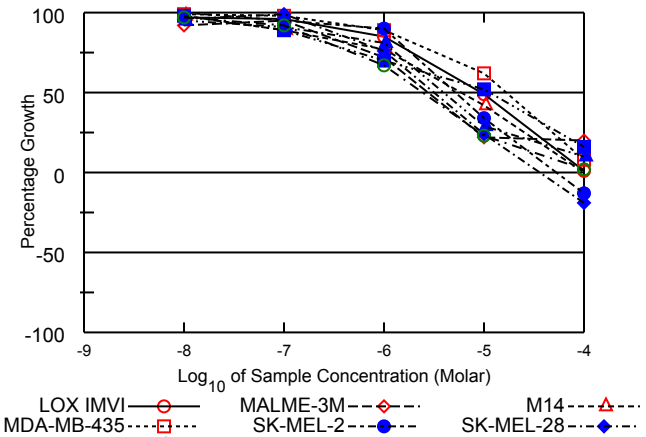
Colon Cancer



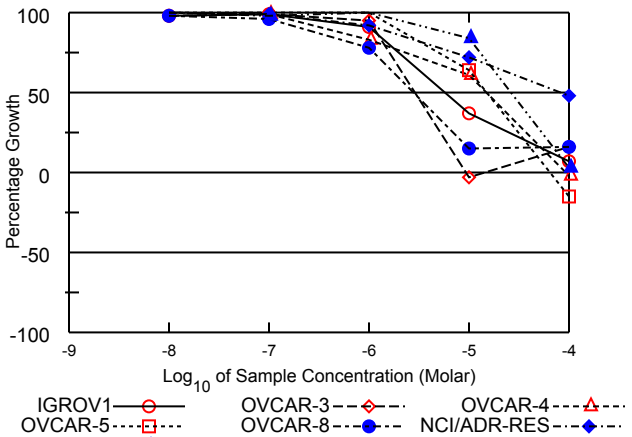
CNS Cancer



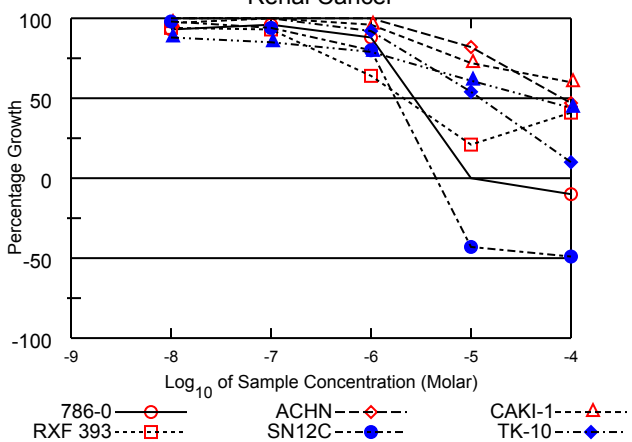
Melanoma



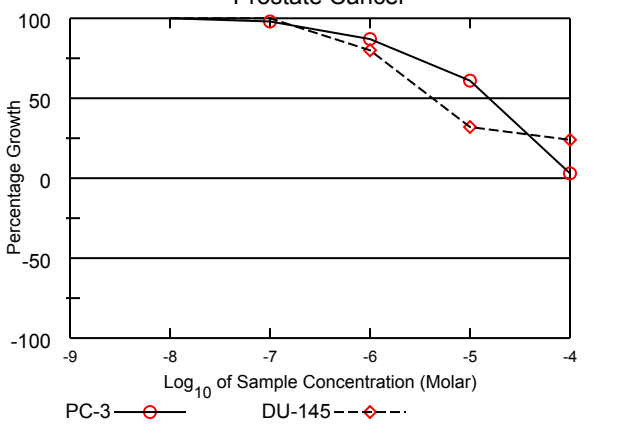
Ovarian Cancer



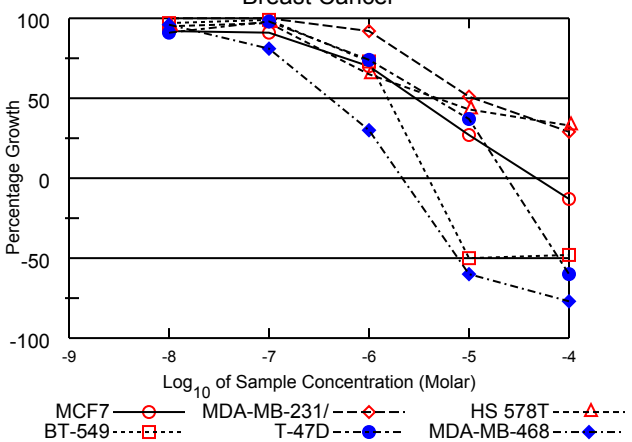
Renal Cancer



Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 758065 / 1	Experiment ID : 1108RS14	Test Type : 08	Units : Molar
Report Date : October 25, 2011	Test Date : August 29, 2011	QNS :	MC :
COMI : KA_aumacro_Bu (104506)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0X1V	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.553	2.031	2.027	1.983	1.580	0.853	0.632	100	97	69	20	5	2.48E-6	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.793	2.566	2.435	2.472	2.225	1.418	0.357	93	95	81	35	-55	4.74E-6	2.46E-5	8.79E-5
K-562	0.213	1.644	1.537	1.545	0.635	0.232	0.232	93	93	29	1	1	4.76E-7	> 1.00E-4	> 1.00E-4
MOLT-4	0.528	1.951	1.851	1.806	1.786	1.302	0.573	93	90	88	54	3	1.22E-5	> 1.00E-4	> 1.00E-4
RPMI-8226	0.970	2.157	2.156	2.201	1.901	1.378	0.903	100	104	78	34	-7	4.42E-6	6.79E-5	> 1.00E-4
SR	0.302	1.331	1.220	1.167	0.663	0.307	0.417	89	84	35	.	11	4.95E-7	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.320	1.524	1.539	1.562	1.450	0.789	0.492	101	103	94	39	14	6.29E-6	> 1.00E-4	> 1.00E-4
EKVX	0.621	1.652	1.591	1.633	1.475	1.079	0.860	94	98	83	44	23	7.17E-6	> 1.00E-4	> 1.00E-4
HOP-62	0.390	1.110	1.087	1.119	1.048	0.311	0.198	97	101	91	-20	-49	2.35E-6	6.58E-6	> 1.00E-4
HOP-92	0.929	1.354	1.376	1.341	1.099	0.803	1.013	105	97	40	-14	20	6.65E-7	.	> 1.00E-4
NCI-H226	0.775	1.919	1.854	1.870	1.814	1.390	0.900	94	96	91	54	11	1.22E-5	> 1.00E-4	> 1.00E-4
NCI-H23	0.531	1.416	1.373	1.341	1.160	0.278	0.424	95	92	71	-48	-20	1.50E-6	3.97E-6	> 1.00E-4
NCI-H322M	0.695	1.755	1.644	1.651	1.679	1.574	0.240	90	90	93	83	-65	1.67E-5	3.62E-5	7.87E-5
NCI-H460	0.228	2.102	2.147	2.137	2.028	1.744	0.274	102	102	96	81	2	2.48E-5	> 1.00E-4	> 1.00E-4
NCI-H522	0.816	1.573	1.516	1.394	0.535	0.291	0.746	92	76	-34	-64	-9	1.73E-7	4.89E-7	.
Colon Cancer															
COLO 205	0.277	1.211	1.277	1.224	1.041	0.596	0.108	107	101	82	34	-61	4.64E-6	2.28E-5	7.63E-5
HCC-2998	0.476	1.539	1.548	1.545	1.519	1.225	0.011	101	101	98	70	-98	1.32E-5	2.62E-5	5.20E-5
HCT-116	0.167	1.282	1.270	1.246	1.121	0.147	0.076	99	97	86	-12	-55	2.31E-6	7.54E-6	7.73E-5
HCT-15	0.319	1.657	1.595	1.737	1.540	1.281	0.510	95	106	91	72	14	2.40E-5	> 1.00E-4	> 1.00E-4
HT29	0.171	0.840	0.885	0.908	0.833	0.371	0.190	107	110	99	30	3	5.11E-6	> 1.00E-4	> 1.00E-4
KM12	0.380	2.135	2.154	2.142	2.101	1.864	0.092	101	100	98	85	-76	1.64E-5	3.36E-5	6.89E-5
SW-620	0.207	1.537	1.539	1.517	1.229	0.376	0.036	100	98	77	13	-83	2.62E-6	1.36E-5	4.55E-5
CNS Cancer															
SF-268	0.378	1.420	1.382	1.330	1.117	0.182	0.288	96	91	71	-52	-24	1.48E-6	3.78E-6	.
SF-295	0.643	2.377	2.314	2.319	2.181	1.618	0.683	96	97	89	56	2	1.30E-5	> 1.00E-4	> 1.00E-4
SF-539	0.631	1.751	1.782	1.781	1.635	0.290	0.551	103	103	90	-54	-13	1.89E-6	4.21E-6	.
SNB-19	0.538	1.842	1.763	1.733	1.619	0.787	0.290	94	92	83	19	-46	3.28E-6	1.96E-5	> 1.00E-4
SNB-75	0.946	1.825	1.783	1.709	1.731	1.381	1.189	95	87	89	49	28	9.71E-6	> 1.00E-4	> 1.00E-4
U251	0.421	1.761	1.816	1.780	1.464	0.201	0.336	104	101	78	-52	-20	1.64E-6	3.97E-6	.
Melanoma															
LOX IMVI	0.334	1.993	1.935	1.921	1.742	1.153	0.344	97	96	85	49	1	9.58E-6	> 1.00E-4	> 1.00E-4
MALME-3M	0.504	1.236	1.179	1.197	1.031	0.668	0.648	92	95	72	22	20	2.77E-6	> 1.00E-4	> 1.00E-4
M14	0.359	1.145	1.130	1.062	0.961	0.687	0.363	98	89	77	42	.	5.79E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.454	1.922	1.900	1.889	1.766	1.370	0.567	99	98	89	62	8	1.69E-5	> 1.00E-4	> 1.00E-4
SK-MEL-2	0.883	1.288	1.287	1.270	1.250	1.023	0.772	100	95	90	34	-13	5.28E-6	5.39E-5	> 1.00E-4
SK-MEL-28	0.508	1.455	1.419	1.450	1.231	0.736	0.414	96	99	76	24	-19	3.18E-6	3.66E-5	> 1.00E-4
SK-MEL-5	0.474	2.749	2.628	2.551	2.312	1.131	0.704	95	91	81	29	10	3.92E-6	> 1.00E-4	> 1.00E-4
UACC-257	0.806	1.753	1.731	1.649	1.465	1.294	0.956	98	89	70	52	16	1.11E-5	> 1.00E-4	> 1.00E-4
UACC-62	0.730	2.427	2.384	2.292	1.868	1.112	0.766	97	92	67	23	2	2.41E-6	> 1.00E-4	> 1.00E-4
Ovarian Cancer															
IGROV1	0.490	1.901	1.877	1.891	1.777	1.007	0.593	98	99	91	37	7	5.68E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.439	1.521	1.504	1.508	1.465	0.424	0.612	98	99	95	-3	16	2.86E-6	.	> 1.00E-4
OVCAR-4	0.554	1.374	1.394	1.366	1.234	1.054	0.541	103	99	83	61	-2	1.49E-5	9.15E-5	> 1.00E-4
OVCAR-5	0.497	1.419	1.466	1.416	1.436	1.091	0.421	105	100	102	64	-15	1.51E-5	6.41E-5	> 1.00E-4
OVCAR-8	0.321	1.530	1.511	1.486	1.265	0.499	0.517	98	96	78	15	16	2.77E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.478	1.629	1.629	1.617	1.542	1.311	1.027	100	99	92	72	48	8.08E-5	> 1.00E-4	> 1.00E-4
SK-OV-3	0.444	1.230	1.230	1.212	1.262	1.105	0.465	100	98	104	84	3	2.62E-5	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.626	2.056	1.952	2.002	1.880	0.625	0.564	93	96	88	.	-10	2.68E-6	9.96E-6	> 1.00E-4
ACHN	0.380	1.412	1.444	1.411	1.442	1.225	0.862	103	100	103	82	47	8.04E-5	> 1.00E-4	> 1.00E-4
CAKI-1	0.601	2.088	2.044	2.119	2.021	1.666	1.494	97	102	96	72	60	> 1.00E-4	> 1.00E-4	> 1.00E-4
RXF 393	0.635	1.228	1.195	1.190	1.017	0.762	0.877	94	93	64	21	41	2.16E-6	> 1.00E-4	> 1.00E-4
SN12C	0.497	2.089	2.060	1.995	1.772	0.283	0.254	98	94	80	-43	-49	1.75E-6	4.47E-6	> 1.00E-4
TK-10	0.557	1.178	1.206	1.210	1.127	0.890	0.622	105	105	92	54	10	1.21E-5	> 1.00E-4	> 1.00E-4
UO-31	0.604	1.713	1.580	1.542	1.481	1.280	1.094	88	85	79	61	44	4.51E-5	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.452	1.552	1.561	1.526	1.407	1.122	0.484	101	98	87	61	3	1.54E-5	> 1.00E-4	> 1.00E-4
DU-145	0.242	1.023	1.031	1.028	0.868	0.489	0.428	101	101	80	32	24	4.17E-6	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.357	2.079	1.934	1.916	1.569	0.828	0.311	92	91	70	27	-13	2.97E-6	4.76E-5	> 1.00E-4
MDA-MB-231/ATCC	0.618	1.813	1.881	1.818	1.722	1.225	0.967	106	100	92	51	29	1.09E-5	> 1.00E-4	> 1.00E-4
HS 578T	0.775	1.521	1.484	1.499	1.260	1.095	1.022	95	97	65	43	33	4.75E-6	> 1.00E-4	> 1.00E-4
BT-549	0.850	1.543	1.524	1.538	1.356	0.425	0.445	97	99	73	-50	-48	1.54E-6	3.92E-6	> 1.00E-4
T-47D	0.377	0.845	0.805	0.838	0.723	0.548	0.150	91	98	74	37	-60	4.37E-6	2.38E-5	7.82E-5
MDA-MB-468	0.571	1.179	1.157	1.062	0.752	0.226	0.130	96	81	30	-60	-77	4.01E-7	2.14E-6	7.66E-6

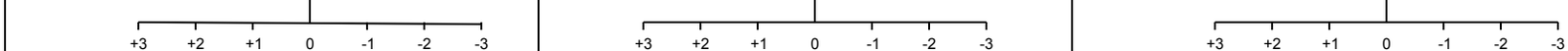
National Cancer Institute Developmental Therapeutics Program

Mean Graphs

NSC : D - 758065/1 | Units :Molar | SSPL :0X1V | EXP. ID :1108RS14

Report Date :October 25, 2011 | Test Date :August 29, 2011

Panel/Cell Line	Log_{10}GI50	GI50	Log_{10}TGI	TGI	Log_{10}LC50	LC50
Leukemia						
CCRF-CEM	-5.60		> -4.00		> -4.00	
HL-60(TB)	-5.32		-4.61		-4.06	
K-562	-6.32		> -4.00		> -4.00	
MOLT-4	-4.91		> -4.00		> -4.00	
RPMI-8226	-5.35		-4.17		> -4.00	
SR	-6.31		> -4.00		> -4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	-5.20		> -4.00		> -4.00	
EKVX	-5.14		> -4.00		> -4.00	
HOP-62	-5.63		-5.18		> -4.00	
HOP-92	-6.18				> -4.00	
NCI-H226	-4.91		> -4.00		> -4.00	
NCI-H23	-5.82		-5.40		> -4.00	
NCI-H322M	-4.78		-4.44		-4.10	
NCI-H460	-4.61		> -4.00		> -4.00	
NCI-H522	-6.76		-6.31			
Colon Cancer						
COLO 205	-5.33		-4.64		-4.12	
HCC-2998	-4.88		-4.58		-4.28	
HCT-116	-5.64		-5.12		-4.11	
HCT-15	-4.62		> -4.00		> -4.00	
HT29	-5.29		> -4.00		> -4.00	
KM12	-4.78		-4.47		-4.16	
SW-620	-5.58		-4.87		-4.34	
CNS Cancer						
SF-268	-5.83		-5.42			
SF-295	-4.88		> -4.00		> -4.00	
SF-539	-5.72		-5.38			
SNB-19	-5.48		-4.71		> -4.00	
SNB-75	-5.01		> -4.00		> -4.00	
U251	-5.79		-5.40			
Melanoma						
LOX IMVI	-5.02		> -4.00		> -4.00	
MALME-3M	-5.56		> -4.00		> -4.00	
M14	-5.24		> -4.00		> -4.00	
MDA-MB-435	-4.77		> -4.00		> -4.00	
SK-MEL-2	-5.28		-4.27		> -4.00	
SK-MEL-28	-5.50		-4.44		> -4.00	
SK-MEL-5	-5.41		> -4.00		> -4.00	
UACC-257	-4.96		> -4.00		> -4.00	
UACC-62	-5.62		> -4.00		> -4.00	
Ovarian Cancer						
IGROV1	-5.25		> -4.00		> -4.00	
OVCAR-3	-5.54				> -4.00	
OVCAR-4	-4.83		-4.04		> -4.00	
OVCAR-5	-4.82		-4.19		> -4.00	
OVCAR-8	-5.56		> -4.00		> -4.00	
NCI/ADR-RES	-4.09		> -4.00		> -4.00	
SK-OV-3	-4.58		> -4.00		> -4.00	
Renal Cancer						
786-0	-5.57		-5.00		> -4.00	
ACHN	-4.09		> -4.00		> -4.00	
CAKI-1	> -4.00		> -4.00		> -4.00	
RXF 393	-5.67		> -4.00		> -4.00	
SN12C	-5.76		-5.35		> -4.00	
TK-10	-4.92		> -4.00		> -4.00	
UO-31	-4.35		> -4.00		> -4.00	
Prostate Cancer						
PC-3	-4.81		> -4.00		> -4.00	
DU-145	-5.38		> -4.00		> -4.00	
Breast Cancer						
MCF7	-5.53		-4.32		> -4.00	
MDA-MB-231/ATCC	-4.96		> -4.00		> -4.00	
HS 578T	-5.32		> -4.00		> -4.00	
BT-549	-5.81		-5.41		> -4.00	
T-47D	-5.36		-4.62		-4.11	
MDA-MB-468	-6.40		-5.67		-5.12	
_MID	-5.28		-4.39		-4.04	
Delta	1.48		1.92		1.08	
Range	2.76		2.31		1.12	



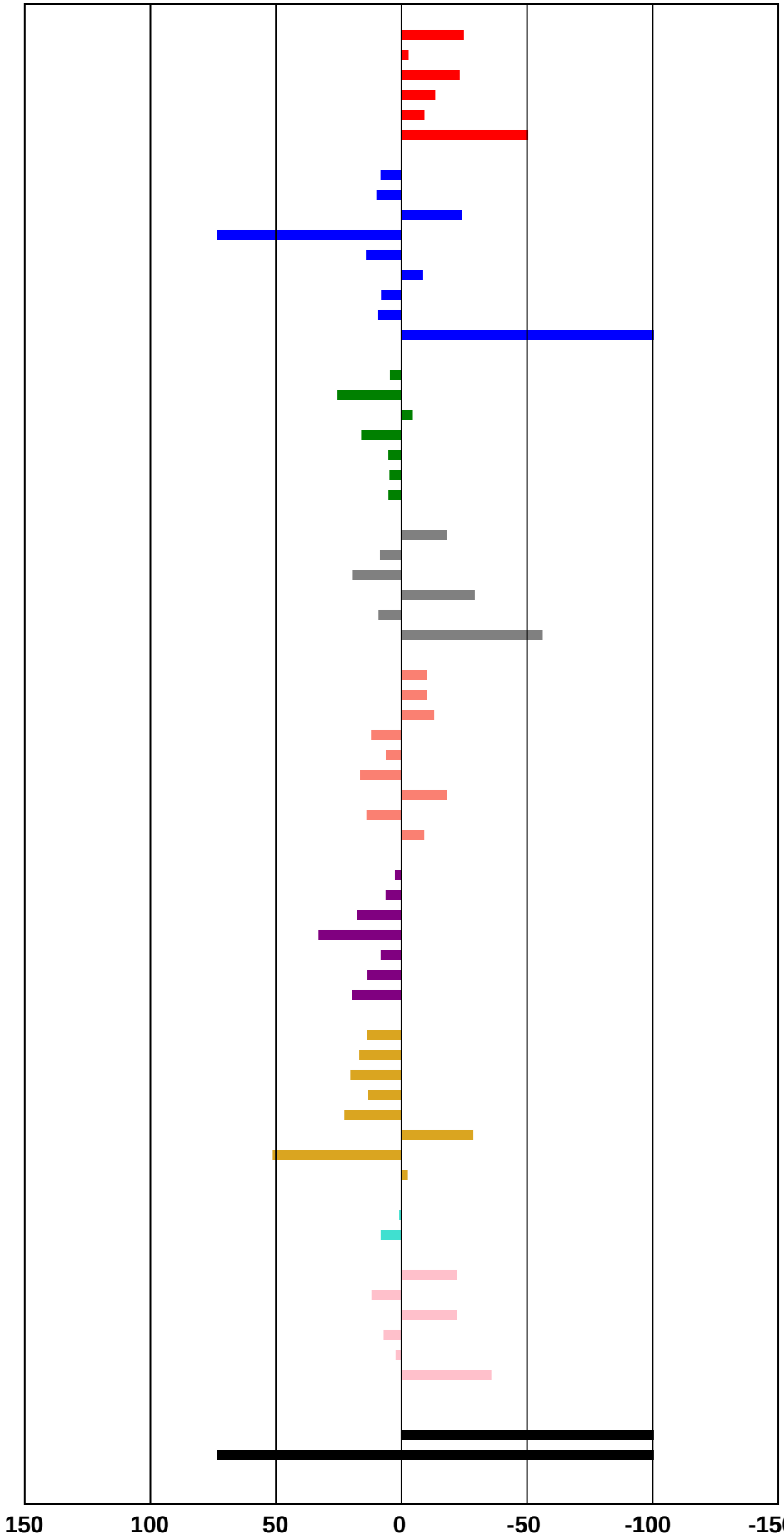
Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-762524 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** Nov 28, 2011
Experiment ID: 1111OS67		**Report Date:** Jan 11, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	60.56
HL-60(TB)	82.57
K-562	62.23
MOLT-4	71.99
RPMI-8226	76.27
SR	34.93
Non-Small Cell Lung Cancer	
A549/ATCC	93.14
EKVX	94.78
HOP-62	61.25
HOP-92	158.06
NCI-H226	98.94
NCI-H23	76.79
NCI-H322M	92.93
NCI-H460	94.03
NCI-H522	-15.08
Colon Cancer	
COLO 205	89.39
HCC-2998	110.23
HCT-116	80.90
HCT-15	100.84
HT29	90.00
KM12	89.58
SW-620	89.97
CNS Cancer	
SF-268	67.48
SF-295	93.36
SF-539	104.16
SNB-19	56.23
SNB-75	93.92
U251	29.16
Melanoma	
LOX IMVI	75.26
MALME-3M	75.24
M14	72.40
MDA-MB-435	96.92
SK-MEL-2	91.03
SK-MEL-28	101.30
SK-MEL-5	67.19
UACC-257	98.76
UACC-62	76.36
Ovarian Cancer	
IGROV1	87.39
OVCAR-3	91.10
OVCAR-4	102.56
OVCAR-5	117.80
OVCAR-8	93.08
NCI/ADR-RES	98.31
SK-OV-3	104.41
Renal Cancer	
786-0	98.37
A498	101.61
ACHN	105.17
CAKI-1	97.99
RXF 393	107.53
SN12C	56.82
TK-10	136.02
UO-31	82.86
Prostate Cancer	
PC-3	85.69
DU-145	93.07
Breast Cancer	
MCF7	63.33
MDA-MB-231/ATCC	96.76
HS 578T	63.28
BT-549	91.87
T-47D	87.12
MDA-MB-468	49.67
Mean	85.08
Delta	100.16
Range	173.14

Mean Growth Percent - Growth Percent



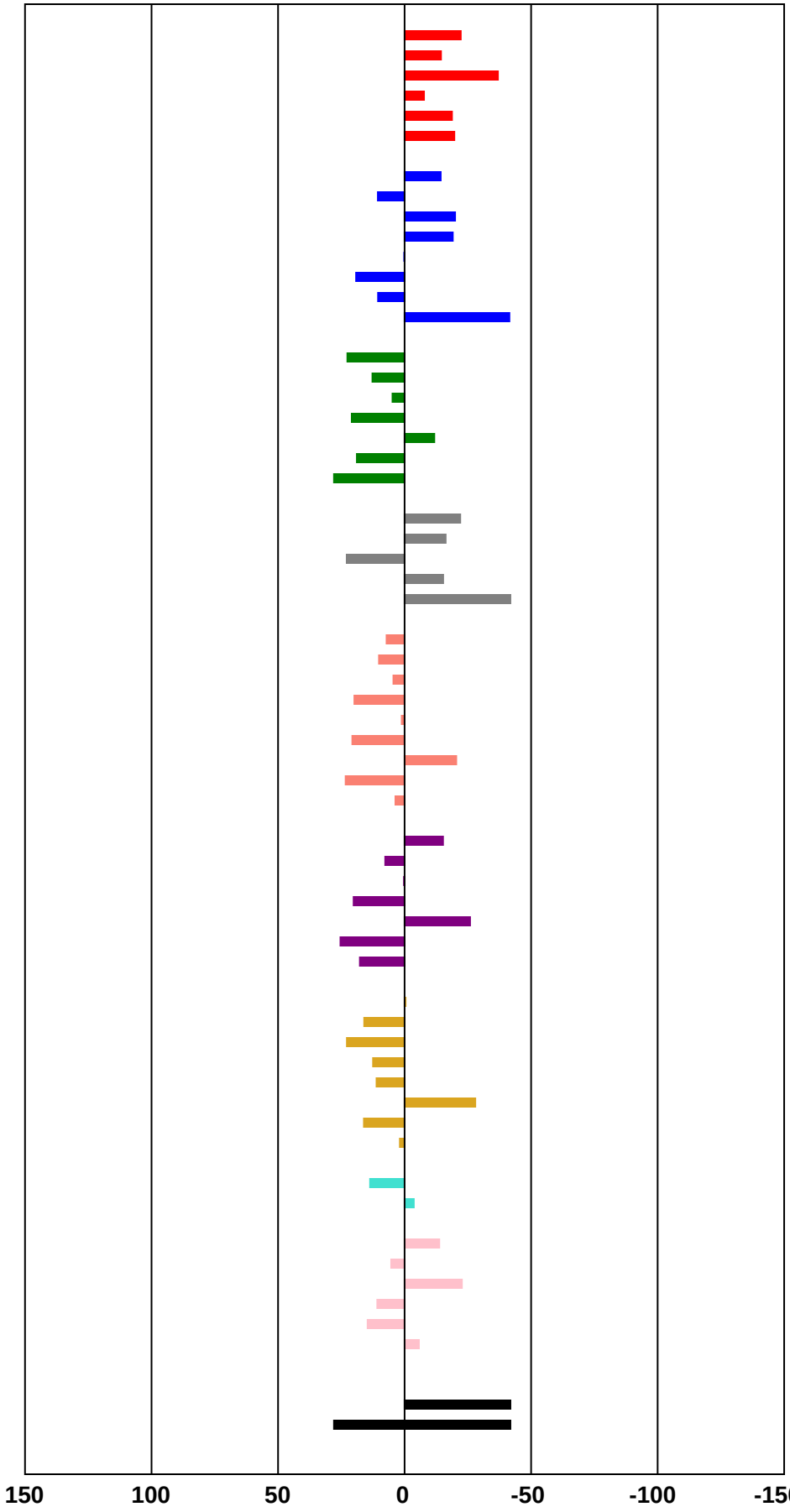
Developmental Therapeutics Program

One Dose Mean Graph

NSC: D-762525 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** Nov 28, 2011
Experiment ID: 1111OS67		**Report Date:** Jan 11, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	56.58
HL-60(TB)	64.39
K-562	41.89
MOLT-4	71.11
RPMI-8226	60.05
SR	59.12
Non-Small Cell Lung Cancer	
A549/ATCC	64.51
EKVX	89.34
HOP-62	58.82
NCI-H226	59.73
NCI-H23	78.90
NCI-H322M	97.94
NCI-H460	89.26
NCI-H522	37.36
Colon Cancer	
COLO 205	101.39
HCC-2998	91.49
HCT-116	83.56
HCT-15	99.66
HT29	67.04
KM12	97.64
SW-620	106.68
CNS Cancer	
SF-268	56.78
SF-295	62.55
SF-539	101.65
SNB-19	63.53
U251	36.96
Melanoma	
LOX IMVI	85.90
MALME-3M	88.90
M14	83.20
MDA-MB-435	98.62
SK-MEL-2	79.90
SK-MEL-28	99.43
SK-MEL-5	58.36
UACC-257	102.08
UACC-62	82.40
Ovarian Cancer	
IGROV1	63.59
OVCAR-3	86.43
OVCAR-4	79.00
OVCAR-5	98.92
OVCAR-8	52.90
NCI/ADR-RES	104.13
SK-OV-3	96.45
Renal Cancer	
786-0	78.38
A498	94.74
ACHN	101.58
CAKI-1	91.24
RXF 393	89.87
SN12C	50.84
TK-10	94.85
UO-31	80.64
Prostate Cancer	
PC-3	92.42
DU-145	75.14
Breast Cancer	
MCF7	65.07
MDA-MB-231/ATCC	84.07
HS 578T	56.14
BT-549	89.57
T-47D	93.39
MDA-MB-468	73.12
Mean	78.78
Delta	41.82
Range	69.72

Mean Growth Percent - Growth Percent



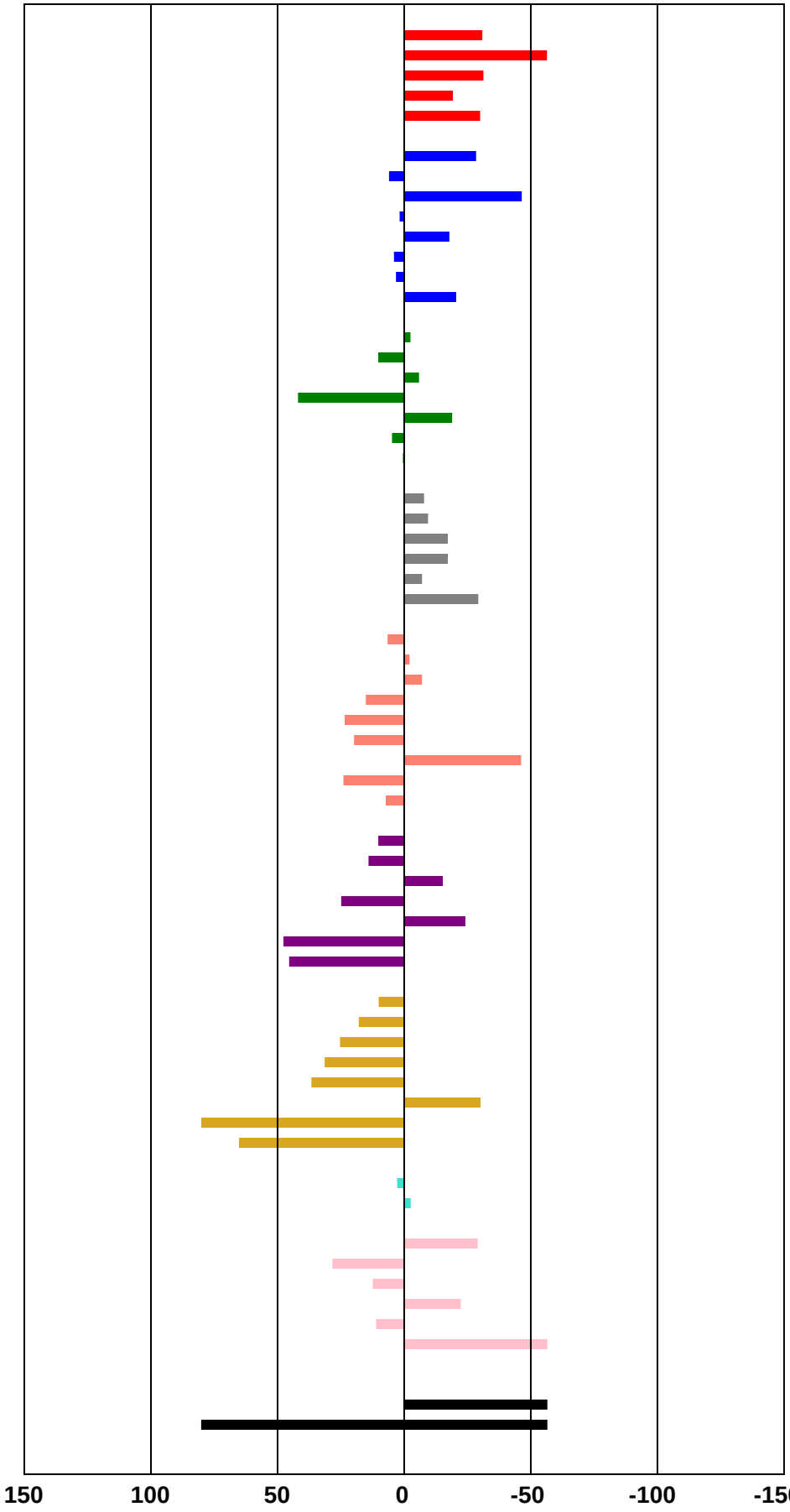
Developmental Therapeutics Program

One Dose Mean Graph

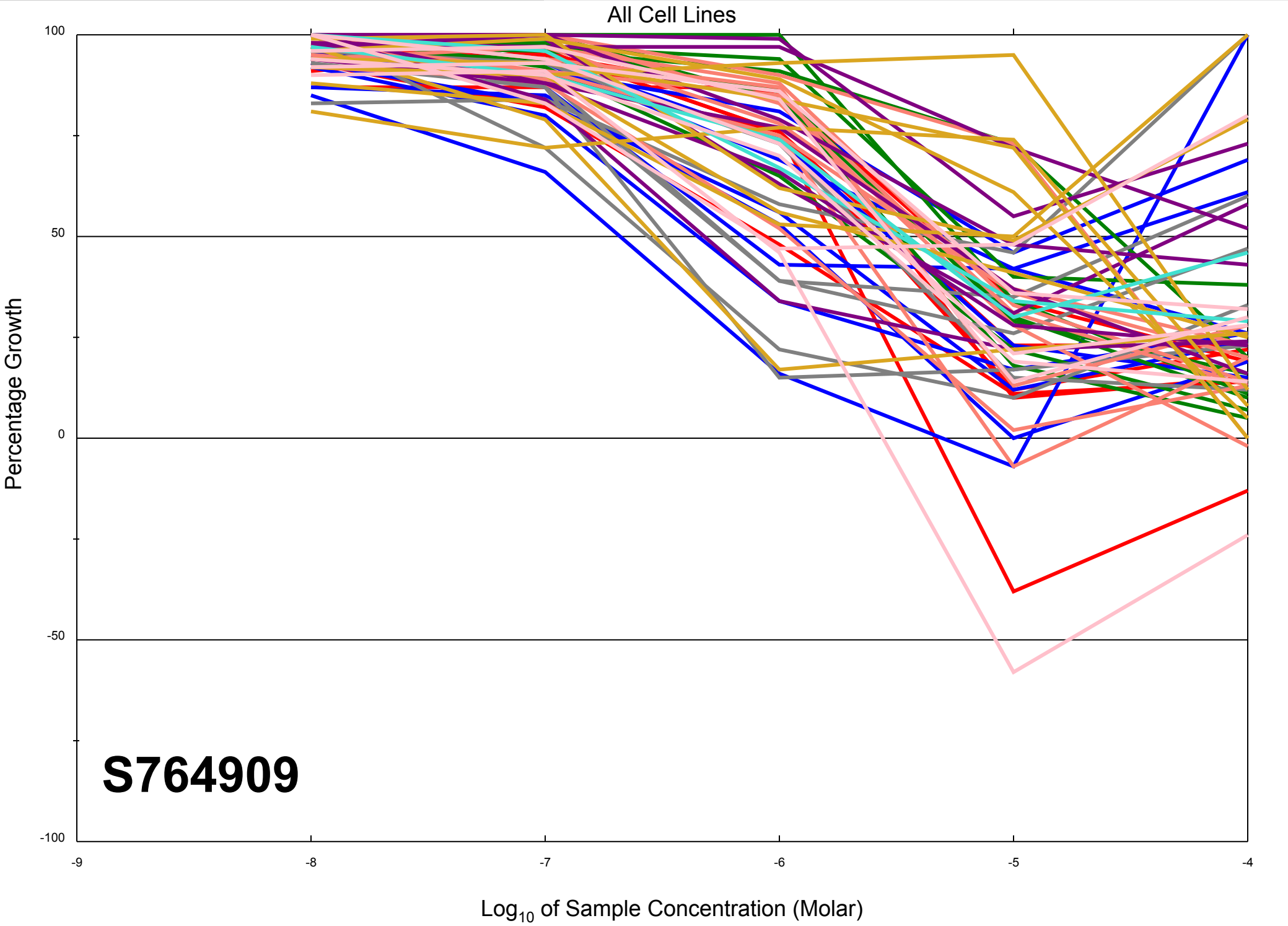
NSC: D-764909 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** May 07, 2012
Experiment ID: 1205OS68		**Report Date:** Jun 09, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	17.44
HL-60(TB)	-8.09
K-562	17.01
MOLT-4	29.05
RPMI-8226	18.31
Non-Small Cell Lung Cancer	
A549/ATCC	19.90
HOP-62	53.62
HOP-92	1.87
NCI-H226	49.44
NCI-H23	30.46
NCI-H322M	51.67
NCI-H460	50.88
NCI-H522	27.76
Colon Cancer	
COLO 205	45.80
HCC-2998	57.89
HCT-116	42.44
HCT-15	89.56
HT29	29.35
KM12	52.45
SW-620	48.13
CNS Cancer	
SF-268	40.45
SF-295	38.88
SF-539	31.08
SNB-19	31.07
SNB-75	41.24
U251	19.04
Melanoma	
LOX IMVI	54.19
MALME-3M	46.18
M14	41.25
MDA-MB-435	62.77
SK-MEL-2	71.12
SK-MEL-28	67.42
SK-MEL-5	2.13
UACC-257	71.61
UACC-62	54.93
Ovarian Cancer	
IGROV1	57.87
OVCAR-3	61.72
OVCAR-4	33.03
OVCAR-5	72.50
OVCAR-8	24.15
NCI/ADR-RES	95.31
SK-OV-3	93.06
Renal Cancer	
786-0	57.69
A498	65.58
ACHN	72.97
CAKI-1	79.04
RXF 393	84.27
SN12C	18.16
TK-10	127.80
UO-31	112.85
Prostate Cancer	
PC-3	50.41
DU-145	45.71
Breast Cancer	
MCF7	19.26
MDA-MB-231/ATCC	76.00
HS 578T	60.01
BT-549	25.94
T-47D	58.72
MDA-MB-468	-8.24
Mean	47.97
Delta	56.21
Range	136.04

Mean Growth Percent - Growth Percent



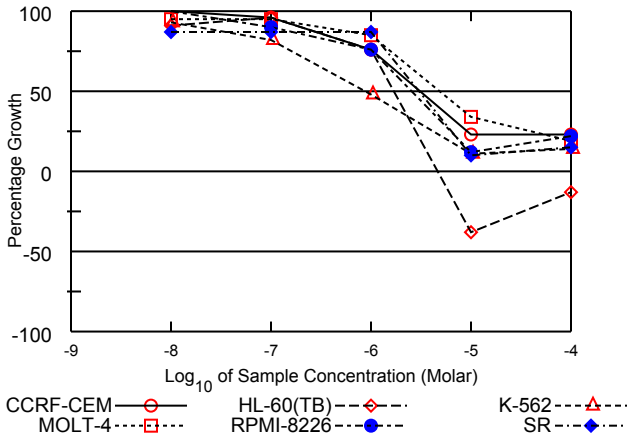
National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 764909/1	SSPL:0X1V	EXP. ID:1206NS96
	Report Date:September 25, 2012	Test Date:June 25, 2012	



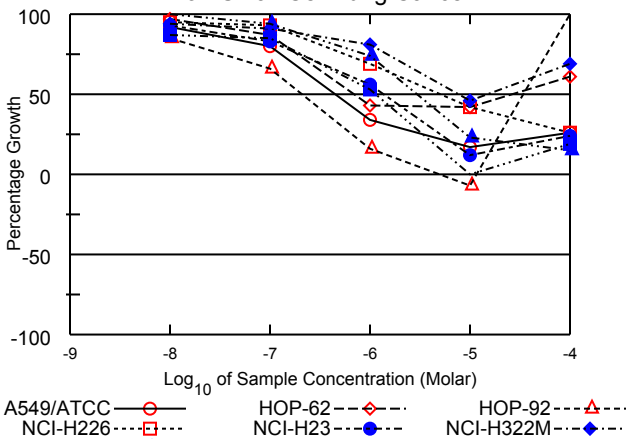
National Cancer Institute Developmental Therapeutics Program
Dose Response Curves

NSC: D - 764909 / 1	SSPL: 0X1V	EXP. ID: 1206NS96
Report Date: September 25, 2012	Test Date: June 25, 2012	

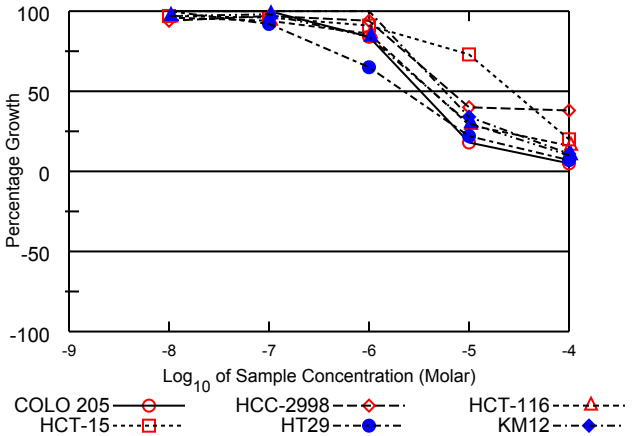
Leukemia



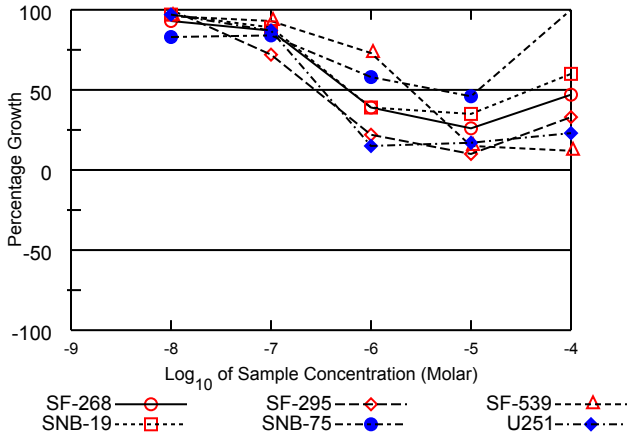
Non-Small Cell Lung Cancer



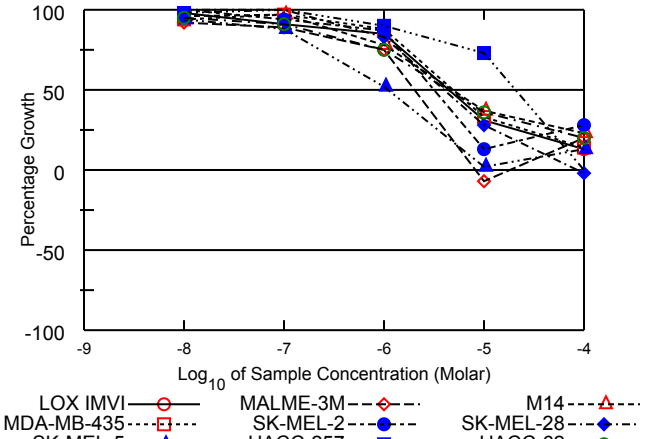
Colon Cancer



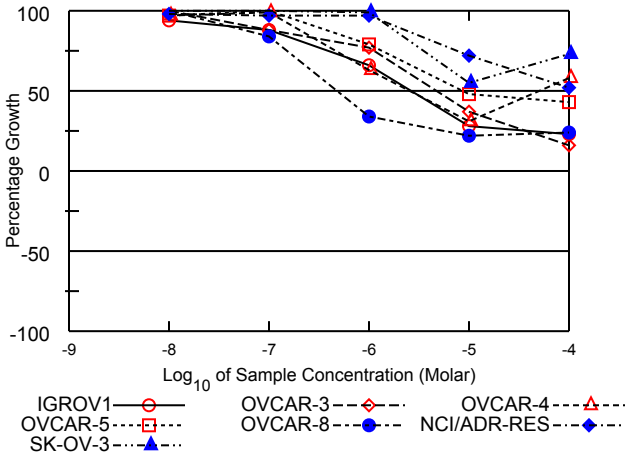
CNS Cancer



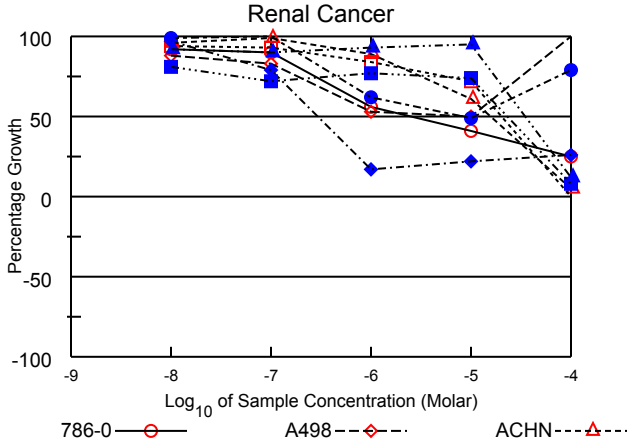
Melanoma



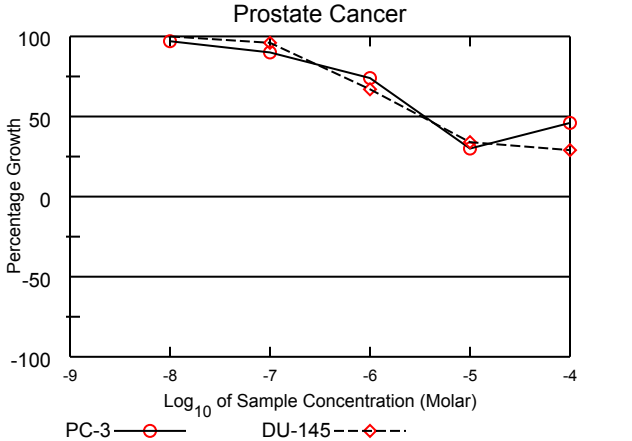
Ovarian Cancer



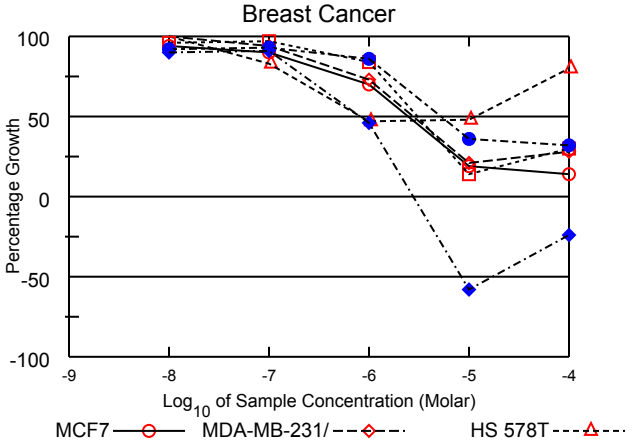
Renal Cancer



Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 764909 / 1	Experiment ID : 1206NS96	Test Type : 08	Units : Molar
Report Date : September 25, 2012	Test Date : June 25, 2012	QNS :	MC :
COMI : KA_AuMeMacro_Pr (117963)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0X1V	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.678	2.530	2.527	2.452	2.086	1.103	1.113	100	96	76	23	23	3.09E-6	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.781	3.004	2.795	2.905	2.471	0.486	0.678	91	96	76	-38	-13	1.69E-6	4.65E-6	> 1.00E-4
K-562	0.228	1.661	1.565	1.397	0.922	0.391	0.422	93	82	48	11	14	8.96E-7	> 1.00E-4	> 1.00E-4
MOLT-4	0.476	1.795	1.726	1.723	1.604	0.923	0.724	95	95	85	34	19	4.87E-6	> 1.00E-4	> 1.00E-4
RPMI-8226	0.800	2.173	2.176	2.034	1.838	0.959	1.104	100	90	76	12	22	2.51E-6	> 1.00E-4	> 1.00E-4
SR	0.354	1.788	1.599	1.596	1.605	0.497	0.567	87	87	87	10	15	3.03E-6	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.328	1.607	1.505	1.350	0.762	0.541	0.662	92	80	34	17	26	4.47E-7	> 1.00E-4	> 1.00E-4
HOP-62	0.271	0.828	0.812	0.756	0.509	0.507	0.611	97	87	43	42	61	.	> 1.00E-4	> 1.00E-4
HOP-92	1.262	1.561	1.516	1.460	1.309	1.171	1.732	85	66	16	-7	157	.	.	> 1.00E-4
NCI-H226	0.742	1.983	1.923	1.894	1.594	1.266	1.063	95	93	69	42	26	5.06E-6	> 1.00E-4	> 1.00E-4
NCI-H23	0.645	1.744	1.665	1.562	1.257	0.778	0.904	93	83	56	12	24	1.35E-6	> 1.00E-4	> 1.00E-4
NCI-H322M	0.687	1.466	1.421	1.396	1.315	1.046	1.226	94	91	81	46	69	.	> 1.00E-4	> 1.00E-4
NCI-H460	0.210	2.145	2.221	2.035	1.651	0.647	0.503	104	94	74	23	15	2.96E-6	> 1.00E-4	> 1.00E-4
NCI-H522	0.739	1.839	1.698	1.669	1.318	0.737	0.948	87	85	53	.	19	1.12E-6	.	> 1.00E-4
Colon Cancer															
COLO 205	0.219	0.979	0.981	1.018	0.857	0.353	0.261	100	105	84	18	5	3.25E-6	> 1.00E-4	> 1.00E-4
HCC-2998	0.919	2.669	2.560	2.625	2.573	1.622	1.585	94	97	94	40	38	6.58E-6	> 1.00E-4	> 1.00E-4
HCT-116	0.166	1.572	1.516	1.491	1.381	0.576	0.386	96	94	86	29	16	4.32E-6	> 1.00E-4	> 1.00E-4
HCT-15	0.218	1.606	1.562	1.545	1.484	1.226	0.499	97	96	91	73	20	2.70E-5	> 1.00E-4	> 1.00E-4
HT29	0.182	1.114	1.121	1.037	0.789	0.383	0.251	101	92	65	22	7	2.22E-6	> 1.00E-4	> 1.00E-4
KM12	0.600	2.569	2.594	2.579	2.576	1.266	0.815	101	101	100	34	11	5.71E-6	> 1.00E-4	> 1.00E-4
SW-620	0.239	1.789	1.747	1.756	1.546	0.706	0.389	97	98	84	30	10	4.30E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.611	1.755	1.680	1.607	1.053	0.912	1.149	93	87	39	26	47	5.83E-7	> 1.00E-4	> 1.00E-4
SF-295	0.615	1.524	1.583	1.273	0.819	0.710	0.915	107	72	22	10	33	2.81E-7	> 1.00E-4	> 1.00E-4
SF-539	0.847	2.245	2.188	2.151	1.870	1.059	1.009	96	93	73	15	12	2.51E-6	> 1.00E-4	> 1.00E-4
SNB-19	0.618	1.819	1.778	1.681	1.082	1.038	1.345	97	89	39	35	60	.	> 1.00E-4	> 1.00E-4
SNB-75	0.914	1.724	1.586	1.593	1.384	1.284	1.786	83	84	58	46	108	.	> 1.00E-4	> 1.00E-4
U251	0.389	1.757	1.715	1.578	0.599	0.621	0.708	97	87	15	17	23	3.28E-7	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.474	2.635	2.599	2.430	2.317	1.142	0.754	98	91	85	31	13	4.46E-6	> 1.00E-4	> 1.00E-4
MALME-3M	0.588	1.048	1.011	0.996	0.933	0.545	0.680	92	89	75	-7	20	2.01E-6	.	> 1.00E-4
M14	0.323	1.257	1.219	1.225	1.055	0.673	0.536	96	97	78	37	23	4.93E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.436	1.892	1.804	1.850	1.711	0.924	0.641	94	97	88	33	14	4.95E-6	> 1.00E-4	> 1.00E-4
SK-MEL-2	0.794	1.491	1.500	1.451	1.398	0.886	0.993	101	94	87	13	28	3.15E-6	> 1.00E-4	> 1.00E-4
SK-MEL-28	0.477	1.396	1.393	1.396	1.239	0.734	0.468	100	100	83	28	-2	3.97E-6	8.58E-5	> 1.00E-4
SK-MEL-5	0.503	2.482	2.359	2.249	1.524	0.543	0.759	94	88	52	2	13	1.08E-6	> 1.00E-4	> 1.00E-4
UACC-257	0.784	1.753	1.733	1.762	1.653	1.496	0.781	98	101	90	73	.	2.08E-5	9.86E-5	> 1.00E-4
UACC-62	0.708	2.194	2.120	2.059	1.818	1.245	1.009	95	91	75	36	20	4.37E-6	> 1.00E-4	> 1.00E-4
Ovarian Cancer															
IGROV1	0.668	1.671	1.614	1.549	1.334	0.949	0.895	94	88	66	28	23	2.67E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.509	1.500	1.518	1.377	1.276	0.880	0.664	102	88	77	37	16	4.85E-6	> 1.00E-4	> 1.00E-4
OVCAR-4	0.527	1.056	1.041	1.051	0.861	0.689	0.835	97	99	63	31	58	.	> 1.00E-4	> 1.00E-4
OVCAR-5	0.455	1.043	1.026	1.054	0.917	0.735	0.711	97	102	79	48	43	8.35E-6	> 1.00E-4	> 1.00E-4
OVCAR-8	0.367	1.459	1.467	1.282	0.735	0.610	0.634	101	84	34	22	24	4.72E-7	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.534	1.724	1.702	1.683	1.685	1.392	1.149	98	97	97	72	52	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-OV-3	0.532	1.268	1.284	1.322	1.263	0.938	1.071	102	107	99	55	73	> 1.00E-4	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.640	2.190	2.062	2.040	1.514	1.277	1.023	92	90	56	41	25	2.62E-6	> 1.00E-4	> 1.00E-4
A498	1.460	2.201	2.110	2.073	1.856	1.829	2.845	88	83	53	50	187	.	> 1.00E-4	> 1.00E-4
ACHN	0.302	1.133	1.104	1.122	1.041	0.811	0.343	96	99	89	61	5	1.58E-5	> 1.00E-4	> 1.00E-4
CAKI-1	0.660	1.966	1.891	1.877	1.760	1.606	0.666	94	93	84	72	.	2.05E-5	> 1.00E-4	> 1.00E-4
RXF 393	0.660	1.158	1.154	1.163	0.970	0.906	1.055	99	101	62	49	79	.	> 1.00E-4	> 1.00E-4
SN12C	0.521	1.936	1.890	1.644	0.762	0.828	0.885	97	79	17	22	26	2.96E-7	> 1.00E-4	> 1.00E-4
TK-10	0.495	1.080	1.032	1.021	1.039	1.048	0.567	92	90	93	95	12	3.48E-5	> 1.00E-4	> 1.00E-4
UO-31	0.712	1.754	1.561	1.468	1.519	1.488	0.797	81	72	77	74	8	2.34E-5	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.535	1.863	1.830	1.728	1.515	0.930	1.147	97	90	74	30	46	3.46E-6	> 1.00E-4	> 1.00E-4
DU-145	0.334	1.279	1.300	1.242	0.963	0.660	0.604	102	96	67	34	29	3.28E-6	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.489	2.148	2.054	1.976	1.651	0.812	0.715	94	90	70	19	14	2.49E-6	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.419	1.055	1.069	1.018	0.881	0.555	0.597	102	94	73	21	28	2.77E-6	> 1.00E-4	> 1.00E-4
HS 578T	1.127	2.010	2.054	1.862	1.546	1.548	1.838	105	83	47	48	80	.	> 1.00E-4	> 1.00E-4
BT-549	0.666	1.536	1.498	1.507	1.393	0.789	0.924	96	97	84	14	30	3.04E-6	> 1.00E-4	> 1.00E-4
T-47D	0.689	1.642	1.563	1.571	1.513	1.037	0.997	92	93	86	36	32	5.36E-6	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.608	1.392	1.312	1.320	0.970	0.257	0.463	90	91	46	-58	-24	8.21E-7	2.78E-6	.

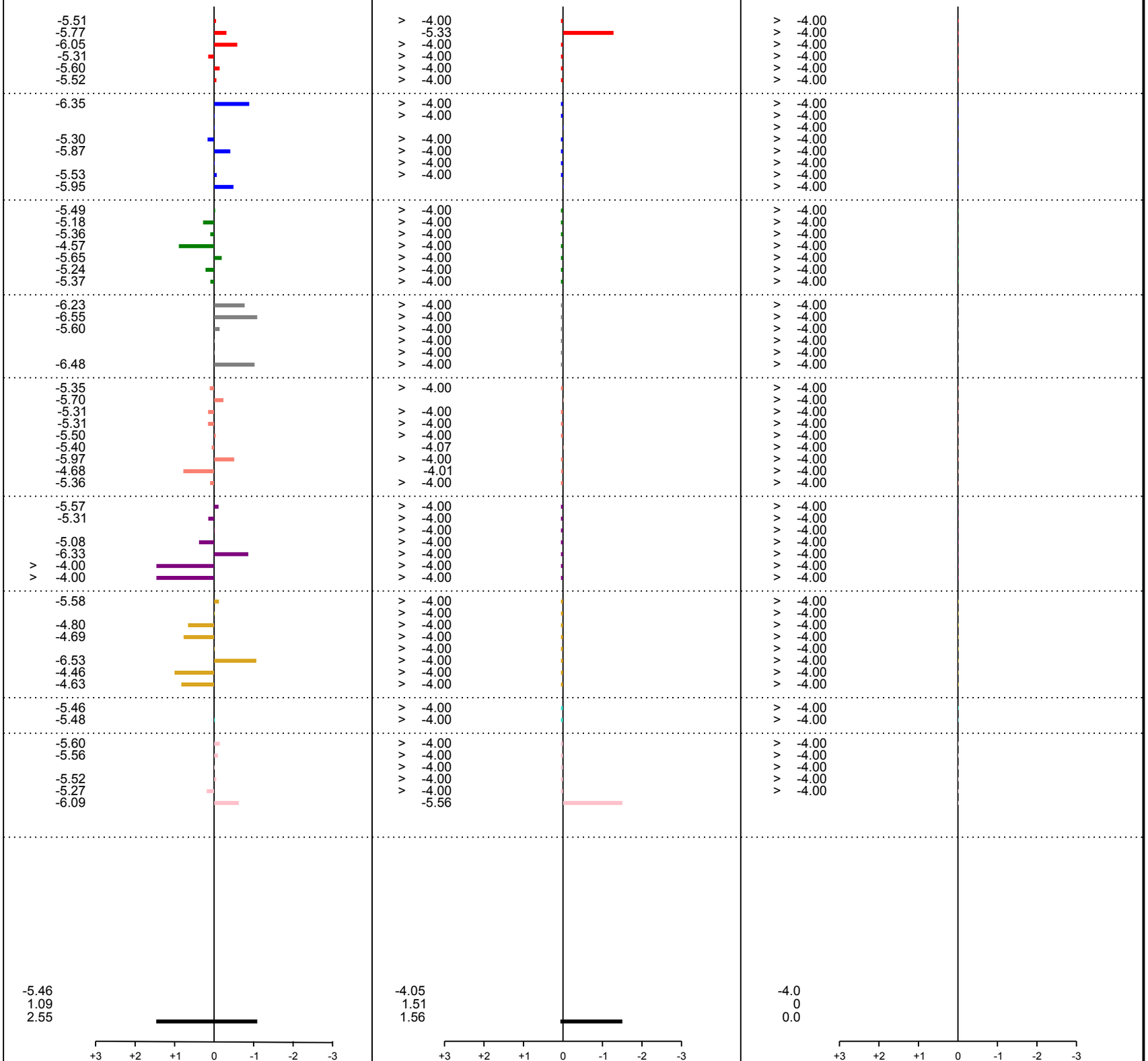
National Cancer Institute Developmental Therapeutics Program

Mean Graphs

NSC : D - 764909/1 | Units :Molar | SSPL :0X1V | EXP. ID :1206NS96

Report Date :September 25, 2012 | Test Date :June 25, 2012

Panel/Cell Line	Log_{10}GI50	Log_{10}TGI	Log_{10}LC50
Leukemia			
CCRF-CEM	-5.51	> -4.00	> -4.00
HL-60(TB)	-5.77	-5.33	> -4.00
K-562	-6.05	> -4.00	> -4.00
MOLT-4	-5.31	> -4.00	> -4.00
RPMI-8226	-5.60	> -4.00	> -4.00
SR	-5.52	> -4.00	> -4.00
Non-Small Cell Lung Cancer			
A549/ATCC	-6.35	> -4.00	> -4.00
HOP-62		> -4.00	> -4.00
HOP-92			> -4.00
NCI-H226	-5.30	> -4.00	> -4.00
NCI-H23	-5.87	> -4.00	> -4.00
NCI-H322M		> -4.00	> -4.00
NCI-H460	-5.53	> -4.00	> -4.00
NCI-H522	-5.95		> -4.00
Colon Cancer			
COLO 205	-5.49	> -4.00	> -4.00
HCC-2998	-5.18	> -4.00	> -4.00
HCT-116	-5.36	> -4.00	> -4.00
HCT-15	-4.57	> -4.00	> -4.00
HT29	-5.65	> -4.00	> -4.00
KM12	-5.24	> -4.00	> -4.00
SW-620	-5.37	> -4.00	> -4.00
CNS Cancer			
SF-268	-6.23	> -4.00	> -4.00
SF-295	-6.55	> -4.00	> -4.00
SF-539	-5.60	> -4.00	> -4.00
SNB-19		> -4.00	> -4.00
SNB-75		> -4.00	> -4.00
U251	-6.48	> -4.00	> -4.00
Melanoma			
LOX IMVI	-5.35	> -4.00	> -4.00
MALME-3M	-5.70		> -4.00
M14	-5.31	> -4.00	> -4.00
MDA-MB-435	-5.31	> -4.00	> -4.00
SK-MEL-2	-5.50	> -4.00	> -4.00
SK-MEL-28	-5.40	-4.07	> -4.00
SK-MEL-5	-5.97	> -4.00	> -4.00
UACC-257	-4.68	-4.01	> -4.00
UACC-62	-5.36	> -4.00	> -4.00
Ovarian Cancer			
IGROV1	-5.57	> -4.00	> -4.00
OVCAR-3	-5.31	> -4.00	> -4.00
OVCAR-4		> -4.00	> -4.00
OVCAR-5	-5.08	> -4.00	> -4.00
OVCAR-8	-6.33	> -4.00	> -4.00
NCI/ADR-RES	> -4.00	> -4.00	> -4.00
SK-OV-3	> -4.00	> -4.00	> -4.00
Renal Cancer			
786-0	-5.58	> -4.00	> -4.00
A498		> -4.00	> -4.00
ACHN	-4.80	> -4.00	> -4.00
CAKI-1	-4.69	> -4.00	> -4.00
RXF 393		> -4.00	> -4.00
SN12C	-6.53	> -4.00	> -4.00
TK-10	-4.46	> -4.00	> -4.00
UO-31	-4.63	> -4.00	> -4.00
Prostate Cancer			
PC-3	-5.46	> -4.00	> -4.00
DU-145	-5.48	> -4.00	> -4.00
Breast Cancer			
MCF7	-5.60	> -4.00	> -4.00
MDA-MB-231/ATCC	-5.56	> -4.00	> -4.00
HS 578T		> -4.00	> -4.00
BT-549	-5.52	> -4.00	> -4.00
T-47D	-5.27	> -4.00	> -4.00
MDA-MB-468	-6.09	-5.56	
_MID	-5.46	-4.05	-4.0
Delta	1.09	1.51	0
Range	2.55	1.56	0.0



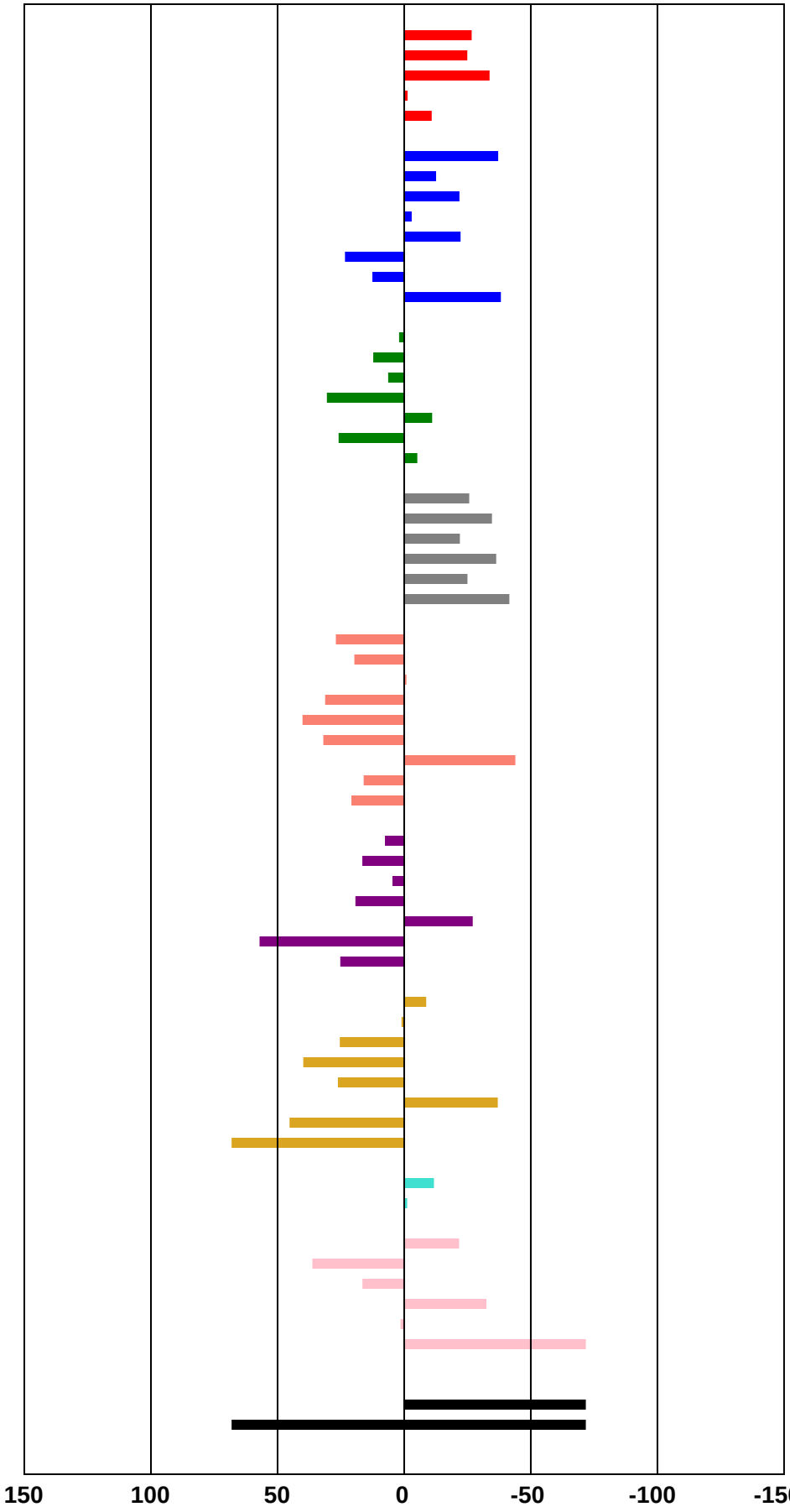
Developmental Therapeutics Program

One Dose Mean Graph

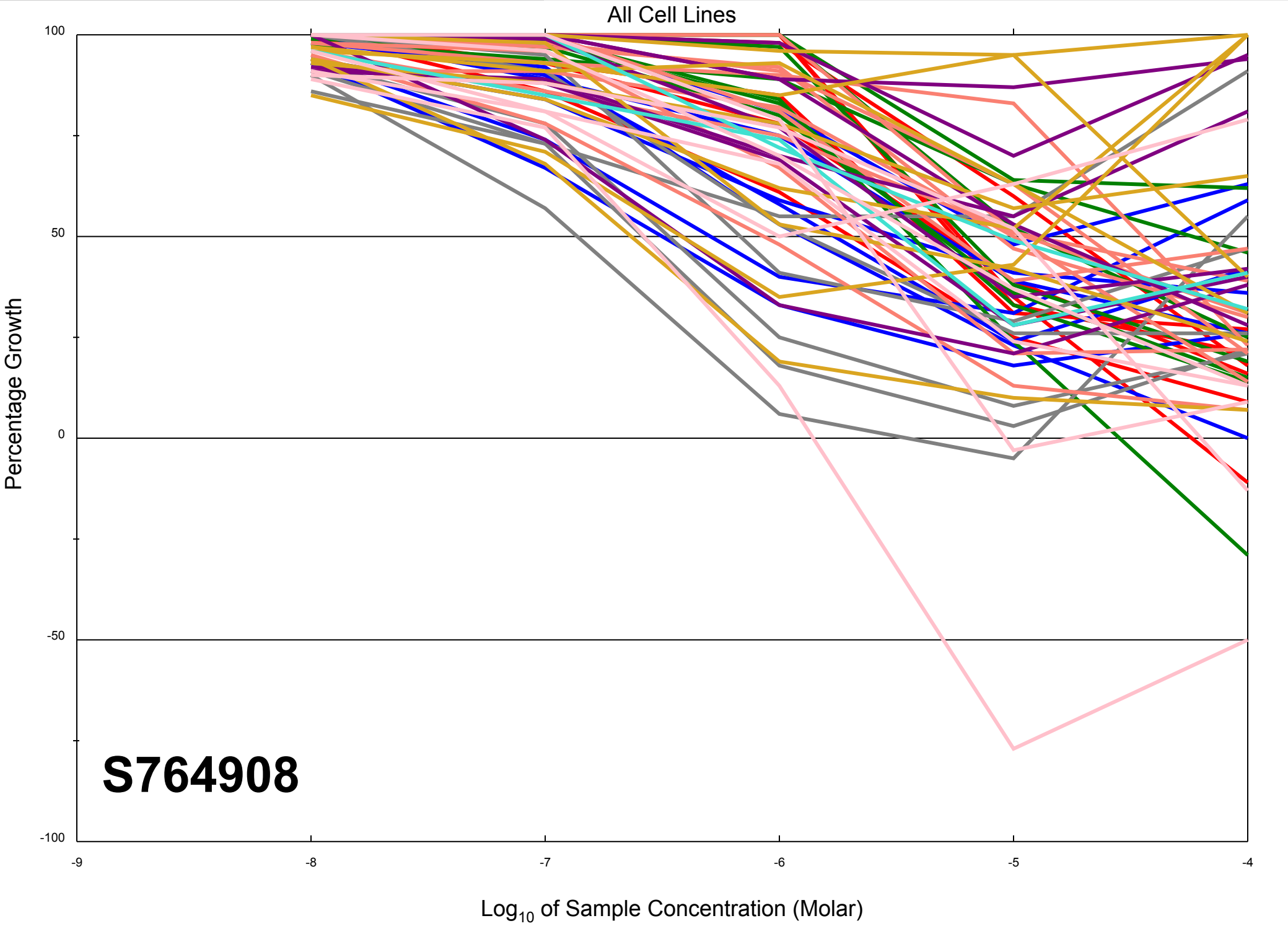
NSC: D-764908 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** May 07, 2012
Experiment ID: 1205OS68		**Report Date:** Jun 09, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	25.49
HL-60(TB)	27.21
K-562	18.42
MOLT-4	50.81
RPMI-8226	41.27
Non-Small Cell Lung Cancer	
A549/ATCC	15.01
HOP-62	39.53
HOP-92	30.32
NCI-H226	49.17
NCI-H23	29.87
NCI-H322M	74.85
NCI-H460	64.03
NCI-H522	13.95
Colon Cancer	
COLO 205	53.49
HCC-2998	63.69
HCT-116	57.80
HCT-15	82.00
HT29	41.09
KM12	77.37
SW-620	46.95
CNS Cancer	
SF-268	26.45
SF-295	17.48
SF-539	30.14
SNB-19	15.80
SNB-75	27.15
U251	10.60
Melanoma	
LOX IMVI	78.46
MALME-3M	71.15
M14	51.25
MDA-MB-435	82.69
SK-MEL-2	91.62
SK-MEL-28	83.41
SK-MEL-5	8.24
UACC-257	67.47
UACC-62	72.32
Ovarian Cancer	
IGROV1	59.07
OVCAR-3	68.00
OVCAR-4	56.12
OVCAR-5	70.73
OVCAR-8	25.07
NCI/ADR-RES	108.58
SK-OV-3	76.71
Renal Cancer	
786-0	43.44
A498	52.52
ACHN	76.89
CAKI-1	91.32
RXF 393	77.65
SN12C	15.18
TK-10	96.74
UO-31	119.62
Prostate Cancer	
PC-3	40.38
DU-145	50.95
Breast Cancer	
MCF7	30.46
MDA-MB-231/ATCC	87.73
HS 578T	67.96
BT-549	19.65
T-47D	52.91
MDA-MB-468	-19.59
Mean	51.80
Delta	71.39
Range	139.21

Mean Growth Percent - Growth Percent



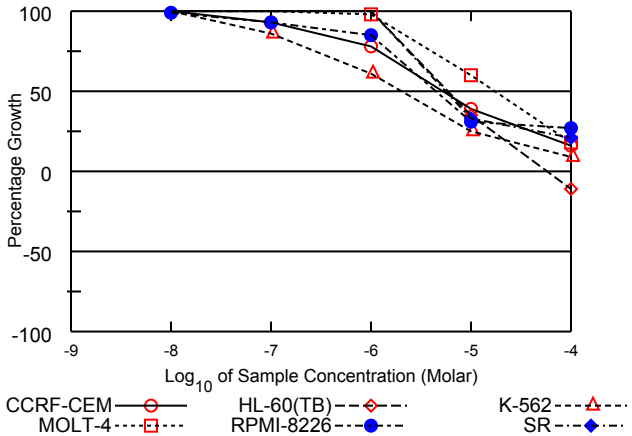
National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 764908/1	SSPL:0X1V	EXP. ID:1206NS96
	Report Date:September 25, 2012	Test Date:June 25, 2012	



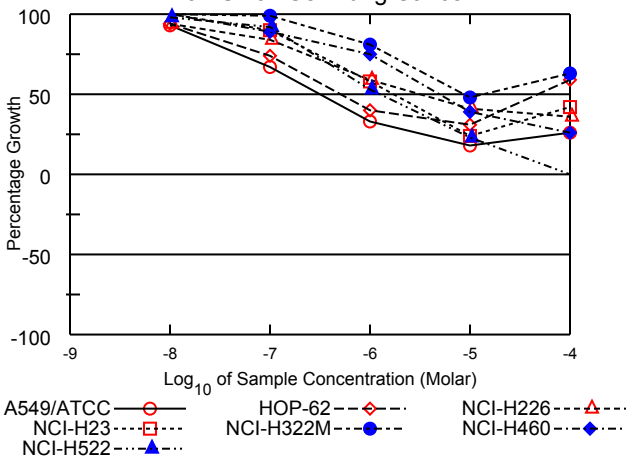
National Cancer Institute Developmental Therapeutics Program
Dose Response Curves

NSC: D - 764908 / 1	SSPL: 0X1V	EXP. ID: 1206NS96
Report Date: September 25, 2012	Test Date: June 25, 2012	

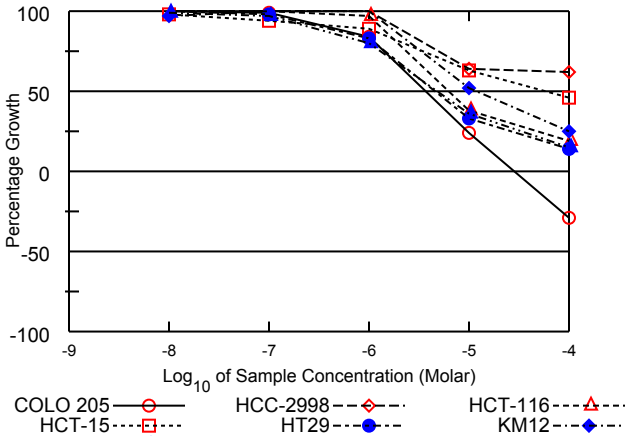
Leukemia



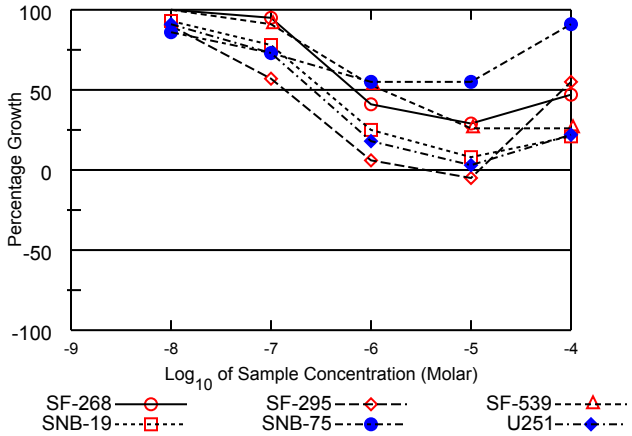
Non-Small Cell Lung Cancer



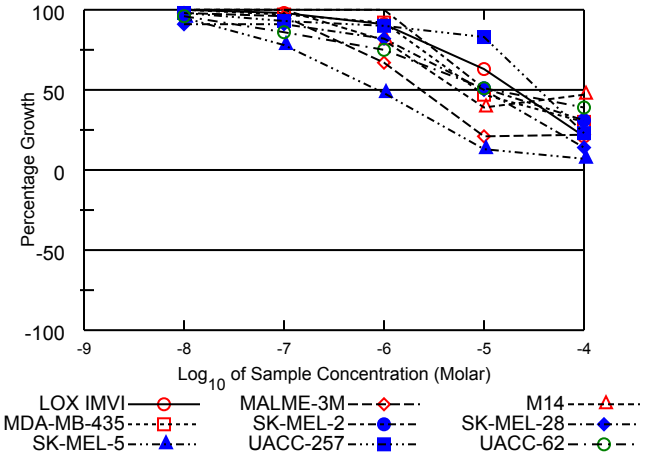
Colon Cancer



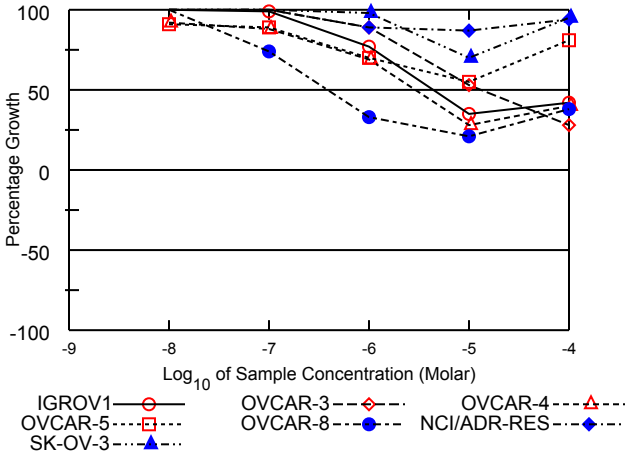
CNS Cancer



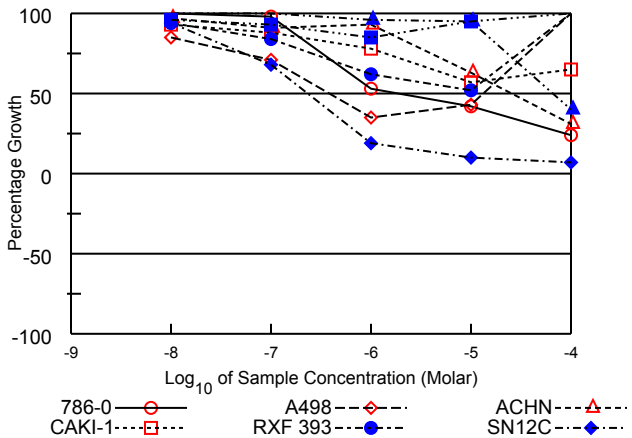
Melanoma



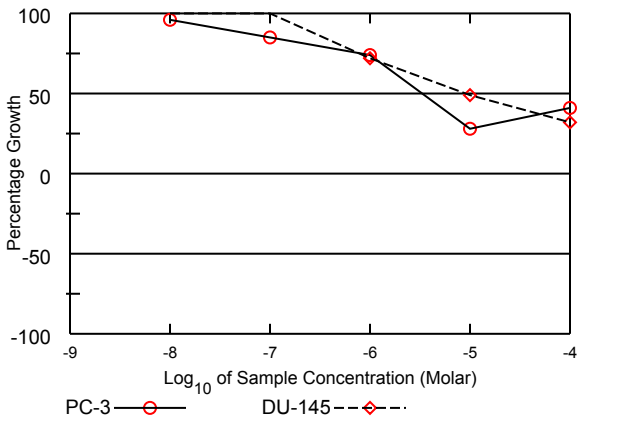
Ovarian Cancer



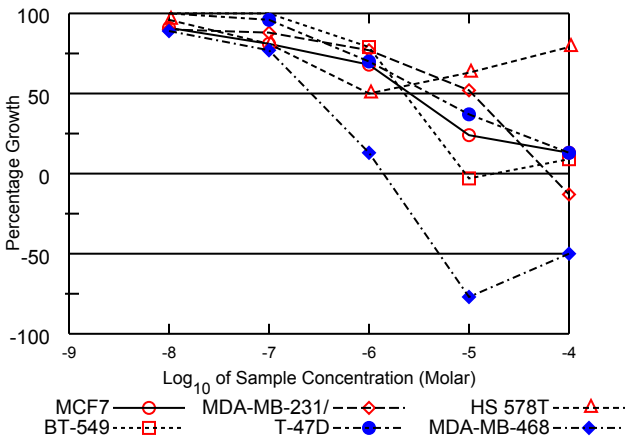
Renal Cancer



Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 764908 / 1	Experiment ID : 1206NS96	Test Type : 08	Units : Molar
Report Date : September 25, 2012	Test Date : June 25, 2012	QNS :	MC :
COMI : KA_AuFmacro_Pr (117962)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0X1V	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.678	2.374	2.377	2.257	2.006	1.344	0.954	100	93	78	39	16	5.31E-6	> 1.00E-4	> 1.00E-4
HL-60(TB)	0.781	2.846	2.995	3.036	2.839	1.512	0.693	107	109	100	35	-11	5.93E-6	5.72E-5	> 1.00E-4
K-562	0.228	1.589	1.635	1.397	1.058	0.568	0.347	103	86	61	25	9	2.01E-6	> 1.00E-4	> 1.00E-4
MOLT-4	0.476	1.723	1.750	1.765	1.703	1.224	0.706	102	103	98	60	18	1.74E-5	> 1.00E-4	> 1.00E-4
RPMI-8226	0.800	2.069	2.058	1.985	1.885	1.194	1.148	99	93	85	31	27	4.48E-6	> 1.00E-4	> 1.00E-4
SR	0.354	1.596	1.597	1.601	1.596	0.762	0.620	100	100	100	33	21	5.55E-6	> 1.00E-4	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.328	1.536	1.446	1.141	0.723	0.540	0.646	93	67	33	18	26	3.15E-7	> 1.00E-4	> 1.00E-4
HOP-62	0.271	0.815	0.780	0.671	0.487	0.439	0.594	94	74	40	31	59	.	> 1.00E-4	> 1.00E-4
NCI-H226	0.742	1.843	1.773	1.664	1.386	1.194	1.134	94	84	59	41	36	3.08E-6	> 1.00E-4	> 1.00E-4
NCI-H23	0.645	1.825	1.829	1.709	1.329	0.926	1.140	100	90	58	24	42	1.71E-6	> 1.00E-4	> 1.00E-4
NCI-H322M	0.687	1.401	1.408	1.393	1.264	1.028	1.136	101	99	81	48	63	.	> 1.00E-4	> 1.00E-4
NCI-H460	0.210	2.194	2.244	1.977	1.700	0.975	0.728	103	89	75	39	26	4.86E-6	> 1.00E-4	> 1.00E-4
NCI-H522	0.739	1.758	1.735	1.677	1.277	0.972	0.737	98	92	53	23	.	1.24E-6	9.67E-5	> 1.00E-4
Colon Cancer															
COLO 205	0.219	0.951	0.953	0.944	0.831	0.392	0.157	100	99	84	24	-29	3.63E-6	2.84E-5	> 1.00E-4
HCC-2998	0.919	2.724	2.847	2.857	2.718	2.075	2.040	107	107	100	64	62	> 1.00E-4	> 1.00E-4	> 1.00E-4
HCT-116	0.166	1.486	1.518	1.499	1.441	0.664	0.421	102	101	97	38	19	6.19E-6	> 1.00E-4	> 1.00E-4
HCT-15	0.218	1.711	1.684	1.625	1.545	1.152	0.912	98	94	89	63	46	6.05E-5	> 1.00E-4	> 1.00E-4
HT29	0.182	1.031	1.062	1.010	0.885	0.458	0.300	104	98	83	33	14	4.50E-6	> 1.00E-4	> 1.00E-4
KM12	0.600	2.627	2.569	2.720	2.674	1.661	1.114	97	105	102	52	25	1.22E-5	> 1.00E-4	> 1.00E-4
SW-620	0.239	1.754	1.733	1.703	1.456	0.781	0.463	99	97	80	36	15	4.79E-6	> 1.00E-4	> 1.00E-4
CNS Cancer															
SF-268	0.611	1.758	1.786	1.700	1.078	0.943	1.155	102	95	41	29	47	6.74E-7	> 1.00E-4	> 1.00E-4
SF-295	0.615	1.470	1.383	1.104	0.666	0.584	1.088	90	57	6	-5	55	.	.	> 1.00E-4
SF-539	0.847	2.264	2.272	2.130	1.603	1.209	1.219	101	91	53	26	26	1.32E-6	> 1.00E-4	> 1.00E-4
SNB-19	0.618	1.854	1.762	1.585	0.932	0.711	0.882	93	78	25	8	21	3.42E-7	> 1.00E-4	> 1.00E-4
SNB-75	0.914	1.703	1.596	1.491	1.351	1.348	1.633	86	73	55	55	91	> 1.00E-4	> 1.00E-4	> 1.00E-4
U251	0.389	1.693	1.570	1.347	0.619	0.434	0.680	91	73	18	3	22	2.63E-7	> 1.00E-4	> 1.00E-4
Melanoma															
LOX IMVI	0.474	2.772	2.790	2.727	2.564	1.929	0.950	101	98	91	63	21	2.05E-5	> 1.00E-4	> 1.00E-4
MALME-3M	0.588	0.976	0.969	0.960	0.850	0.670	0.673	98	96	67	21	22	2.38E-6	> 1.00E-4	> 1.00E-4
M14	0.323	1.207	1.206	1.225	1.039	0.672	0.735	100	102	81	39	47	5.57E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.436	1.767	1.763	1.721	1.659	1.064	0.836	100	97	92	47	30	8.66E-6	> 1.00E-4	> 1.00E-4
SK-MEL-2	0.794	1.445	1.527	1.513	1.457	1.128	0.998	113	110	102	51	31	1.16E-5	> 1.00E-4	> 1.00E-4
SK-MEL-28	0.477	1.399	1.316	1.315	1.235	0.941	0.604	91	91	82	50	14	1.02E-5	> 1.00E-4	> 1.00E-4
SK-MEL-5	0.503	2.285	2.199	1.897	1.359	0.729	0.635	95	78	48	13	7	8.61E-7	> 1.00E-4	> 1.00E-4
UACC-257	0.784	1.779	1.759	1.712	1.681	1.607	1.014	98	93	90	83	23	3.54E-5	> 1.00E-4	> 1.00E-4
UACC-62	0.708	2.179	2.114	1.977	1.808	1.461	1.287	96	86	75	51	39	1.26E-5	> 1.00E-4	> 1.00E-4
Ovarian Cancer															
IGROV1	0.668	1.590	1.617	1.581	1.381	0.990	1.052	103	99	77	35	42	4.40E-6	> 1.00E-4	> 1.00E-4
OVCAR-3	0.509	1.462	1.545	1.507	1.356	1.017	0.781	109	105	89	53	28	1.36E-5	> 1.00E-4	> 1.00E-4
OVCAR-4	0.527	1.057	1.013	0.992	0.892	0.673	0.738	92	88	69	28	40	2.86E-6	> 1.00E-4	> 1.00E-4
OVCAR-5	0.455	1.122	1.059	1.050	0.919	0.823	0.995	91	89	70	55	81	> 1.00E-4	> 1.00E-4	> 1.00E-4
OVCAR-8	0.367	1.442	1.439	1.159	0.717	0.591	0.776	100	74	33	21	38	3.77E-7	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.534	1.811	1.908	1.911	1.671	1.640	1.730	108	108	89	87	94	> 1.00E-4	> 1.00E-4	> 1.00E-4
SK-OV-3	0.532	1.275	1.314	1.323	1.258	1.055	1.239	105	106	98	70	95	> 1.00E-4	> 1.00E-4	> 1.00E-4
Renal Cancer															
786-0	0.640	2.048	2.095	2.015	1.383	1.235	0.980	103	98	53	42	24	1.83E-6	> 1.00E-4	> 1.00E-4
A498	1.460	2.240	2.125	2.011	1.737	1.795	2.559	85	71	35	43	141	.	> 1.00E-4	> 1.00E-4
ACHN	0.302	1.180	1.156	1.102	1.115	0.854	0.571	97	91	93	63	31	2.50E-5	> 1.00E-4	> 1.00E-4
CAKI-1	0.660	1.836	1.755	1.697	1.581	1.333	1.426	93	88	78	57	65	> 1.00E-4	> 1.00E-4	> 1.00E-4
RXF 393	0.660	1.104	1.077	1.034	0.934	0.890	1.329	94	84	62	52	151	> 1.00E-4	> 1.00E-4	> 1.00E-4
SN12C	0.521	1.953	1.868	1.495	0.799	0.662	0.623	94	68	19	10	7	2.34E-7	> 1.00E-4	> 1.00E-4
TK-10	0.495	1.056	1.054	1.087	1.036	1.029	0.718	100	105	96	95	40	6.51E-5	> 1.00E-4	> 1.00E-4
UO-31	0.712	1.653	1.612	1.583	1.515	1.610	1.687	96	93	85	95	104	> 1.00E-4	> 1.00E-4	> 1.00E-4
Prostate Cancer															
PC-3	0.535	1.853	1.798	1.655	1.516	0.906	1.073	96	85	74	28	41	3.37E-6	> 1.00E-4	> 1.00E-4
DU-145	0.334	1.291	1.378	1.306	1.023	0.805	0.636	109	102	72	49	32	9.25E-6	> 1.00E-4	> 1.00E-4
Breast Cancer															
MCF7	0.489	2.225	2.061	1.903	1.677	0.913	0.722	91	81	68	24	13	2.62E-6	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.419	1.023	0.964	0.948	0.887	0.733	0.366	90	88	77	52	-13	1.07E-5	6.35E-5	> 1.00E-4
HS 578T	1.127	2.088	2.052	1.908	1.609	1.733	1.885	96	81	50	63	79	> 1.00E-4	> 1.00E-4	> 1.00E-4
BT-549	0.666	1.515	1.571	1.581	1.341	0.644	0.739	107	108	79	-3	9	2.27E-6	.	> 1.00E-4
T-47D	0.689	1.639	1.636	1.606	1.358	1.041	0.811	100	96	70	37	13	4.08E-6	> 1.00E-4	> 1.00E-4
MDA-MB-468	0.608	1.316	1.241	1.151	0.699	0.139	0.305	89	77	13	-77	-50	2.62E-7	1.39E-6	.

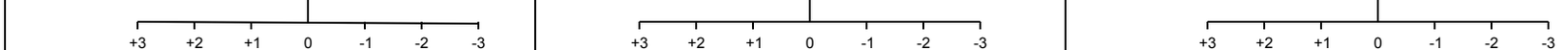
National Cancer Institute Developmental Therapeutics Program

Mean Graphs

NSC : D - 764908/1 | Units :Molar | SSPL :0X1V | EXP. ID :1206NS96

Report Date :September 25, 2012 | Test Date :June 25, 2012

Panel/Cell Line	Log_{10}GI50	GI50	Log_{10}TGI	TGI	Log_{10}LC50	LC50
Leukemia						
CCRF-CEM	-5.27		> -4.00		> -4.00	
HL-60(TB)	-5.23		-4.24		> -4.00	
K-562	-5.70		> -4.00		> -4.00	
MOLT-4	-4.76		> -4.00		> -4.00	
RPMI-8226	-5.35		> -4.00		> -4.00	
SR	-5.26		> -4.00		> -4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	-6.50		> -4.00		> -4.00	
HOP-62			> -4.00		> -4.00	
NCI-H226	-5.51		> -4.00		> -4.00	
NCI-H23	-5.77		> -4.00		> -4.00	
NCI-H322M			> -4.00		> -4.00	
NCI-H460	-5.31		> -4.00		> -4.00	
NCI-H522	-5.91		-4.01		> -4.00	
Colon Cancer						
COLO 205	-5.44		-4.55		> -4.00	
HCC-2998	> -4.00		> -4.00		> -4.00	
HCT-116	-5.21		> -4.00		> -4.00	
HCT-15	-4.22		> -4.00		> -4.00	
HT29	-5.35		> -4.00		> -4.00	
KM12	-4.91		> -4.00		> -4.00	
SW-620	-5.32		> -4.00		> -4.00	
CNS Cancer						
SF-268	-6.17		> -4.00		> -4.00	
SF-295					> -4.00	
SF-539	-5.88		> -4.00		> -4.00	
SNB-19	-6.47		> -4.00		> -4.00	
SNB-75	> -4.00		> -4.00		> -4.00	
U251	-6.58		> -4.00		> -4.00	
Melanoma						
LOX IMVI	-4.69		> -4.00		> -4.00	
MALME-3M	-5.62		> -4.00		> -4.00	
M14	-5.25		> -4.00		> -4.00	
MDA-MB-435	-5.06		> -4.00		> -4.00	
SK-MEL-2	-4.94		> -4.00		> -4.00	
SK-MEL-28	-4.99		> -4.00		> -4.00	
SK-MEL-5	-6.07		> -4.00		> -4.00	
UACC-257	-4.45		> -4.00		> -4.00	
UACC-62	-4.90		> -4.00		> -4.00	
Ovarian Cancer						
IGROV1	-5.36		> -4.00		> -4.00	
OVCAR-3	-4.87		> -4.00		> -4.00	
OVCAR-4	-5.54		> -4.00		> -4.00	
OVCAR-5	> -4.00		> -4.00		> -4.00	
OVCAR-8	-6.42		> -4.00		> -4.00	
NCI/ADR-RES	> -4.00		> -4.00		> -4.00	
SK-OV-3	> -4.00		> -4.00		> -4.00	
Renal Cancer						
786-0	-5.74		> -4.00		> -4.00	
A498			> -4.00		> -4.00	
ACHN	-4.60		> -4.00		> -4.00	
CAKI-1	> -4.00		> -4.00		> -4.00	
RXF 393	> -4.00		> -4.00		> -4.00	
SN12C	-6.63		> -4.00		> -4.00	
TK-10	-4.19		> -4.00		> -4.00	
UO-31	> -4.00		> -4.00		> -4.00	
Prostate Cancer						
PC-3	-5.47		> -4.00		> -4.00	
DU-145	-5.03		> -4.00		> -4.00	
Breast Cancer						
MCF7	-5.58		> -4.00		> -4.00	
MDA-MB-231/ATCC	-4.97		-4.20		> -4.00	
HS 578T	> -4.00		> -4.00		> -4.00	
BT-549	-5.64				> -4.00	
T-47D	-5.39		> -4.00		> -4.00	
MDA-MB-468	-6.58		-5.86			
_MID	-5.19		-4.05		-4.0	
Delta	1.44		1.81		0	
Range	2.63		1.86		0.0	



Developmental Therapeutics Program

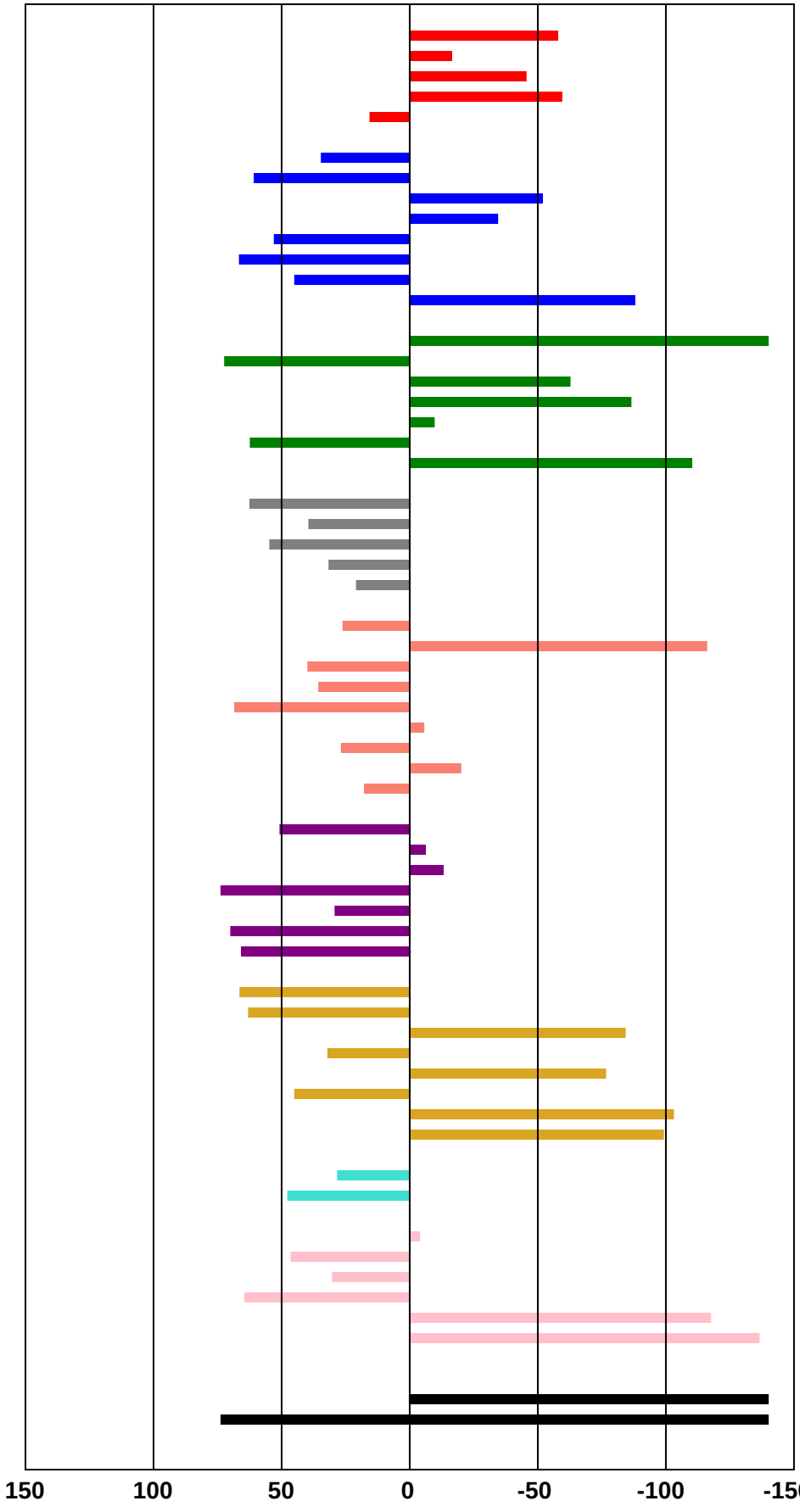
One Dose Mean Graph

NSC: D-765698 / 1 | **Conc:** 1.00E-5 Molar | **Test Date:** Jun 11, 2012

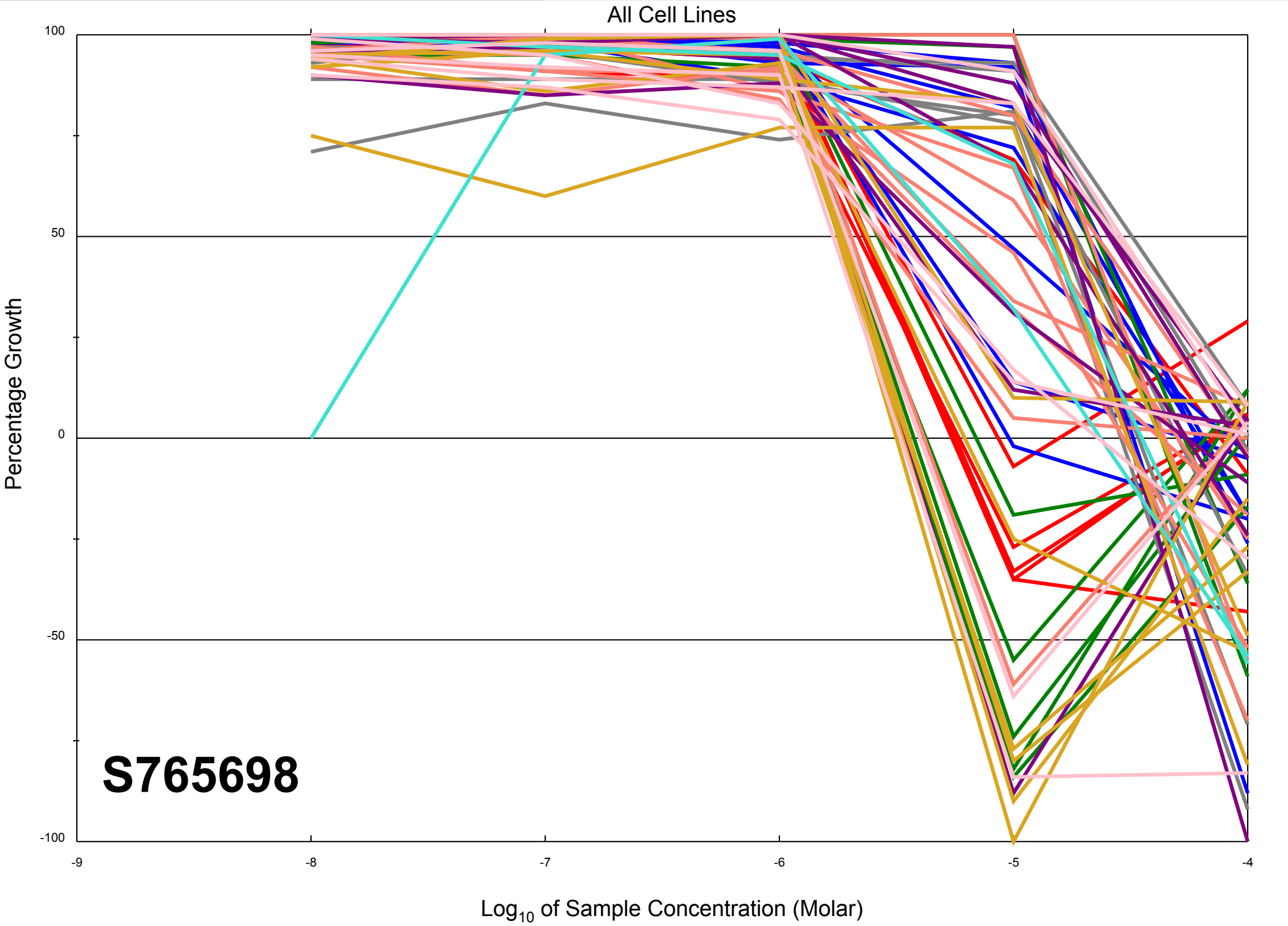
Experiment ID: 1206OS93 | **Report Date:** Jul 16, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-12.41
HL-60(TB)	28.95
K-562	-0.07
MOLT-4	-14.02
RPMI-8226	60.58
Non-Small Cell Lung Cancer	
A549/ATCC	79.57
HOP-62	105.77
HOP-92	-6.46
NCI-H226	11.02
NCI-H23	97.93
NCI-H322M	111.55
NCI-H460	89.96
NCI-H522	-42.52
Colon Cancer	
COLO 205	-94.58
HCC-2998	117.32
HCT-116	-17.23
HCT-15	-41.01
HT29	35.79
KM12	107.31
SW-620	-64.76
CNS Cancer	
SF-268	107.48
SF-539	84.44
SNB-19	99.71
SNB-75	76.58
U251	65.86
Melanoma	
LOX IMVI	71.10
MALME-3M	-70.58
M14	84.84
MDA-MB-435	80.59
SK-MEL-2	113.40
SK-MEL-28	39.84
SK-MEL-5	71.74
UACC-257	25.39
UACC-62	62.74
Ovarian Cancer	
IGROV1	95.72
OVCAR-3	39.22
OVCAR-4	32.28
OVCAR-5	118.74
OVCAR-8	74.21
NCI/ADR-RES	114.92
SK-OV-3	110.76
Renal Cancer	
786-0	111.33
A498	107.97
ACHN	-38.77
CAKI-1	77.04
RXF 393	-31.13
SN12C	89.95
TK-10	-57.59
UO-31	-53.70
Prostate Cancer	
PC-3	73.22
DU-145	92.66
Breast Cancer	
MCF7	41.48
MDA-MB-231/ATCC	91.39
HS 578T	75.22
BT-549	109.45
T-47D	-72.11
MDA-MB-468	-91.03
Mean	45.21
Delta	139.79
Range	213.32

Mean Growth Percent - Growth Percent



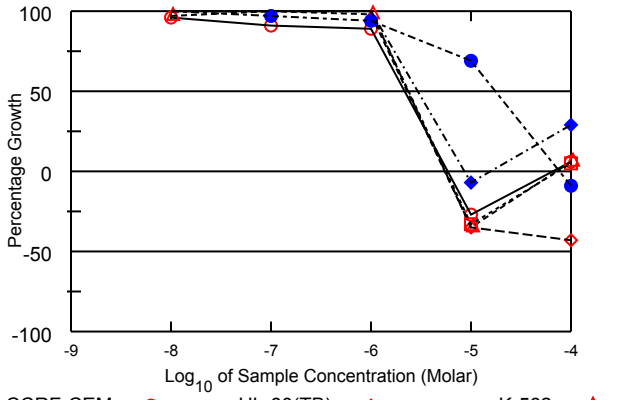
National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 765698/1	SSPL:0X1V	EXP. ID:1207NS08
	Report Date:September 25, 2012	Test Date:July 16, 2012	



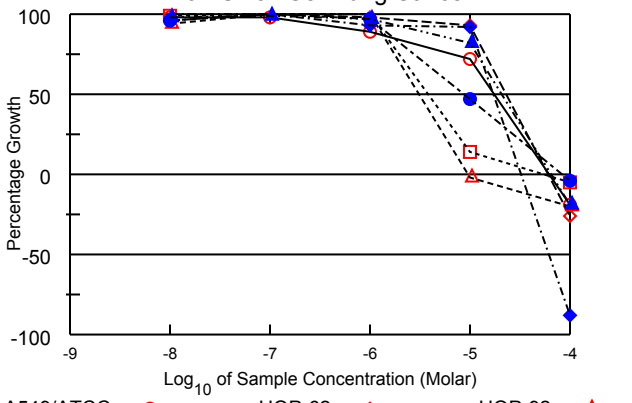
National Cancer Institute Developmental Therapeutics Program
Dose Response Curves

NSC: D - 765698 / 1	SSPL: 0X1V	EXP. ID: 1207NS08
Report Date: September 25, 2012	Test Date: July 16, 2012	

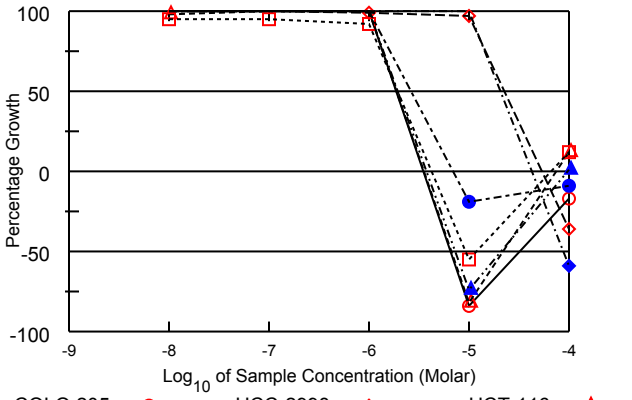
Leukemia



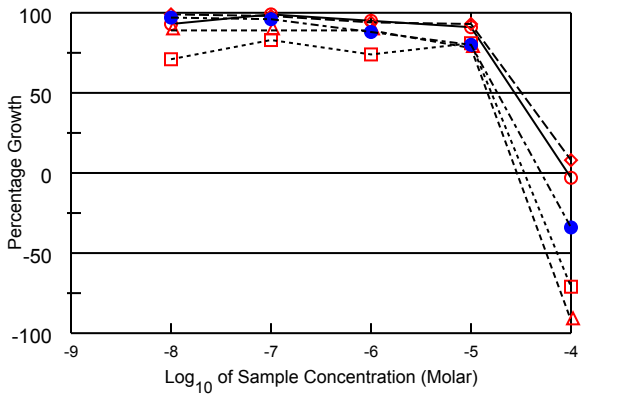
Non-Small Cell Lung Cancer



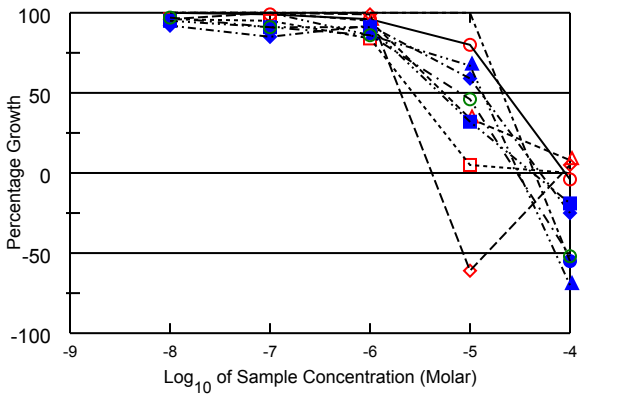
Colon Cancer



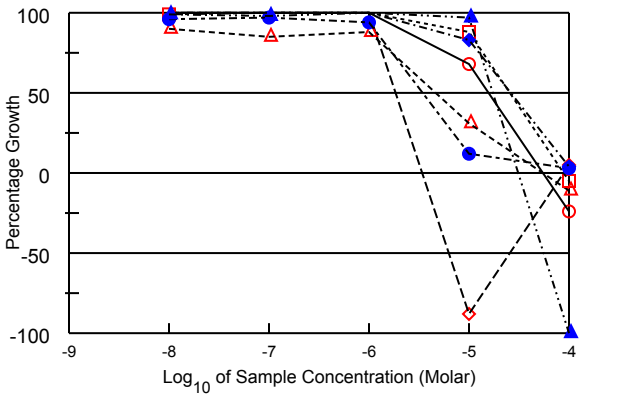
CNS Cancer



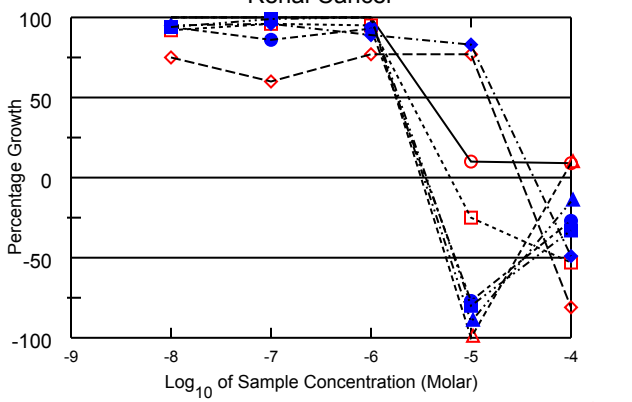
Melanoma



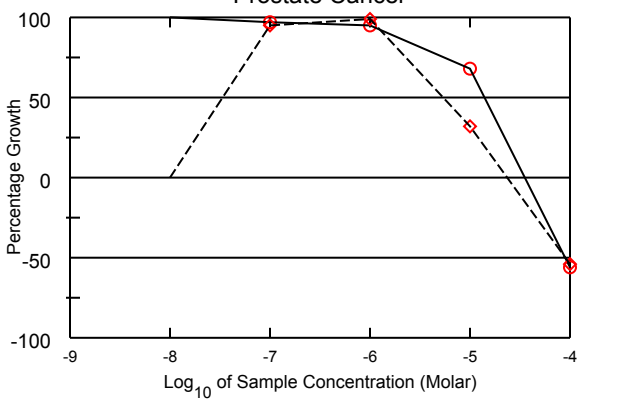
Ovarian Cancer



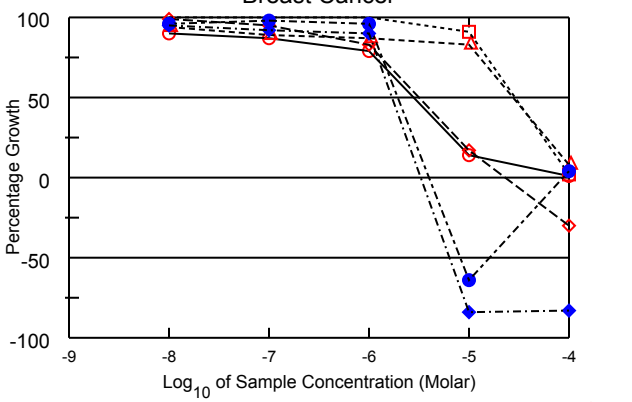
Renal Cancer



Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 765698 / 1	Experiment ID : 1207NS08	Test Type : 08	Units : Molar
Report Date : September 25, 2012	Test Date : July 16, 2012	QNS :	MC :
COMI : KA_Au_pseudomacro_Et (118827)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0X1V	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.627	2.784	2.694	2.585	2.556	0.458	0.754	96	91	89	-27	6	2.18E-6	.	> 1.00E-4
HL-60(TB)	0.895	2.548	2.885	2.842	2.915	0.582	0.509	120	118	122	-35	-43	2.88E-6	5.99E-6	> 1.00E-4
K-562	0.240	2.030	1.981	2.156	2.000	0.156	0.348	97	107	98	-35	6	2.30E-6	.	> 1.00E-4
MOLT-4	0.664	2.194	2.313	2.398	2.194	0.448	0.733	108	113	100	-33	5	2.38E-6	.	> 1.00E-4
RPMI-8226	1.272	3.040	3.035	2.988	2.933	2.498	1.155	100	97	94	69	-9	1.76E-5	7.63E-5	> 1.00E-4
SR	0.221	0.611	0.631	0.616	0.625	0.205	0.334	105	101	103	-7	29	3.04E-6	.	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.400	1.687	1.660	1.665	1.551	1.322	0.323	98	98	89	72	-19	1.73E-5	6.14E-5	> 1.00E-4
HOP-62	0.410	1.352	1.317	1.359	1.330	1.285	0.305	96	101	98	93	-26	2.30E-5	6.07E-5	> 1.00E-4
HOP-92	1.410	1.991	1.956	2.000	2.069	1.381	1.127	94	102	113	-2	-20	3.54E-6	9.59E-6	> 1.00E-4
NCI-H226	0.904	2.471	2.462	2.548	2.605	1.120	0.861	99	105	109	14	-5	4.15E-6	5.53E-5	> 1.00E-4
NCI-H23	0.821	2.397	2.340	2.416	2.343	1.567	0.791	96	101	97	47	-4	8.82E-6	8.46E-5	> 1.00E-4
NCI-H322M	0.815	1.699	1.707	1.706	1.639	1.630	0.095	101	101	93	92	-88	1.71E-5	3.24E-5	6.13E-5
NCI-H460	0.264	2.645	2.592	2.612	2.569	2.222	0.213	98	99	97	82	-19	2.08E-5	6.45E-5	> 1.00E-4
Colon Cancer															
COLO 205	0.380	1.761	1.869	1.850	2.067	0.061	0.315	108	106	122	-84	-17	2.24E-6	3.91E-6	.
HCC-2998	1.199	3.287	3.324	3.327	3.264	3.223	0.763	102	102	99	97	-36	2.25E-5	5.33E-5	> 1.00E-4
HCT-116	0.187	1.860	1.830	1.977	1.958	0.034	0.382	98	107	106	-82	12	1.98E-6	.	.
HCT-15	0.160	2.185	2.078	2.084	2.019	0.072	0.413	95	95	92	-55	12	1.92E-6	.	.
HT29	0.303	1.475	1.538	1.644	1.656	0.246	0.276	105	114	115	-19	-9	3.07E-6	7.22E-6	> 1.00E-4
KM12	0.409	1.991	2.053	2.040	2.060	2.076	0.167	104	103	104	105	-59	2.17E-5	4.37E-5	8.80E-5
SW-620	0.247	2.052	2.052	2.115	2.150	0.065	0.258	100	104	105	-74	1	2.04E-6	.	.
CNS Cancer															
SF-268	0.562	1.922	1.831	1.908	1.852	1.800	0.545	93	99	95	91	-3	2.73E-5	9.29E-5	> 1.00E-4
SF-539	0.493	2.609	2.583	2.568	2.481	2.466	0.654	99	98	94	93	8	3.20E-5	> 1.00E-4	> 1.00E-4
SNB-19	0.824	2.236	2.079	2.081	2.080	1.925	0.068	89	89	89	78	-92	1.46E-5	2.88E-5	5.67E-5
SNB-75	1.227	2.045	1.809	1.910	1.834	1.886	0.357	71	83	74	81	-71	1.59E-5	3.40E-5	7.28E-5
U251	0.496	1.928	1.891	1.867	1.761	1.643	0.328	97	96	88	80	-34	1.84E-5	5.04E-5	> 1.00E-4
Melanoma															
LOX IMVI	0.715	3.209	3.200	3.190	3.119	2.721	0.684	100	99	96	80	-4	2.28E-5	8.87E-5	> 1.00E-4
MALME-3M	0.563	1.138	1.118	1.163	1.131	0.219	0.589	96	104	99	-61	5	2.02E-6	.	.
M14	0.445	1.801	1.816	1.819	1.727	0.911	0.548	101	101	95	34	8	5.50E-6	> 1.00E-4	> 1.00E-4
MDA-MB-435	0.376	1.618	1.565	1.558	1.421	0.434	0.381	96	95	84	5	.	2.69E-6	> 1.00E-4	> 1.00E-4
SK-MEL-2	1.033	1.833	1.869	1.921	1.856	1.834	0.466	105	111	103	100	-55	2.11E-5	4.42E-5	9.30E-5
SK-MEL-28	0.539	1.418	1.345	1.289	1.350	1.055	0.407	92	85	92	59	-25	1.27E-5	5.06E-5	> 1.00E-4
SK-MEL-5	0.676	2.991	3.010	2.991	2.673	2.220	0.204	101	100	86	67	-70	1.33E-5	3.08E-5	7.16E-5
UACC-257	0.900	2.213	2.150	2.095	2.091	1.317	0.725	95	91	91	32	-19	4.91E-6	4.17E-5	> 1.00E-4
UACC-62	1.049	2.864	2.810	2.706	2.611	1.880	0.506	97	91	86	46	-52	7.86E-6	2.95E-5	9.59E-5
Ovarian Cancer															
IGROV1	0.638	1.760	1.867	1.855	1.808	1.396	0.483	110	108	104	68	-24	1.55E-5	5.43E-5	> 1.00E-4
OVCAR-3	0.485	1.545	1.615	1.668	1.676	0.059	0.539	107	112	112	-88	5	2.05E-6	.	.
OVCAR-4	0.769	1.550	1.474	1.431	1.458	1.011	0.685	90	85	88	31	-11	4.66E-6	5.47E-5	> 1.00E-4
OVCAR-5	0.434	1.502	1.490	1.503	1.544	1.369	0.411	99	100	104	88	-5	2.54E-5	8.77E-5	> 1.00E-4
OVCAR-8	0.417	1.746	1.688	1.704	1.663	0.572	0.459	96	97	94	12	3	3.41E-6	> 1.00E-4	> 1.00E-4
NCI/ADR-RES	0.748	2.340	2.367	2.440	2.358	2.066	0.818	102	106	101	83	4	2.62E-5	> 1.00E-4	> 1.00E-4
SK-OV-3	0.592	1.336	1.326	1.323	1.405	1.317	0.001	99	98	109	97	-100	1.74E-5	3.12E-5	5.59E-5
Renal Cancer															
786-0	0.838	2.914	2.958	3.055	2.967	1.056	1.034	102	107	103	10	9	3.72E-6	> 1.00E-4	> 1.00E-4
A498	1.396	2.140	1.953	1.846	1.968	1.969	0.261	75	60	77	77	-81	1.48E-5	3.06E-5	6.34E-5
ACHN	0.259	1.788	1.814	1.837	1.793	-0.001	0.395	102	103	100	-100	9	1.78E-6	.	.
CAKI-1	1.099	2.958	2.807	2.886	2.873	0.823	0.513	92	96	95	-25	-53	2.38E-6	6.19E-6	7.63E-5
RXF 393	0.885	1.298	1.272	1.241	1.270	0.206	0.646	94	86	93	-77	-27	1.79E-6	3.53E-6	.
SN12C	0.958	2.854	2.750	2.770	2.638	2.533	0.491	95	96	89	83	-49	1.78E-5	4.27E-5	> 1.00E-4
TK-10	0.779	1.317	1.344	1.429	1.496	0.075	0.665	105	121	133	-90	-15	2.36E-6	3.94E-6	.
UO-31	0.680	2.119	2.032	2.110	2.135	0.138	0.454	94	99	101	-80	-33	1.92E-6	3.62E-6	.
Prostate Cancer															
PC-3	0.518	2.390	2.425	2.325	2.301	1.795	0.229	102	97	95	68	-56	1.40E-5	3.55E-5	8.98E-5
DU-145	0.389	1.734	.	1.661	1.722	0.814	0.179	.	95	99	32	-54	5.34E-6	2.34E-5	8.98E-5
Breast Cancer															
MCF7	0.424	2.292	2.104	2.044	1.895	0.686	0.452	90	87	79	14	1	2.78E-6	> 1.00E-4	> 1.00E-4
MDA-MB-231/ATCC	0.677	1.392	1.383	1.360	1.273	0.799	0.476	99	95	83	17	-30	3.18E-6	2.31E-5	> 1.00E-4
HS 578T	0.912	2.038	1.974	1.919	1.893	1.848	1.003	94	89	87	83	8	2.76E-5	> 1.00E-4	> 1.00E-4
BT-549	0.746	1.988	1.998	2.069	2.027	1.878	0.765	101	106	103	91	2	2.88E-5	> 1.00E-4	> 1.00E-4
T-47D	0.684	1.623	1.589	1.603	1.587	0.248	0.719	96	98	96	-64	4	1.94E-6	.	.
MDA-MB-468	0.767	1.651	1.607	1.578	1.567	0.123	0.133	95	92	90	-84	-83	1.71E-6	3.30E-6	6.39E-6

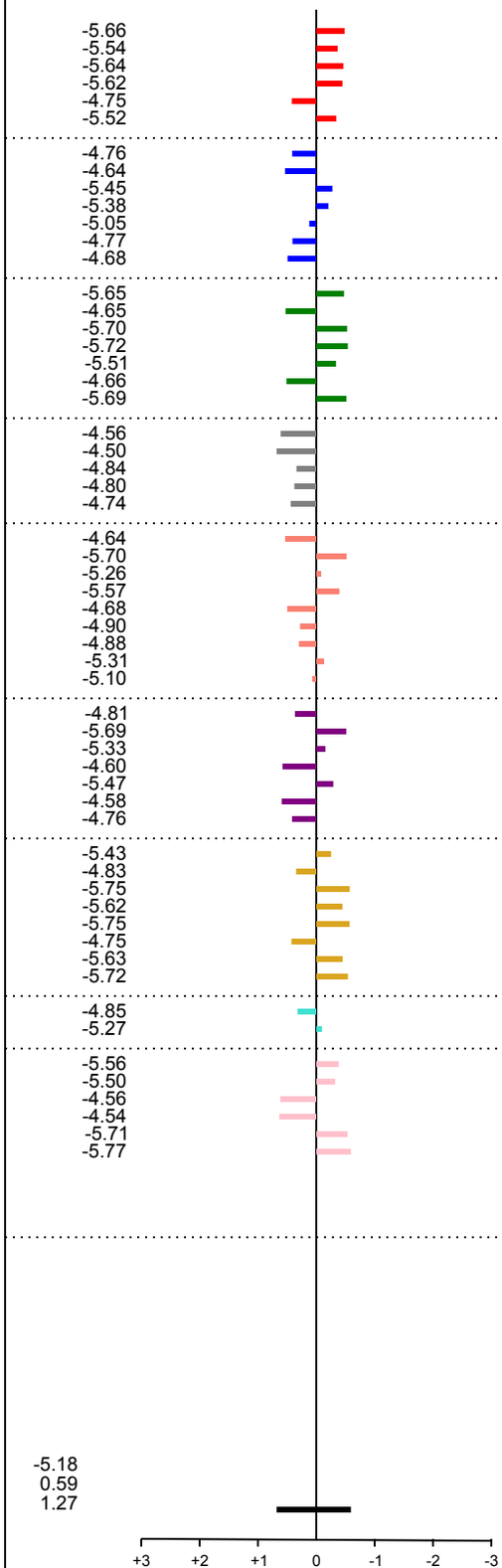
National Cancer Institute Developmental Therapeutics Program

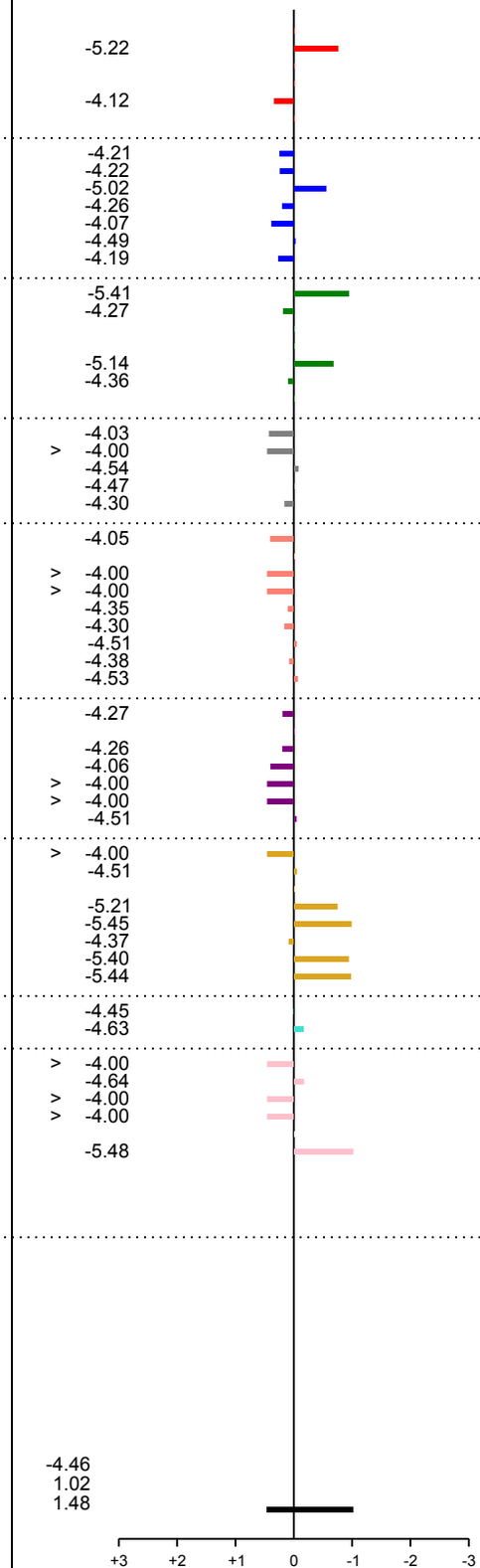
Mean Graphs

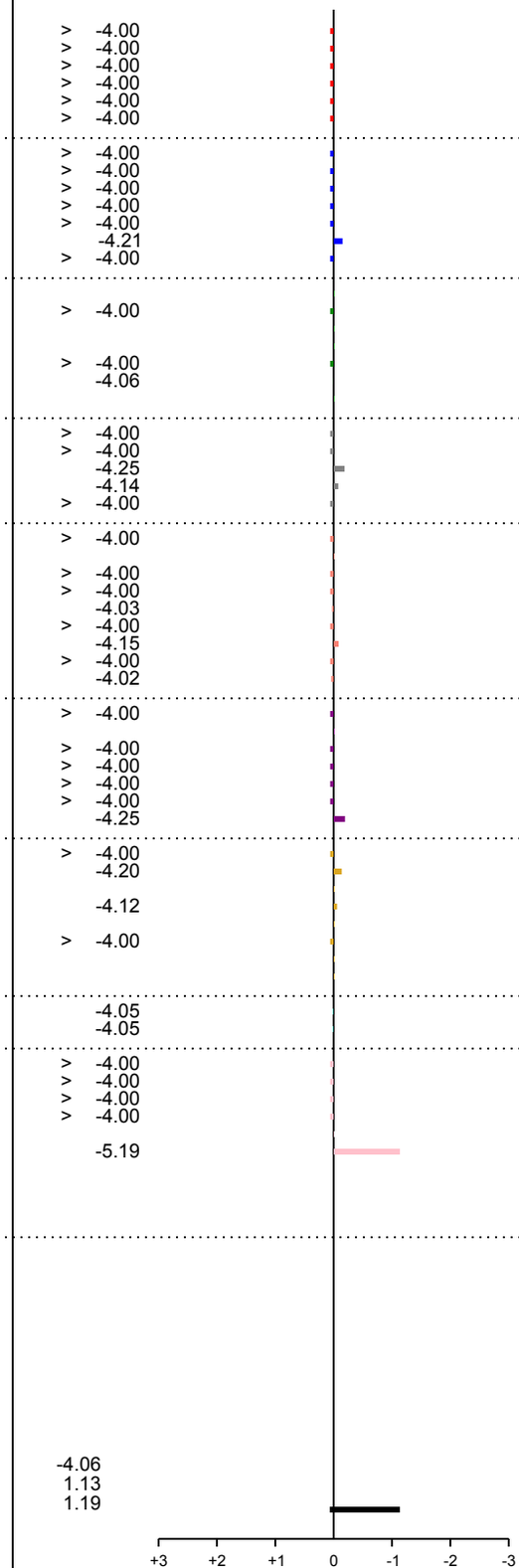
NSC : D - 765698/1 | Units :Molar | SSPL :0X1V | EXP. ID :1207NS08

Report Date :September 25, 2012 | Test Date :July 16, 2012

Panel/Cell Line	Log_{10}GI50	Log_{10}TGI	Log_{10}LC50
Leukemia			
CCRF-CEM	-5.66		> -4.00
HL-60(TB)	-5.54	-5.22	> -4.00
K-562	-5.64		> -4.00
MOLT-4	-5.62		> -4.00
RPMI-8226	-4.75	-4.12	> -4.00
SR	-5.52		> -4.00
Non-Small Cell Lung Cancer			
A549/ATCC	-4.76	-4.21	> -4.00
HOP-62	-4.64	-4.22	> -4.00
HOP-92	-5.45	-5.02	> -4.00
NCI-H226	-5.38	-4.26	> -4.00
NCI-H23	-5.05	-4.07	> -4.00
NCI-H322M	-4.77	-4.49	-4.21
NCI-H460	-4.68	-4.19	> -4.00
Colon Cancer			
COLO 205	-5.65	-5.41	
HCC-2998	-4.65	-4.27	> -4.00
HCT-116	-5.70		
HCT-15	-5.72		
HT29	-5.51	-5.14	> -4.00
KM12	-4.66	-4.36	-4.06
SW-620	-5.69		
CNS Cancer			
SF-268	-4.56	-4.03	> -4.00
SF-539	-4.50	> -4.00	> -4.00
SNB-19	-4.84	-4.54	-4.25
SNB-75	-4.80	-4.47	-4.14
U251	-4.74	-4.30	> -4.00
Melanoma			
LOX IMVI	-4.64	-4.05	> -4.00
MALME-3M	-5.70		
M14	-5.26	> -4.00	> -4.00
MDA-MB-435	-5.57	> -4.00	> -4.00
SK-MEL-2	-4.68	-4.35	-4.03
SK-MEL-28	-4.90	-4.30	> -4.00
SK-MEL-5	-4.88	-4.51	-4.15
UACC-257	-5.31	-4.38	> -4.00
UACC-62	-5.10	-4.53	-4.02
Ovarian Cancer			
IGROV1	-4.81	-4.27	> -4.00
OVCAR-3	-5.69		
OVCAR-4	-5.33	-4.26	> -4.00
OVCAR-5	-4.60	-4.06	> -4.00
OVCAR-8	-5.47	> -4.00	> -4.00
NCI/ADR-RES	-4.58	> -4.00	> -4.00
SK-OV-3	-4.76	-4.51	-4.25
Renal Cancer			
786-0	-5.43	> -4.00	> -4.00
A498	-4.83	-4.51	-4.20
ACHN	-5.75		
CAKI-1	-5.62	-5.21	-4.12
RXF 393	-5.75	-5.45	
SN12C	-4.75	-4.37	> -4.00
TK-10	-5.63	-5.40	
UO-31	-5.72	-5.44	
Prostate Cancer			
PC-3	-4.85	-4.45	-4.05
DU-145	-5.27	-4.63	-4.05
Breast Cancer			
MCF7	-5.56	> -4.00	> -4.00
MDA-MB-231/ATCC	-5.50	-4.64	> -4.00
HS 578T	-4.56	> -4.00	> -4.00
BT-549	-4.54	> -4.00	> -4.00
T-47D	-5.71		
MDA-MB-468	-5.77	-5.48	-5.19
_MID	-5.18	-4.46	-4.06
Delta	0.59	1.02	1.13
Range	1.27	1.48	1.19







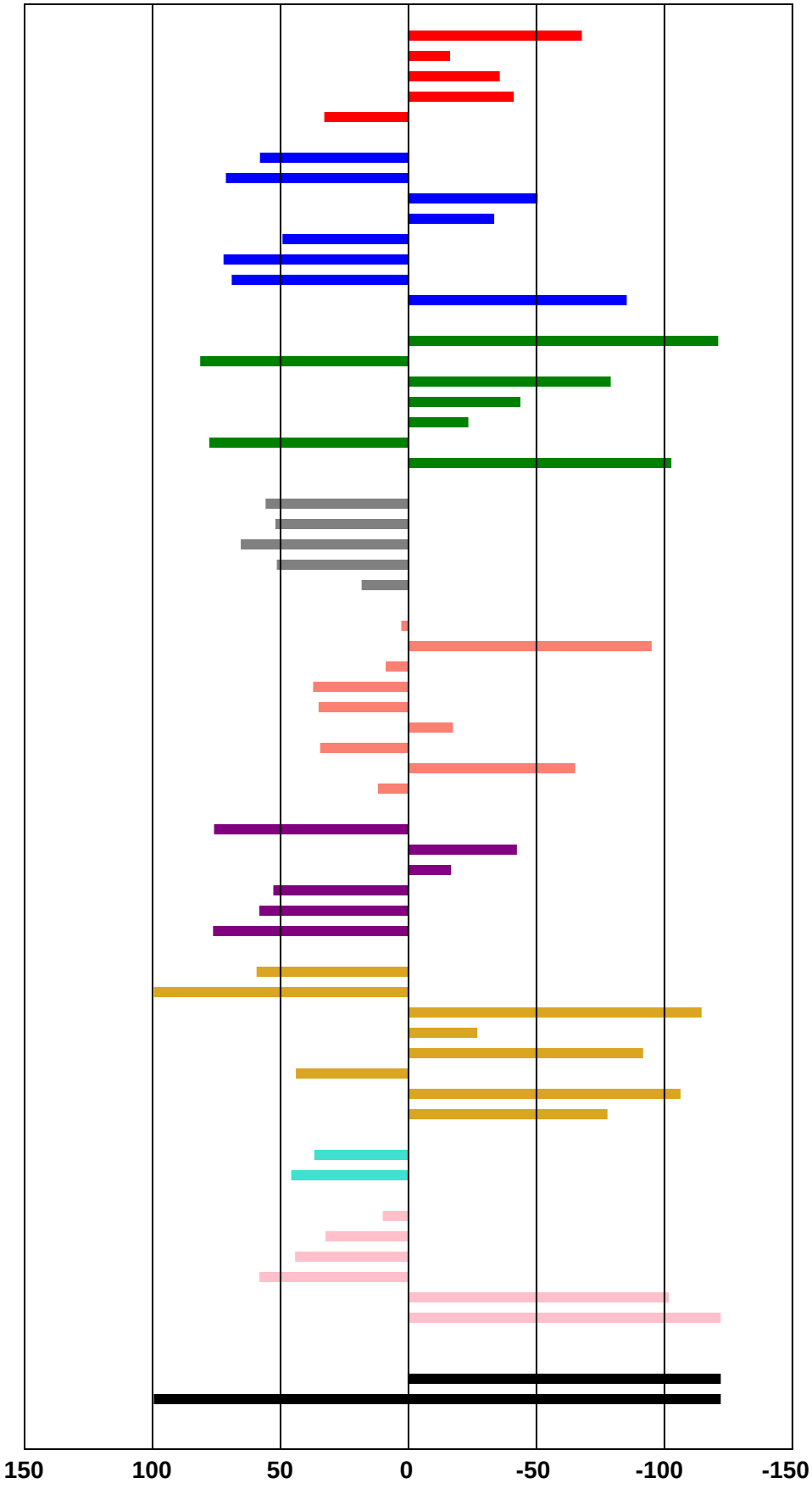
Developmental Therapeutics Program

One Dose Mean Graph

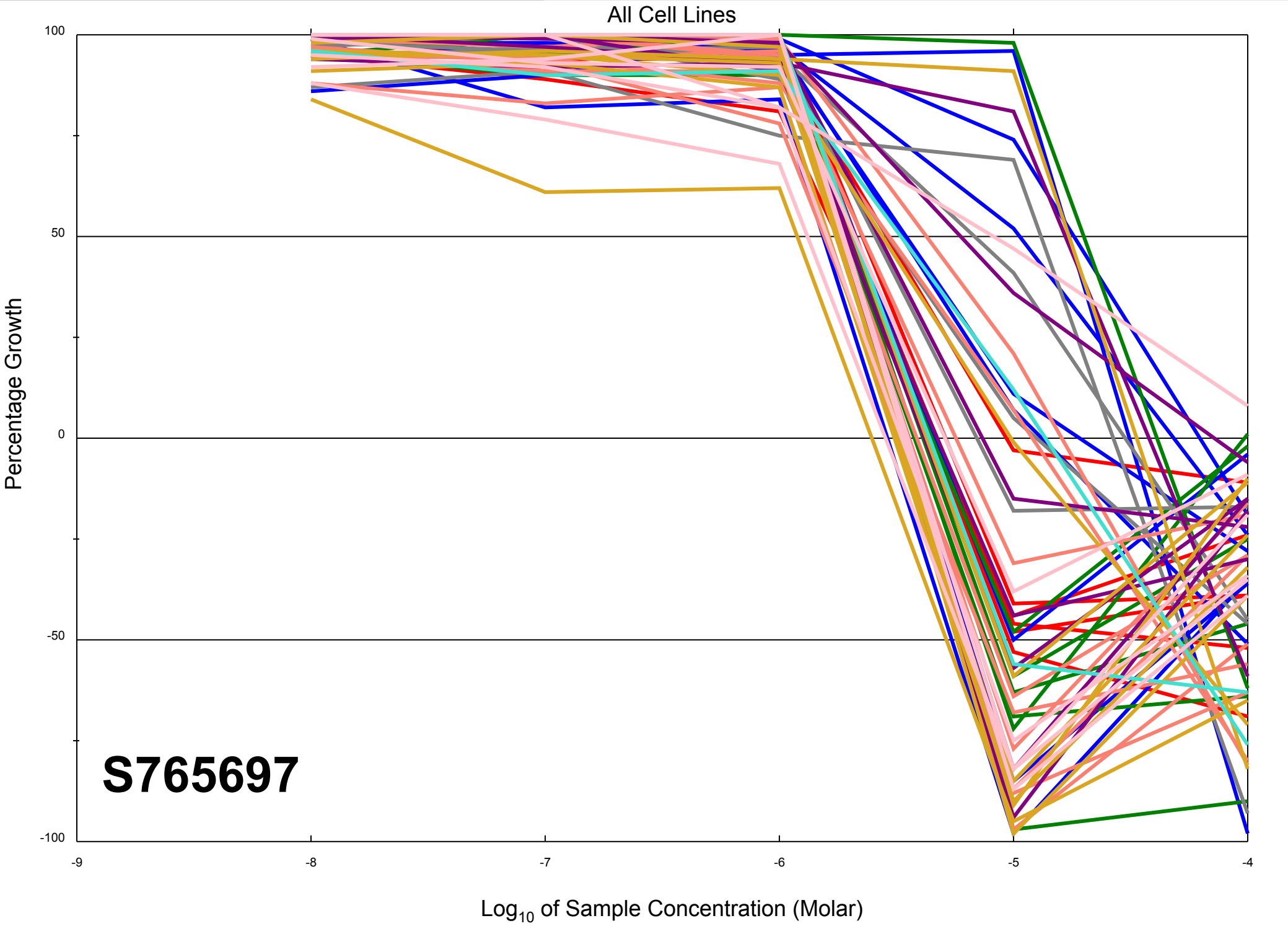
NSC: D-765697 / 1	**Conc:** 1.00E-5 Molar	**Test Date:** Jun 11, 2012
Experiment ID: 1206OS93		**Report Date:** Jul 27, 2012

Panel/Cell Line	Growth Percent
Leukemia	
CCRF-CEM	-36.78
HL-60(TB)	14.74
K-562	-4.70
MOLT-4	-10.18
RPMI-8226	63.20
Non-Small Cell Lung Cancer	
A549/ATCC	88.33
HOP-62	101.65
HOP-92	-19.49
NCI-H226	-2.53
NCI-H23	79.53
NCI-H322M	102.57
NCI-H460	99.37
NCI-H522	-54.31
Colon Cancer	
COLO 205	-90.05
HCC-2998	111.68
HCT-116	-48.05
HCT-15	-12.75
HT29	7.58
KM12	108.12
SW-620	-71.75
CNS Cancer	
SF-268	86.14
SF-539	82.31
SNB-19	95.82
SNB-75	81.75
U251	48.61
Melanoma	
LOX IMVI	33.11
MALME-3M	-64.05
M14	39.21
MDA-MB-435	67.56
SK-MEL-2	65.41
SK-MEL-28	13.60
SK-MEL-5	64.83
UACC-257	-34.18
UACC-62	42.24
Ovarian Cancer	
IGROV1	106.27
OVCAR-3	-11.39
OVCAR-4	14.31
OVCAR-5	83.11
NCI/ADR-RES	88.59
SK-OV-3	106.66
Renal Cancer	
786-0	89.66
A498	129.79
ACHN	-83.54
CAKI-1	4.06
RXF 393	-60.69
SN12C	74.29
TK-10	-75.33
UO-31	-46.77
Prostate Cancer	
PC-3	67.11
DU-145	76.13
Breast Cancer	
MCF7	40.37
MDA-MB-231/ATCC	62.73
HS 578T	74.60
BT-549	88.55
T-47D	-70.77
MDA-MB-468	-91.04
Mean	30.63
Delta	121.67
Range	220.83

Mean Growth Percent - Growth Percent



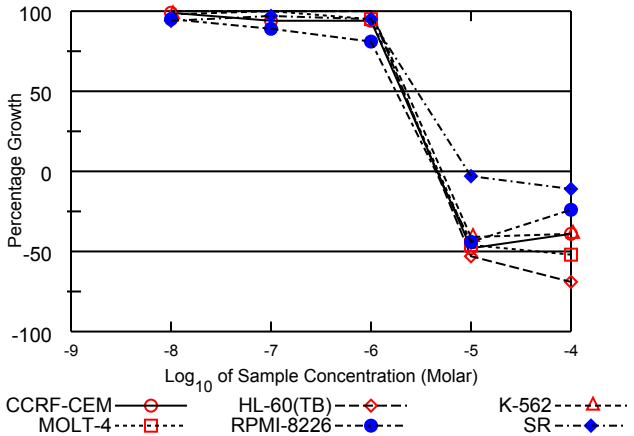
National Cancer Institute Developmental Therapeutics Program Dose Response Curves	NSC : D - 765697/1	SSPL:0X1V	EXP. ID:1207NS11
	Report Date:September 25, 2012	Test Date:July 23, 2012	



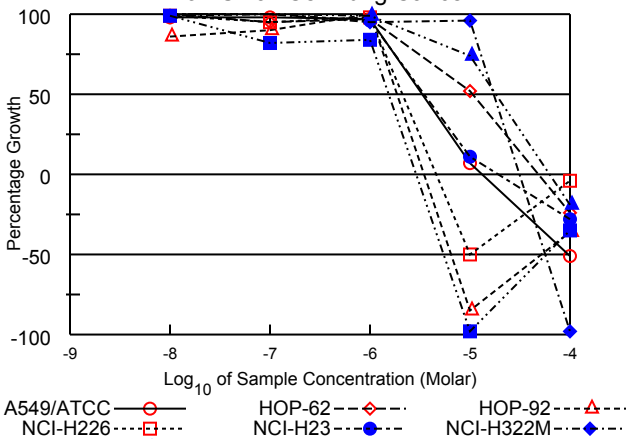
National Cancer Institute Developmental Therapeutics Program
Dose Response Curves

NSC: D - 765697 / 1	SSPL: 0X1V	EXP. ID: 1207NS11
Report Date: September 25, 2012	Test Date: July 23, 2012	

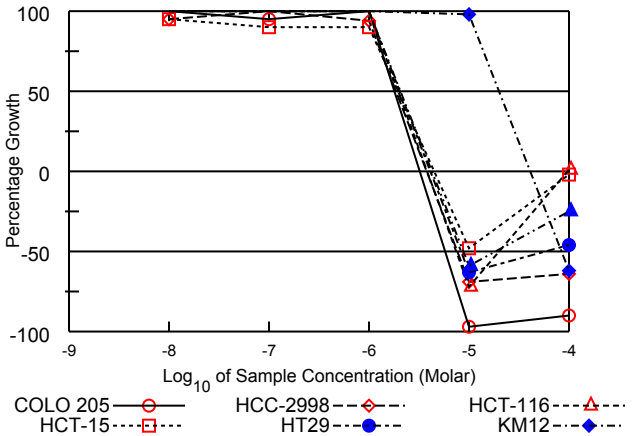
Leukemia



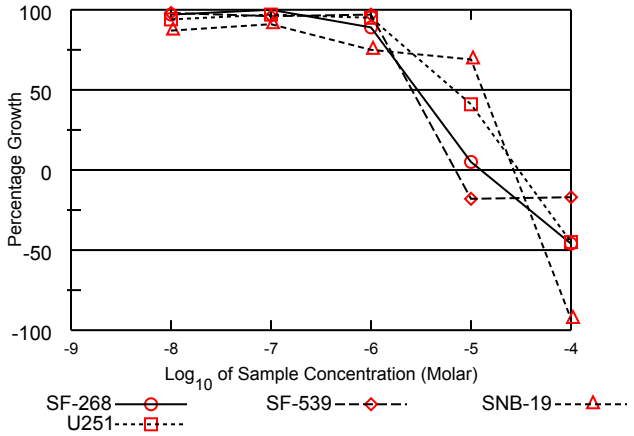
Non-Small Cell Lung Cancer



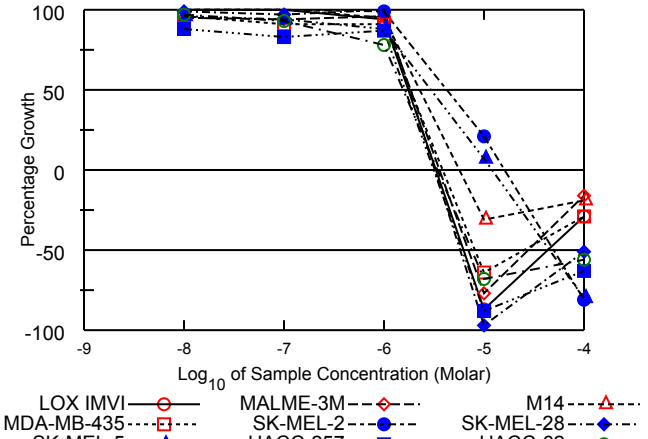
Colon Cancer



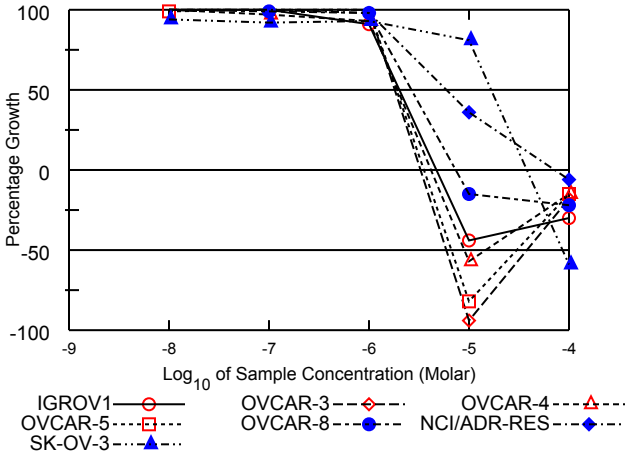
CNS Cancer



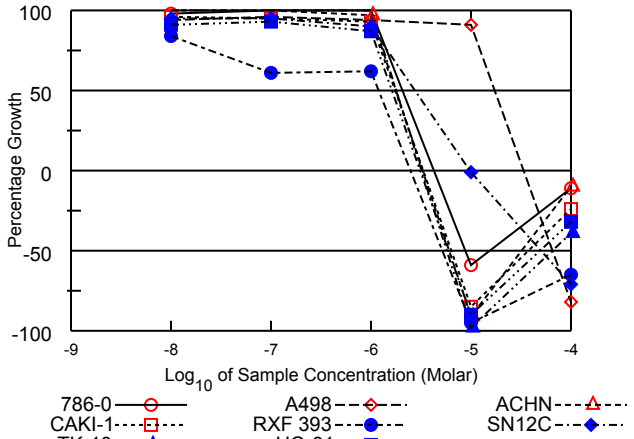
Melanoma



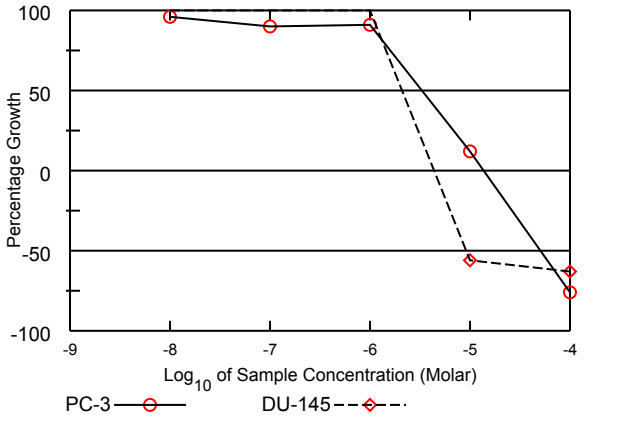
Ovarian Cancer



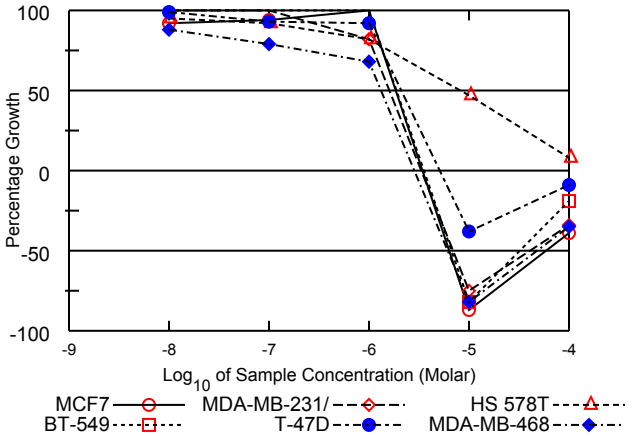
Renal Cancer



Prostate Cancer



Breast Cancer



National Cancer Institute Developmental Therapeutics Program
In-Vitro Testing Results

NSC : D - 765697 / 1	Experiment ID : 1207NS11	Test Type : 08	Units : Molar
Report Date : September 25, 2012	Test Date : July 23, 2012	QNS :	MC :
COMI : KA_Au_pseudomacro_EtOH (118825)	Stain Reagent : SRB Dual-Pass Related	SSPL : 0X1V	

			Log10 Concentration												
	Time		Mean Optical Densities					Percent Growth							
Panel/Cell Line	Zero	Ctrl	-8.0	-7.0	-6.0	-5.0	-4.0	-8.0	-7.0	-6.0	-5.0	-4.0	GI50	TGI	LC50
Leukemia															
CCRF-CEM	0.516	2.077	2.067	1.980	1.976	0.270	0.317	99	94	94	-48	-39	2.03E-6	4.59E-6	> 1.00E-4
HL-60(TB)	0.673	2.327	2.471	2.335	2.378	0.314	0.207	109	100	103	-53	-69	2.18E-6	4.56E-6	9.52E-6
K-562	0.353	2.450	2.404	2.446	2.475	0.209	0.216	98	100	101	-41	-39	2.29E-6	5.16E-6	> 1.00E-4
MOLT-4	0.609	2.114	2.234	2.306	2.039	0.332	0.290	108	113	95	-46	-52	2.09E-6	4.74E-6	4.39E-5
RPMI-8226	0.999	2.531	2.461	2.364	2.240	0.555	0.763	95	89	81	-44	-24	1.77E-6	4.42E-6	> 1.00E-4
SR	0.194	0.670	0.643	0.656	0.645	0.189	0.174	94	97	95	-3	-11	2.87E-6	9.35E-6	> 1.00E-4
Non-Small Cell Lung Cancer															
A549/ATCC	0.413	1.581	1.558	1.557	1.550	0.497	0.202	98	98	97	7	-51	3.35E-6	1.33E-5	9.58E-5
HOP-62	0.514	1.557	1.580	1.510	1.529	1.059	0.391	102	95	97	52	-24	1.07E-5	4.84E-5	> 1.00E-4
HOP-92	1.087	1.309	1.277	1.287	1.343	0.168	0.692	86	90	115	-85	-36	2.12E-6	3.77E-6	.
NCI-H226	0.746	2.180	2.172	2.114	2.152	0.371	0.714	99	95	98	-50	-4	2.11E-6	4.58E-6	.
NCI-H23	1.173	2.957	2.949	2.994	2.889	1.374	0.845	100	102	96	11	-28	3.50E-6	1.93E-5	> 1.00E-4
NCI-H322M	0.689	1.631	1.622	1.629	1.580	1.593	0.014	99	100	95	96	-98	1.72E-5	3.12E-5	5.65E-5
NCI-H460	0.271	2.624	2.733	2.613	2.602	2.015	0.221	105	100	99	74	-19	1.82E-5	6.30E-5	> 1.00E-4
NCI-H522	0.986	1.913	1.901	1.750	1.764	0.022	0.640	99	82	84	-98	-35	1.54E-6	2.90E-6	.
Colon Cancer															
COLO 205	0.374	1.217	1.238	1.172	1.260	0.013	0.039	102	95	105	-97	-90	1.87E-6	3.32E-6	5.87E-6
HCC-2998	0.542	1.539	1.493	1.543	1.475	0.167	0.194	95	100	94	-69	-64	1.85E-6	3.75E-6	7.61E-6
HCT-116	0.192	1.679	1.820	1.810	1.930	0.054	0.209	109	109	117	-72	1	2.26E-6	.	.
HCT-15	0.249	2.174	2.072	1.979	1.987	0.129	0.244	95	90	90	-48	-2	1.95E-6	4.49E-6	> 1.00E-4
HT29	0.300	1.457	1.489	1.561	1.574	0.112	0.162	103	109	110	-63	-46	2.23E-6	4.34E-6	.
KM12	0.515	2.481	2.542	2.583	2.528	2.447	0.195	103	105	102	98	-62	2.00E-5	4.10E-5	8.40E-5
SW-620	0.251	2.085	2.100	2.152	2.139	0.103	0.189	101	104	103	-59	-25	2.12E-6	4.31E-6	.
CNS Cancer															
SF-268	0.737	2.104	2.058	2.105	1.960	0.801	0.400	97	100	89	5	-46	2.92E-6	1.24E-5	> 1.00E-4
SF-539	0.797	2.736	2.703	2.650	2.683	0.652	0.660	98	96	97	-18	-17	2.57E-6	6.96E-6	> 1.00E-4
SNB-19	0.753	2.215	2.029	2.076	1.852	1.756	0.056	87	91	75	69	-93	1.30E-5	2.67E-5	5.44E-5
U251	0.678	2.206	2.120	2.158	2.123	1.300	0.373	94	97	95	41	-45	6.71E-6	2.98E-5	> 1.00E-4
Melanoma															
LOX IMVI	0.552	2.887	2.929	2.923	2.747	0.070	0.394	102	102	94	-87	-29	1.75E-6	3.30E-6	.
MALME-3M	0.673	1.354	1.319	1.313	1.327	0.153	0.569	95	94	96	-77	-16	1.84E-6	3.58E-6	.
M14	0.425	1.873	1.907	1.932	1.807	0.295	0.346	102	104	95	-31	-19	2.29E-6	5.72E-6	> 1.00E-4
MDA-MB-435	0.396	1.854	1.799	1.721	1.724	0.141	0.280	96	91	91	-64	-29	1.84E-6	3.85E-6	.
SK-MEL-2	1.283	2.267	2.295	2.329	2.254	1.490	0.249	103	106	99	21	-81	4.24E-6	1.61E-5	5.00E-5
SK-MEL-28	0.449	1.100	1.091	1.078	1.108	0.012	0.222	99	97	101	-97	-51	1.81E-6	3.23E-6	5.77E-6
SK-MEL-5	0.729	3.095	3.010	2.949	2.812	0.892	0.147	96	94	88	7	-80	2.94E-6	1.20E-5	4.53E-5
UACC-257	0.996	1.736	1.651	1.614	1.642	0.124	0.366	88	83	87	-88	-63	1.63E-6	3.16E-6	6.10E-6
UACC-62	0.857	2.829	2.779	2.681	2.401	0.271	0.374	97	93	78	-68	-56	1.56E-6	3.42E-6	7.49E-6
Ovarian Cancer															
IGROV1	0.662	2.071	2.112	2.129	1.943	0.372	0.466	103	104	91	-44	-30	2.01E-6	4.73E-6	> 1.00E-4
OVCAR-3	0.601	1.752	1.893	1.801	1.827	0.037	0.492	112	104	106	-94	-18	1.91E-6	3.40E-6	.
OVCAR-4	0.644	1.133	1.140	1.121	1.100	0.280	0.546	101	97	93	-57	-15	1.94E-6	4.19E-6	.
OVCAR-5	0.406	1.305	1.298	1.340	1.324	0.075	0.347	99	104	102	-82	-15	1.92E-6	3.60E-6	.
OVCAR-8	0.564	2.030	2.059	2.013	2.004	0.477	0.442	102	99	98	-15	-22	2.66E-6	7.32E-6	> 1.00E-4
NCI/ADR-RES	0.868	2.702	2.739	2.840	2.656	1.519	0.820	102	108	98	36	-6	5.84E-6	7.31E-5	> 1.00E-4
SK-OV-3	0.651	1.409	1.365	1.351	1.359	1.266	0.268	94	92	93	81	-59	1.67E-5	3.80E-5	8.65E-5
Renal Cancer															
786-0	0.732	2.664	2.628	2.740	2.732	0.303	0.650	98	104	104	-59	-11	2.14E-6	4.35E-6	.
A498	1.207	1.999	1.954	1.968	1.948	1.931	0.217	94	96	94	91	-82	1.73E-5	3.37E-5	6.54E-5
ACHN	0.340	1.740	1.759	1.768	1.702	0.030	0.305	101	102	97	-91	-10	1.78E-6	3.28E-6	.
CAKI-1	0.946	3.084	3.000	2.967	2.945	0.146	0.723	96	95	93	-85	-24	1.75E-6	3.35E-6	.
RXF 393	0.779	1.031	0.991	0.933	0.936	0.036	0.275	84	61	62	-95	-65	1.19E-6	2.48E-6	5.15E-6
SN12C	0.721	2.622	2.535	2.525	2.441	0.714	0.210	95	95	90	-1	-71	2.77E-6	9.74E-6	5.02E-5
TK-10	0.770	1.393	1.394	1.476	1.505	0.017	0.467	100	113	118	-98	-39	2.06E-6	3.52E-6	.
UO-31	0.706	2.245	2.113	2.143	2.044	0.072	0.482	91	93	87	-90	-32	1.62E-6	3.10E-6	.
Prostate Cancer															
PC-3	0.651	1.952	1.898	1.826	1.842	0.810	0.154	96	90	91	12	-76	3.34E-6	1.37E-5	5.03E-5
DU-145	0.333	1.296	1.364	1.338	1.313	0.147	0.124	107	104	102	-56	-63	2.13E-6	4.42E-6	9.16E-6
Breast Cancer															
MCF7	0.380	1.741	1.633	1.656	1.737	0.048	0.233	92	94	100	-87	-39	1.84E-6	3.41E-6	.
MDA-MB-231/ATCC	0.625	1.418	1.449	1.481	1.276	0.159	0.413	104	108	82	-75	-34	1.60E-6	3.34E-6	.
HS 578T	0.954	2.190	2.132	2.086	1.971	1.539	1.057	95	92	82	47	8	8.38E-6	> 1.00E-4	> 1.00E-4
BT-549	0.918	1.984	2.017	2.143	2.150	0.166	0.741	103	115	116	-82	-19	2.15E-6	3.85E-6	.
T-47D	0.681	1.671	1.658	1.602	1.594	0.424	0.617	99	93	92	-38	-9	2.11E-6	5.12E-6	> 1.00E-4
MDA-MB-468	0.679	1.528	1.425	1.348	1.257	0.119	0.439	88	79	68	-82	-35	1.32E-6	2.83E-6	.

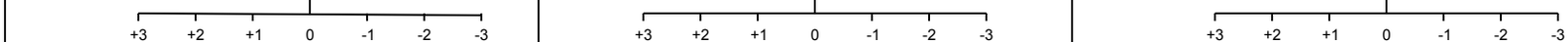
National Cancer Institute Developmental Therapeutics Program

Mean Graphs

NSC : D - 765697/1 | Units :Molar | SSPL :0X1V | EXP. ID :1207NS11

Report Date :September 25, 2012 | Test Date :July 23, 2012

Panel/Cell Line	Log_{10}GI50	GI50	Log_{10}TGI	TGI	Log_{10}LC50	LC50
Leukemia						
CCRF-CEM	-5.69		-5.34		> -4.00	
HL-60(TB)	-5.66		-5.34		-5.02	
K-562	-5.64		-5.29		> -4.00	
MOLT-4	-5.68		-5.32		-4.36	
RPMI-8226	-5.75		-5.35		> -4.00	
SR	-5.54		-5.03		> -4.00	
Non-Small Cell Lung Cancer						
A549/ATCC	-5.47		-4.88		-4.02	
HOP-62	-4.97		-4.32		> -4.00	
HOP-92	-5.67		-5.42			
NCI-H226	-5.68		-5.34			
NCI-H23	-5.46		-4.71		> -4.00	
NCI-H322M	-4.76		-4.51		-4.25	
NCI-H460	-4.74		-4.20		> -4.00	
NCI-H522	-5.81		-5.54			
Colon Cancer						
COLO 205	-5.73		-5.48		-5.23	
HCC-2998	-5.73		-5.43		-5.12	
HCT-116	-5.65					
HCT-15	-5.71		-5.35		> -4.00	
HT29	-5.65		-5.36			
KM12	-4.70		-4.39		-4.08	
SW-620	-5.67		-5.37			
CNS Cancer						
SF-268	-5.53		-4.91		> -4.00	
SF-539	-5.59		-5.16		> -4.00	
SNB-19	-4.88		-4.57		-4.26	
U251	-5.17		-4.53		> -4.00	
Melanoma						
LOX IMVI	-5.76		-5.48			
MALME-3M	-5.73		-5.45			
M14	-5.64		-5.24		> -4.00	
MDA-MB-435	-5.74		-5.41			
SK-MEL-2	-5.37		-4.79		-4.30	
SK-MEL-28	-5.74		-5.49		-5.24	
SK-MEL-5	-5.53		-4.92		-4.34	
UACC-257	-5.79		-5.50		-5.21	
UACC-62	-5.81		-5.47		-5.13	
Ovarian Cancer						
IGROV1	-5.70		-5.33		> -4.00	
OVCAR-3	-5.72		-5.47			
OVCAR-4	-5.71		-5.38			
OVCAR-5	-5.72		-5.44			
OVCAR-8	-5.58		-5.14		> -4.00	
NCI/ADR-RES	-5.23		-4.14		> -4.00	
SK-OV-3	-4.78		-4.42		-4.06	
Renal Cancer						
786-0	-5.67		-5.36			
A498	-4.76		-4.47		-4.18	
ACHN	-5.75		-5.48			
CAKI-1	-5.76		-5.48			
RXF 393	-5.92		-5.61		-5.29	
SN12C	-5.56		-5.01		-4.30	
TK-10	-5.69		-5.45			
UO-31	-5.79		-5.51			
Prostate Cancer						
PC-3	-5.48		-4.86		-4.30	
DU-145	-5.67		-5.35		-5.04	
Breast Cancer						
MCF7	-5.73		-5.47			
MDA-MB-231/ATCC	-5.80		-5.48			
HS 578T	-5.08		> -4.00		> -4.00	
BT-549	-5.67		-5.41			
T-47D	-5.68		-5.29		> -4.00	
MDA-MB-468	-5.88		-5.55			
_MID	-5.54		-5.14		-4.33	
Delta	0.38		0.47		0.96	
Range	1.22		1.61		1.29	



NSC: 758065

It was tested against the following disease types and cell lines:

Experiment ID: HF1900

Panel Name	Cell Name	Schedule	Route	High Dose
Breast Cancer	MDA-MB-231	QD X 4	IP	150 mg/kg/dose
Non-Small Cell Lung Cancer	NCI-H23	QD X 4	IP	150 mg/kg/dose
Colon Cancer	SW-620	QD X 4	IP	150 mg/kg/dose

Experiment ID: HF1901

Panel Name	Cell Name	Schedule	Route	High Dose
Colon Cancer	COLO 205	QD X 4	IP	150 mg/kg/dose
Melanoma	LOX IMVI	QD X 4	IP	150 mg/kg/dose
Ovarian Cancer	OVCAR-3	QD X 4	IP	150 mg/kg/dose

Experiment ID: HF1902

Panel Name	Cell Name	Schedule	Route	High Dose
Non-Small Cell Lung Cancer	NCI-H522	QD X 4	IP	150 mg/kg/dose
CNS Cancer	U251	QD X 4	IP	150 mg/kg/dose
Melanoma	UACC-62	QD X 4	IP	150 mg/kg/dose

Experiment ID: HF1903

Panel Name	Cell Name	Schedule	Route	High Dose
Melanoma	MDA-MB-435	QD X 4	IP	150 mg/kg/dose
Ovarian Cancer	OVCAR-5	QD X 4	IP	150 mg/kg/dose
CNS Cancer	SF-295	QD X 4	IP	150 mg/kg/dose

Your compound was scored as follows:

IP Score	4 out of 48
SC Score	0 out of 48
Total	4 out of 96
Cell Kill	N

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(71) Applicant *(for all designated States except US)*: **UNIVERSITY OF KWAZULU-NATAL** [ZA/ZA]; Office of Registrar, University Road, Chiltern Hills, 3629 Westville (ZA).

(72) Inventors; and

(75) Inventors/Applicants *(for US only)*: **MUNRO, Orde, Quentin** [ZA/ZA]; 59A Warwick Road, Ferncliffe, 3201 Pietermaritzburg (ZA). **AKERMAN, Kate, Julie** [ZA/ZA]; 25 Natalie Place, 2 Kay Road, Hayfields, Pietermaritzburg 3201 (ZA). **AKERMAN, Piers** [ZA/ZA]; 25 Natalie Place, 2 Kay Road, Hayfields, Pietermaritzburg 3201 (ZA).

(74) Agents: **FORBES, Craig, Paul** et al.; Adams & Adams, PO Box 1014, 0001 Pretoria (ZA).

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[Continued on next page]

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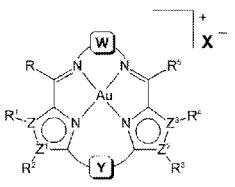

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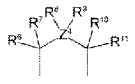

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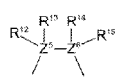

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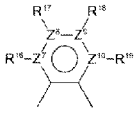

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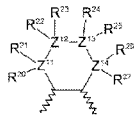

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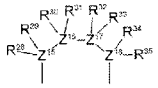

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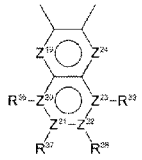

Y1

(57) Abstract: The invention provides compounds of the Formula (I), in which W is independently selected from W^1, W^2, W^3, W^4, W^5, or W represents a pair of substituents independently selected from H, alkyl, aryl or amide in which the amide is optionally part of a linking chain, and the Z^n-Z^n bonds (n = 4-17; n' = n + 1) are optionally of any whole or partial bond order, Y is Y^1 or Y represents a pair of substituents independently selected from H, C-$_1$-C$_6$ alkyl, Z_5 or Z_6 aryl, or Y is optionally a bridging structure that may comprise one or more C-$_1$-C$_6$ amide, C-$_1$-C$_6$ ether, or C-$_1$-C$_6$ ester groups, R-R^{39} are independently selected from no substituent, a lone pair of electrons, H, halogen, C_5-C_6 aryl, C_1- C_{12} alkyl, amine, C-$_1$-C$_6$ alkylamine, C-$_1$-C$_6$ amide, nitro, cyano, carboxyl, C-$_1$-C$_6$ ester, phosphane, thiol, C-$_1$-C$_6$ thioether, OR^{40}, and suitable pairs of adjacent R groups (R-R^{39}) may optionally together form part of a C_5 or C_6 aryl ring, a Z_5 or Z_6 ring, R^{40} is independently selected from H, C-$_1$-C$_6$ alkyl, Z_5 or Z_6 aryl, C-$_1$-C$_6$ ester, poly(-C_2O-), amine, and C-$_1$-C$_6$ alkylamine, Z-Z^{24} are independently selected from C, N, P, O, and S, and X^- is a pharmaceutically acceptable anion, for the treatment of cancer.

WO 2011/158176 A2

SM, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

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GOLD COMPLEXES

THIS INVENTION relates to novel chemotherapeutic agents. It relates in particular to novel bis(pyrrolide-imine) and bis(imidazolato-imine) gold(III) Schiff base complexes as chemotherapeutic agents.

General Background

The use of metal complexes in medicine can be traced back to 3500 BC and due to its particular physical and chemical properties gold has always been one of the many metals in use[1,2] Despite its wide use most of the gold based drugs have not been designed specifically for their function, and their mode of action is often unknown[2] The use of gold(0) is limited and is mostly used as a non-irritating food decoration and additive[1] Most of the gold-based drugs employ gold(I) and gold(III).[1]

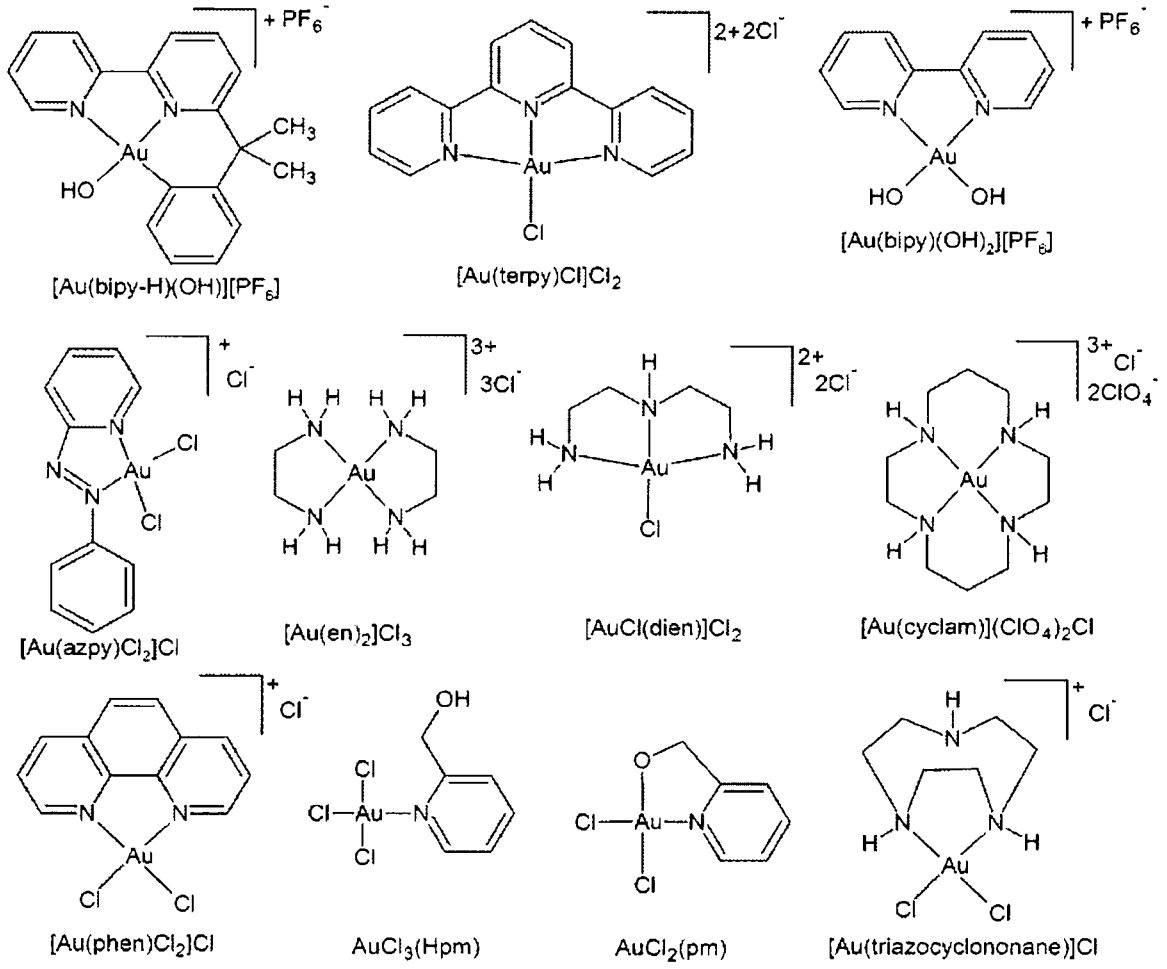
The use of gold(I) based drugs has until recently been the main focus of medicinal research.[3,4] Their usefulness has mostly been in the treatment of rheumatoid arthritis, but testing against different cancer cell lines has been reported.[3] Gold(I) is a soft d^{10} metal ion. The most common coordination geometry for gold(I) complexes is linear, with the molecules usually consisting of a central gold(I) ion coordinated by either phosphorous or sulfur donor ligands.[4,5] Au(I) complexes undergo facile ligand exchange in aqueous solutions, with the rate of ligand exchange increasing in the order $R_3P < RS^- < X^-$. The lability of the ligands contributes to both the therapeutic activity of Au(I) antiarthritic compounds and the side effects observed with these drugs.[4] One of the most well known of the gold(I) drugs is Auranofin (Scheme 1) which is widely used in the treatment of rheumatoid arthritis.

Auranofin and its many derivatives have also become the focus of research into gold(I) based anti-cancer agents. Several complexes have been found to exhibit cytotoxicity greater than that of cisplatin against melanoma and leukemia cancer cell

lines in particular.[5] The *in vitro* test results of many gold(I) chelates against various human cancer cell lines have been promising.[4,5]

However, many of these complexes have never entered into clinical trials, since they have been associated with cardiotoxicity in preclinical trials.[2] Due to this cardiotoxicity of gold(I) chelates, gold(III) has become the focus of research into gold based chemotherapeutic agents.[5,6]

One of the first metal based drugs that was used in the treatment of cancer was cisplatin.[6,7] Cisplatin is still widely used today in the treatment of several types of tumors, particularly testicular cancer. Its use is, however, hindered by some clinical problems such as a severe toxicity towards non-cancerous tissue and the frequent occurrence of initial and acquired resistance to the treatment.[6] The most concerning adverse side effect is nephrotoxicity correlated to platinum binding and inactivation of renal thiol-containing enzymes.[6] These drawbacks to the success of cisplatin in anticancer chemotherapy has raised great interest in the study of metal complexes to be used as antitumor agents, instigating the ongoing investigation of alternative metal-based drugs. The allure of gold(III) as an anti-tumor agent is that it has a d^8 electron configuration, with vacant $d(x^2-y^2)$ orbitals, and therefore adopts a rigorously square planar coordination geometry. Gold(III) is therefore isostructural and isoelectronic to platinum(II).[8] Despite the similarity to platinum(II) literature relating to the use of gold(III) as a chemotherapeutic agent is scarce.[6] The rarity of data on gold(III) complexes probably derives from their high redox potential and relatively poor stability, which make their use rather problematic under physiological conditions.[5,6] The gold(III) ion can be readily reduced to the more stable gold(I) ion or even metallic gold(0) under the *in vivo* reducing conditions, characteristic of the mammalian environment.[5] The coordination of a ligand, which is a strong σ-donor and π-acceptor ligand that can stabilize the gold(III) ion under physiological conditions is therefore critical if gold(III) is to be used in the treatment of cancer.[5,9]



Gold(III) complexes with Au-N bonds that have been tested for cytotoxicity against human cancer cell lines.[10]

Scheme 2

There are currently no commercially available gold(III) compounds being used as chemotherapeutic agents. There are, however, many gold(III) complexes that have shown very promising *in vitro* and *in vivo* activity against many different human cancer cell lines.[10] The structures of a range of gold(III) chelates, which have Au–N bonds, that have been tested for cytotoxicity are shown in Scheme 2.

The two pyridyl gold(III) species, $[AuCl_3(Hpm)]$ and $[AuCl_2(pm)]$ (Scheme 2) have good cytotoxicity towards a range of human cancer cell lines, particularly human ovarian cancer cell lines. The results of these tests although promising were comparable to the

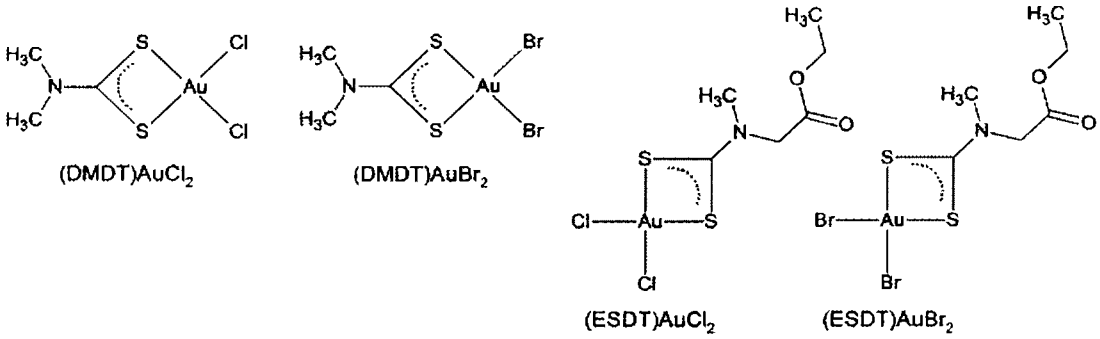
screening results of $NaAuCl_4$ which is their parent compound.[10] The other drawback of these compounds is that although stable in organic solutions, they are susceptible to reduction in aqueous buffer media, which limits their practical usefulness.[10,11] The bipyridine type complexes, $[Au(bipy)(OH)_2][PF_6]$ and [Au(bipy-H)(OH)][PF_6] were, on the other hand, found to be stable in aqueous buffer media. Unfortunately they were found to interact with calf thymus DNA only weakly. Despite this weak interaction with calf thymus DNA, both bipyridyl gold(III) complexes show IC_{50} values falling into the micromolar range against an ovarian carcinoma cell line. [Au(bipy-H)(OH)][PF_6] is the most active of the two compounds. The results of the tests against other ovarian cancer cell lines as well as leukemia cell lines were less encouraging.[9]

The gold(III) complexes with multidentate N-donor ligands; $[Au(phen)Cl_2]Cl$, $[Au(terpy)Cl]Cl_2$, $[AuCl(dien)]Cl_2$, $[Au(cyclam)](ClO_4)_2Cl$ and $[Au(en)_2]Cl_2$, showed reasonable stability in physiological buffer solutions at 37 °C. These gold(III) complexes have been greatly stabilized by the chelation of the gold(III) ion to polyamine ligands. This stabilization was evidenced by measurements of the reduction potentials of the complexes.[8,10] The stabilization was less evident for the less basic phenanthrene and terpyridine ligands.[8] With the exception of the complex $[Au(cyclam)](ClO_4)_2Cl$, all complexes exhibited good cytotoxicity against the human ovarian cancer cell line A2780. These complexes also exhibited good cytotoxicity towards the cisplatin-resistant A2780 ovarian cancer cell line; this suggests that gold(III) compounds might overcome the phenomenon of drug resistance.[8,10] The free ligands that were coordinated to a gold(III) ion to give the complexes were also screened against the same cancer cell lines to ensure that the cytotoxicity was a result of the presence of the gold(III) ion. These test results showed that the free ethylenediamine ligand was devoid of any activity. The potency of free phenanthrene and terpyridine, on the other hand, was comparable to that of the respective gold(III)complexes making the screening results of these chelates difficult to interpret. The study did, however, prove that the cytotoxicity of $[Au(en)_2]Cl_2$ was a direct consequence of the presence of the gold(III) ion.[10]

The complex $[Au(azpy)Cl_2]Cl$, which contains a bidentate N-donor ligand, exhibited promising cytotoxic activity in cisplatin-sensitive and cisplatin-resistant ovarian carcinoma and leukemia cancer cell lines. Interestingly, solutions of $[Au(azpy)Cl_2]Cl$

underwent a cyclization reaction under physiological conditions leading to the formation of a tricyclic cationic organic compound, which also exhibited good cytotoxic activity.[10,12]

The gold(III) dithiocarbamate complexes, are examples of gold(III) chelates with Au–S bond which are bound to ligands through a sulfur atom. Examples of dithiocarbamate complexes that have been screened against various cancer cell lines are shown below in Scheme 3.



Gold(III) chelates with sulfur-bound ligands.

Scheme 3

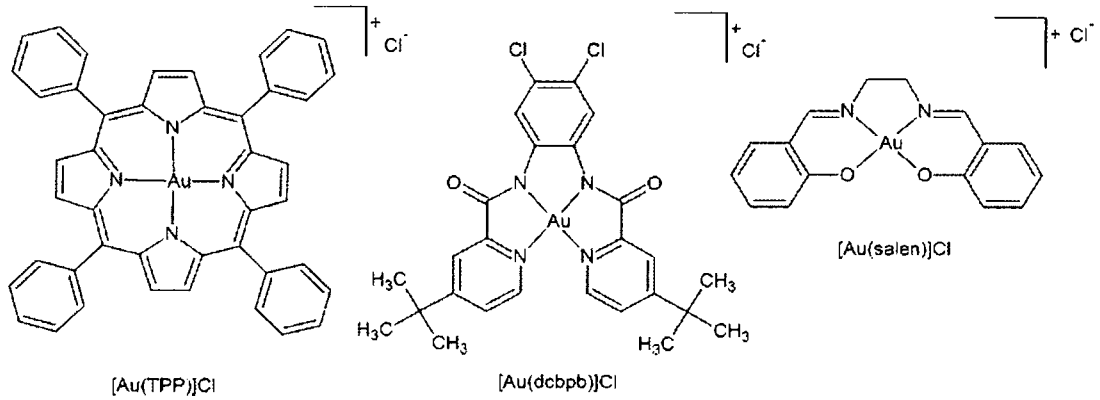
The Gold(III) dithiocarbamate complexes that have been screened against various human cancer cell lines exhibited greater cytotoxic effects compared to cisplatin. The complexes were also bioactive against drug resistant cancer cell lines and induced apoptosis.[6,7] The compounds have proven to be stabile under physiological conditions and readily bind to calf thymus DNA, inhibiting both DNA and RNA synthesis. Experiments on red blood cells indicated that haemolytic properties might contribute significantly to the bioactivity of the agents. The complexes triggered cancer cell death via apoptotic and non-apoptotic pathways and affected mitochondrial functions.[6,7,10] The free ligand ESDT (Scheme 3) did not exhibit proteosome inhibitory activity and the parent gold salts $KAuCl_4$ and $KAuBr_4$ also showed weaker inhibitory activities than $(ESDT)AuBr_2$.

Although the *in vitro* anti-cancer activity of gold(III) compounds has been documented for more than three decades, very few demonstrate promising *in vivo* anti-

cancer activities. Among the gold(III)compounds in the literature that have undergone *in vivo* testing are the gold(III) dithiocarbamate compounds, which inhibited approximately 50% growth of breast cancer cells a month after the first dose of the compound.[13]

Detailed background relating to the invention

The gold(III) chelates of this invention have tetradentate dianion ligands. More specifically they are $N_2N'_2$ tetradentate ligands and therefore are closely related to the highly cytotoxic gold(III) tetraarylporphyrins. The advantage of tetradentate ligands is that they are better able to stabilize the gold(III) cation against reduction under physiological conditions and are therefore potentially more useful as drugs.[5,9] Coordination of a tetradentate dianionic ligand to gold(III) gives a mono-cationic gold(III) compound having a planar geometry. These mono-cationic complexes have a similar overall structure to lipophilic organic cations, which have proven to be effective chemotherapeutic agents.[13] The structures of a selection of known gold(III) chelates with tetradentate, dianionic ligands[13] are set out in Scheme 4.



The structures of a selection of gold(III) chelates with tetradentate, dianionic ligands.[13]

Scheme 4

The gold(III) porphyrins have proven to be stable under physiological conditions. The complexes [Au(dcbpb)]Cl and [Au(salen)]Cl, on the other hand, show signs of slow decomposition under similar conditions.[13] [Au(TPP)]Cl has displayed promising anticancer activities toward a panel of human cancer cell lines including

nasopharyngeal carcinoma, promyelocytic leukaemia, hepatocellular carcinoma, cervical epithelioid carcinoma, and oral epidermoid carcinoma.[13] The IC_{50} values of [Au(TPP)]Cl ranged between 0.11 and 0.73 μM. These IC_{50} values show that [Au(TPP)]Cl is several hundred times more cytotoxic than cisplatin. This compound also shows significant cytotoxicity against KB-3-1 and its multi-drug resistant (KB-V1) variant. The latter possesses a high level of membrane P-glycoproteins, which exclude drugs such as vinblastine and doxorubicin.[13] To investigate the cytotoxic effect of [Au(TPP)]Cl on non-cancerous cells, the cytotoxicity toward peripheral blood mononuclear cells (PBMCs) from healthy individuals and CCD-19Lu cells, which is a fibroblast cell line derived from normal lung tissue, were examined. Results by MTT assay revealed that [Au(TPP)]Cl exhibits at least ten-fold higher cytotoxicity to cancer cells than non-cancerous cells.[13] The presence of gold(III) ions has been proven to be critical for the observed *in vitro* chemotherapeutic properties. This conclusion is based on the inactivity of $[Zn^{II}(TPP)]$. The zinc(II) analogue of [Au(TPP)]Cl exhibits an IC_{50} value greater than 50 μM. The gold(III) ion is unstable under physiological conditions as it undergoes reduction to colloidal gold. The porphyrin ligand is, however able to stabilize the gold(III) ion and it is hypothesized that $[Au(TPP)]^+$ acts as a stable lipophilic planar cation for binding to bio-molecular target(s) through non-covalent interactions.[13]

The cytotoxic properties of the gold(III) salen Schiff base complexes and the bis(pyridyl)carboxamide gold(III) complexes have also been evaluated.[13] These compounds have been shown to exhibit a cytotoxicity comparable to that of cisplatin with a IC_{50} values in the range of 10-30 μM.

There are two different pathways via which a compound can cause cell death, these are apoptosis and necrosis. Apoptosis is characterized by an ordered series of biochemical and biophysical reactions that are regulated by various genes, this is in contrast to necrosis which is premature cell death. While apoptosis often provides beneficial effects to the organism, necrosis is almost always detrimental, and can be fatal. Apoptosis does not trigger inflammatory tissue reactions, and thus is advantageous for cytotoxic chemotherapeutic agents to be able to induce apoptotic cell death as opposed to necrosis. The compound [Au(TPP)]Cl induced cytotoxicity in NPC cells via an apoptotic pathway.[13] By means of confocal imaging, typical apoptotic morphological changes were detected, including the formation of apoptotic bodies,

chromatin condensation and DNA fragmentation. The induced apoptosis was also confirmed by the oligonucleosomic degradation of cellular DNA, as this type of chromatin degradation is characteristic of apoptosis. These experiments confirm that [Au(TPP)]Cl induces apoptotic cell death in NPC cells as opposed to necrosis.[13] The dithiocarbamate gold(III) complexes were also found to cause apoptosis as opposed to necrosis[6,7] this would suggest that gold(III) chelates could potentially favour an apoptotic pathway as opposed to a necrotic pathway. This would make them more attractive chemotherapeutic agents.

Tetradentate Schiff base ligands comprising two pyrrole groups bridged by a synthetically variable di(azomethine) unit have been known for several decades.[14] However, studies of both the free base ligands as well as their metal chelates are quite limited.[14] Coordination of this class of ligands to a metal cation usually occurs with the concomitant deprotonation of the pyrrole NH groups, this means that they are $N_2N'_2$ tetradentate, dianionic ligands. The ligands have been previously bound to Ru(II), Pd(II), Ni(II), Co(III), Mn(II), Cu(II), Sm(II), Pt(II) and Fe(III).[15-23] Chelation of the former by the dianionic ligand will result in a neutral metal chelate, with the exception of Co(III) and Fe(III), which will give a monocationic complex. These metal chelates have been used as hydrogenation catalysts when coordinated to Pd(II)[16] as well as high efficiency red electrophosphorescence materials when chelated to Pt(II).[22] The complexes also show a similar coordination geometry, regardless of the electronic configuration of the metal ion. The metal ions exhibiting a nominally square planar coordination geometry, regardless of whether the bis(imine) linkage is aromatic or a straight or substituted alkyl group. The bridging does, however, affect the extent to which the metal ion is distorted from the optimum square planar geometry. Short bridges, of two carbons in length, whether aromatic or alkyl result in a smaller bite angle of the ligand. This small bite angle manifests itself as an acute N_{imine}–M–N_{imine} bond angle.[16,23] The longer three carbon bridge allows for a larger bite angle and the N_{imine}–M–N_{imine} bond angle therefore tends towards a right angle.[16]

The free base bis(pyrrole-imine) compounds have been shown to exhibit fascinating supramolecular structures both with aromatic[24] and alkyl[14] bridges. The pyrrole N-H and imine type nitrogen atoms form a highly predictable hydrogen bonding motif. The compounds with aromatic bridges have even been used to form distinct

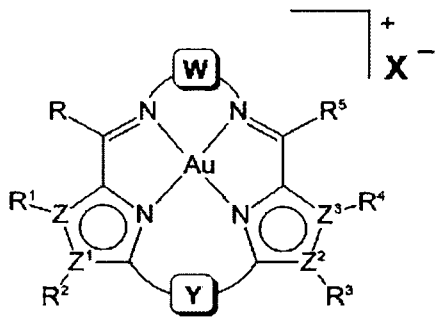
nanostructures, with the effect of isomeric molecules being examined in an attempt to try and further understand the self assembly of organic molecules into distinct nanostructures.[24]

The invention

The present invention provides new classes of gold(III) bis(pyrrolide-imine) and bis(imidazolato-imine) compounds. Several of these compounds have been shown to be cytotoxic towards a wide range of human cancer cell lines having an activity similar to, or better than, cisplatin which is currently the industry standard. The most active compound has been proven *in vitro* to be a poison of topoisomerase II at low concentrations (EC_{50} = 0.5 μM) and a catalytic inhibitor of the enzyme at higher concentrations (50 μM).

An extensive search of the literature as well as the Cambridge Structural Database (CSD) has confirmed that the gold(III) chelates of the invention are new. Neither the structures nor the syntheses of the bis(pyrrolide-imine) and bis(imidazolato-imine) gold(III) Schiff base complexes of the invention have been reported and, accordingly, there has been no report of the use of the gold(III) chelates of the invention as cytotoxic agents for the treatment of cancer.

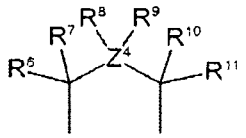
According to a first aspect of the invention, there is provided a compound selected from compounds of the Formula (I),



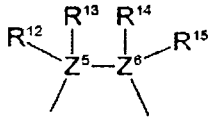
(I)

in which

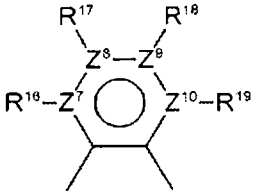
W is independently selected from W^1, W^2, W^3, W^4, W^5,



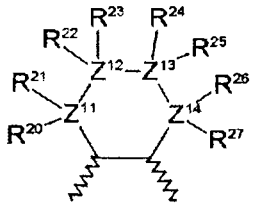
W^1



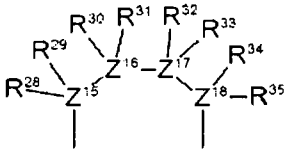
W^2



W^3



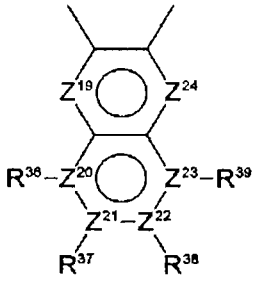
W^4



W^5

or W represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl or C_1-C_6 amide in which the amide is optionally part of a linking chain, and the Z^n–$Z^{n'}$ bonds (n = 4–17; n' = n + 1) are optionally of any whole or partial bond order,

Y is Y^1



Y^1

or Y represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl,

or Y is optionally a bridging structure that may comprise one or more C_1-C_6 amide, C_1-C_6 ether, or C_1-C_6 ester groups,

$R–R^{39}$ are independently selected from no substituent, a lone pair of electrons, H, halogen, C_5-C_6 aryl, C_1-C_{12} alkyl, amine, C_1-C_6 alkylamine, C_1-C_6 amide, nitro, cyano, carboxyl, C_1-C_6 ester, phosphane, thiol, C_1-C_6 thioether, OR^{40}, and suitable pairs of adjacent R groups ($R–R^{39}$) may optionally together form part of a C_5 or C_6 aryl ring, a Z_5 or Z_6 ring,

R^{40} is independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl, C_1-C_6 ester, poly(-C_2O-), amine, and C_1-C_6 alkylamine,

$Z–Z^{24}$ are independently selected from C, N, P, O, and S, and

X^- is a pharmaceutically acceptable anion.

The anion X^- may be selected from halide, hexafluorophosphate, nitrate, and triflate.

Examples of representative structurally characterized and tested compounds of the invention are the following compounds.

Compound 1.1a (MA_AuPr) in which chelate substituents $R–R^5$ are H, $Z–Z^3$ are C, the bridge W is $–CH_2CH_2CH_2–$, Y is 2H, and the anion X is Cl^-.
Compound 1.1b (MA_AuDM) in which chelate substituents $R–R^5$ are H, $Z–Z^3$ are C, the bridge W is $–CH_2C(CH_3)_2CH_2–$, Y is 2H, and the anion X is Cl^-.
Compound 1.1c (MA_AuOH) in which chelate substituents $R–R^5$ are H, $Z–Z^3$ are C, the bridge W is $–CH_2CH(OH)CH_2–$, Y is 2H, and the anion X is Cl^-.
Compound 1.1Y^1a (KA_AumacroPr) in which chelate substituents $R–R^5$ are H, $Z–Z^3$ are C, the bridge W is $–CH_2CH_2CH_2–$, Y is Y^1, where $R^{46}–R^{49}$ are H, Z^{29} and Z^{34} are N, $Z^{30}–Z^{33}$ are C, and the anion X is PF_6^-.
Compound 1.1Y^1b (KA_AumacroDM) in which chelate substituents $R–R^5$ are H, $Z–Z^3$ are C, the bridge W is $–CH_2C(CH_3)_2CH_2–$, Y is Y^1, where $R^{46}–R^{49}$ are H, Z^{29} and Z^{34} are N, $Z^{30}–Z^{33}$ are C, and the anion X is PF_6^-.
Compound 1.5Y^1a (KA_AumacroBu) in which chelate substituents $R–R^5$ are H, $Z–Z^3$ are C, the bridge W is $–CH_2CH_2CH_2CH_2–$, Y is Y^1, where $R^{46}–R^{49}$ are H, Z^{29} and Z^{34} are N, $Z^{30}–Z^{33}$ are C, and the anion X is PF_6^-.

Compound 1.1f (KA_AuMeImPr) in which chelate substituents R and R^5 are H, R^1 and R^4 are CH_3, R^2 and R^3 are lone pairs of electrons, Z and Z^3 are C, Z^1 and Z^2 are N, the bridge W is $-CH_2CH_2CH_2-$, Y is 2H, and the anion X is PF_6^-.
Compound 1.1g (KA_AuMeImDM) in which chelate substituents R and R^5 are H, R^1 and R^4 are CH_3, R^2 and R^3 are lone pairs of electrons, Z and Z^3 are C, Z^1 and Z^2 are N, the bridge W is $-CH_2C(CH_3)CH_2-$, Y is 2H, and the anion X is PF_6^-

Schemes 5a, 5b, and 5c show, by way of illustration of the parent derivatives of each new class of gold(III) chelates, partially labeled thermal ellipsoid diagrams of the X-ray crystal structures of MA_AuPr (compound 1.1a), KA_AumacroPr (compound $1.1Y^1a$), and KA_AuMeImPr (compound 1.1f), respectively.

The single crystal X-ray structural data for compounds 1.1a, 1.1f, and $1.1Y^1a$ are summarized in Table 1. Other crystallographically characterized complexes of the invention are summarized in Table 2.

Table 1

Crystal data and structure refinement details for MA_AuPr (1.1a), KA_AumacroPr ($1.1Y^1a$), and KA_AuMeImPr (1.1f).

Compound	MA_AuPr	KA_AumacroPr	KA_AuMeImPr
Formula	$C_{13}H_{14}AuClN_4$	$C_{21}H_{16}AuN_6F_6P$	$C_{13}H_{16}AuF_6N_6P$
Cell setting	Triclinic	Monoclinic	Monoclinic
Space group	P-1	*P2/c*	*Cc*
Formula weight	458.70	694.33	598.25
a/Å, b/Å, c/Å	7.5888(4), 9.4183(3), 10.5118(4)	16.473(5), 6.980(5), 18.804(5)	16.348(5), 12.015(5), 9.488(5)
α/°, β/°, γ/°	68.707(4), 72.787(4), 72.194(4)	90, 105.675(5), 90	90, 106.865(5), 90
T / K	140(2)	173(2)	295(2)
Z	2	4	4
V / Å^3	651.86(5)	2081.7(17)	1783.5(13)

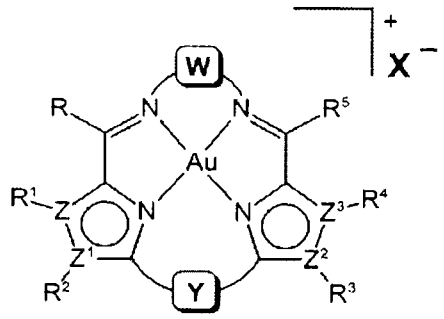
Density (g cm^{-3})	2.337	2.2155	2.228
μ (mm^{-1})	11.479	7.220	8.410
Crystal Dimensions (mm^3)	0.10 x 0.10 x 0.10	0.50 × 0.02 × 0.01	0.45 × 0.25 × 0.15
Radiation λ (Å)	0.71073	0.71073	0.71073
Total Data Collected	10737	14581	6002
Unique Data	4510 [R(int)] = 0.0173	4010 [R(int)] = 0.060	2635 [R(int)] = 0.032
Refinement Method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Goodness-of-fit on F^2	1.032	0.940	1.020
Final *R* indices [I>2sigma(I)]	R_1 = 0.0165 wR_2 = 0.0403	R_1 = 0.0320 wR_2 = 0.0703	R_1 = 0.0271 wR_2 = 0.0660
Final *R* indices [all data]	R_1 = 0.0189 wR_2 = 0.0406	R_1 = 0.0452 wR_2 = 0.0733	R_1 = 0.0288 wR_2 = 0.0655
Largest diff. peak/hole	1.697/-1.902	2.282/-1.453	0.134/ -1.296

It is noteworthy that other anions may be used to crystallize the cations of this invention. For example, we have recently acquired X-ray data for the triflate salt of KA_aumacroDM ($C_{24}H_{20}AuF_3N_6O_3S$, monoclinic space group *Cc*, *a* = 17.092(5) Å, *b* = 25.520(5) Å, *c* = 13.625(5) Å, α = 90°, β = 119.057(5)°, γ = 90°, *V* = 5195(3) $Å^3$, *Z* = 8, *T* = -153(2) °C).

The Applicant has found that MA_AuPr (1.1a), by way of example, has several advantages over currently available inorganic chemotherapeutic agents in clinical use. Firstly, the synthesis of the ligands belonging to the 1.1a–1.1f series of compounds is a simple one-pot reaction, requiring minimal purification. Chelation of the ligand to gold(III) is simple and gives a clean easily re-crystallized product. Derivatization of the parent ligand was found to be possible and different derivatives showed varying activity, suggesting that there is a structure/activity relationship between the different derivatives. *In vitro* testing showed that the chelate 1.1a was more effective than cisplatin against *ca.* 25% of the 60 human cancer cell lines against which it was tested.

The *in vitro* mechanism of action of the drug has been established and is highly specific. This indicates that the activity of the drug can be carefully controlled.

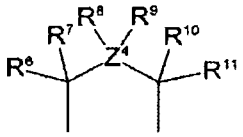
According to a second aspect of the invention, there is provided a compound selected from compounds of the Formula (I),



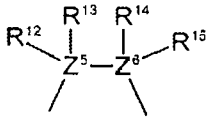
(I)

in which

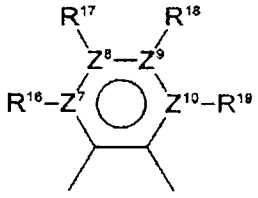
W is independently selected from W^1, W^2, W^3, W^4, W^5,



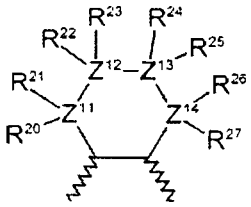
W^1



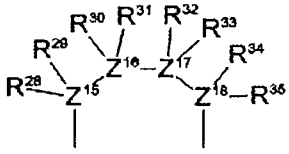
W^2



W^3



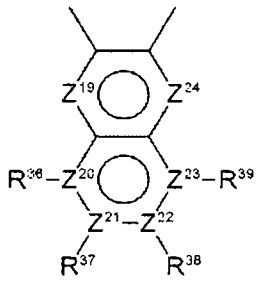
W^4



W^5

or W represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl or C_1-C_6 amide in which the amide is optionally part of a linking chain, and the Z^n–$Z^{n'}$ bonds (n = 4–17; n' = n + 1) are optionally of any whole or partial bond order,

Y is Y^1



Y^1

or Y represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl,

or Y is optionally a bridging structure that may comprise one or more C_1-C_6 amide, C_1-C_6 ether, or C_1-C_6 ester groups,

R–R^{39} are independently selected from no substituent, a lone pair of electrons, H, halogen, C_5-C_6 aryl, C_1-C_{12} alkyl, amine, C_1-C_6 alkylamine, C_1-C_6 amide, nitro, cyano, carboxyl, C_1-C_6 ester, phosphane, thiol, C_1-C_6 thioether, OR^{40}, and suitable pairs of adjacent R groups (R–R^{39}) may optionally together form part of a C_5 or C_6 aryl ring, a Z_5 or Z_6 ring,

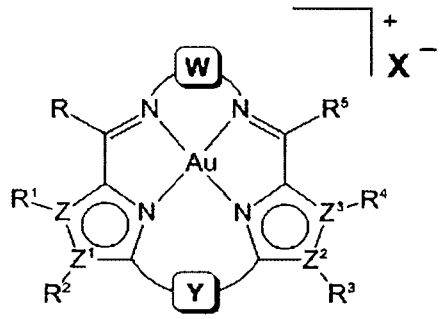
R^{40} is independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl, C_1-C_6 ester, poly(-C_2O-), amine, and C_1-C_6 alkylamine,

Z–Z^{24} are independently selected from C, N, P, O, and S, and

X^- is a pharmaceutically acceptable anion for the treatment of cancer.

The anion X^- may be selected from halide, hexafluorophosphate, nitrate, and triflate.

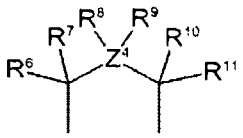
According to a third aspect of the invention, there is provided a pharmaceutical composition, the composition including at least one compound selected from compounds of the Formula (I),



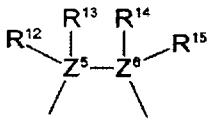
(I)

in which

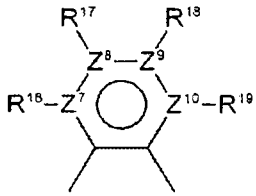
W is independently selected from W^1, W^2, W^3, W^4, W^5,



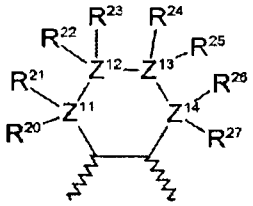
W^1



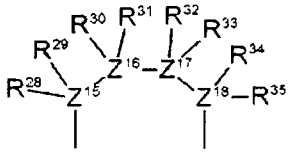
W^2



W^3



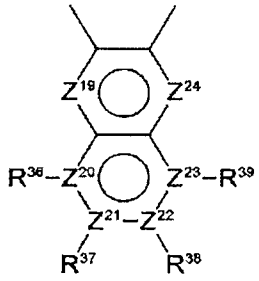
W^4



W^5

or W represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl or C_1-C_6 amide in which the amide is optionally part of a linking chain, and the Z^n–$Z^{n'}$ bonds (n = 4–17; n' = n + 1) are optionally of any whole or partial bond order,

Y is Y^1



Y^1

or Y represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl,

or Y is optionally a bridging structure that may comprise one or more C_1-C_6 amide, C_1-C_6 ether, or C_1-C_6 ester groups,

R–R^{39} are independently selected from no substituent, a lone pair of electrons, H, halogen, C_5-C_6 aryl, C_1-C_{12} alkyl, amine, C_1-C_6 alkylamine, C_1-C_6 amide, nitro, cyano, carboxyl, C_1-C_6 ester, phosphane, thiol, C_1-C_6 thioether, OR^{40}, and suitable pairs of adjacent R groups (R–R^{39}) may optionally together form part of a C_5 or C_6 aryl ring, a Z_5 or Z_6 ring,

R^{40} is independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl, C_1-C_6 ester, poly(-C_2O-), amine, and C_1-C_6 alkylamine,

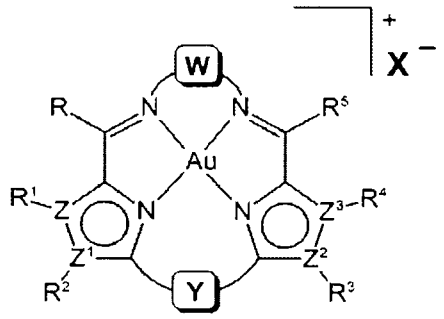
Z–Z^{24} are independently selected from C, N, P, O, and S, and

X^- is a pharmaceutically acceptable anion.

The anion X^- may be selected from halide, hexafluorophosphate, nitrate, and triflate.

The pharmaceutical composition may be for use in the treatment of cancer.

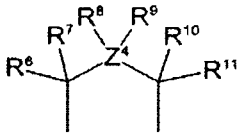
According to a fourth aspect of the invention, there is provided a method of treating cancer, the method including the step of administering, to a subject in need of treatment, a pharmaceutically effective amount of at least one compound selected from compounds of Formula (I),



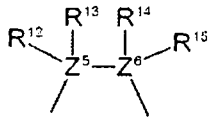
(I)

in which

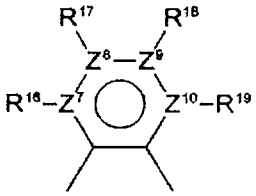
W is independently selected from W^1, W^2, W^3, W^4, W^5,



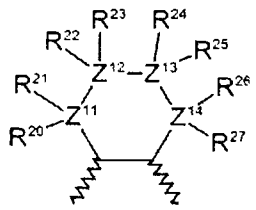
W^1



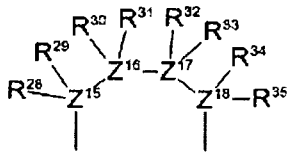
W^2



W^3



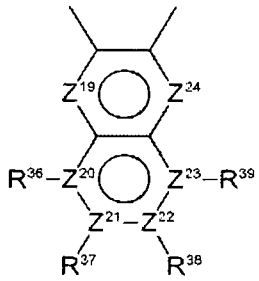
W^4



W^5

or W represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl or C_1-C_6 amide in which the amide is optionally part of a linking chain, and the Z^n–$Z^{n'}$ bonds (n = 4–17; n' = n + 1) are optionally of any whole or partial bond order,

Y is Y^1



Y^1

or Y represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl,

or Y is optionally a bridging structure that may comprise one or more C_1-C_6 amide, C_1-C_6 ether, or C_1-C_6 ester groups,

R–R^{39} are independently selected from no substituent, a lone pair of electrons, H, halogen, C_5-C_6 aryl, C_1-C_{12} alkyl, amine, C_1-C_6 alkylamine, C_1-C_6 amide, nitro, cyano, carboxyl, C_1-C_6 ester, phosphane, thiol, C_1-C_6 thioether, OR^{40}, and suitable pairs of adjacent R groups (R–R^{39}) may optionally together form part of a C_5 or C_6 aryl ring, a Z_5 or Z_6 ring,

R^{40} is independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl, C_1-C_6 ester, poly(-C_2O-), amine, and C_1-C_6 alkylamine,

Z–Z^{24} are independently selected from C, N, P, O, and S, and

X^- is a pharmaceutically acceptable anion.

The anion X^- may be selected from halide, hexafluorophosphate, nitrate, and triflate.

According to a fifth aspect of the invention, there is provided the use of a compound selected from compounds of Formula (I) has hereinbefore described in the manufacture of a medicament for the treatment of cancer.

The invention described thus provides a new class of gold(III) bis(pyrrolide-imine) and bis(imidazolato-imine) Schiff base complexes for use as novel anticancer chemotherapeutic agents. These complexes consist of a central gold(III) ion chelated by a $N_2N'_2$ tetradentate bis(N-heterocycle-imine) type ligand. Upon coordination of the gold(III) ion, the two pyrrole-type nitrogen atoms (N–H groups) are deprotonated, giving the ligand an overall charge of –2. The metal ion complex therefore has an overall charge of +1; hence the chelates are associated with an anion. The complexes were designed to be predominantly planar which allows the gold(III) chelates to intercalate between DNA base pairs. The overall charge on the cation allows for favorable electrostatic interactions with the negatively charged phosphate backbone of the DNA double helix. The molecular target for the gold(III) complexes is thus DNA (and possibly also related nucleotides). Once the drug has intercalated genomic DNA in cells, it prevents DNA transcription (and thus cell growth), separation of daughter chromatids during mitosis (and thus cell division), and/or maintenance of the DNA duplex by interfering specifically with the normal functioning of either of the essential enzymes topoisomerase I or topoisomerase II. Compound 1.1a, for example, acts as a topoisomerase II poison at low concentrations and an inhibitor of the enzyme at high concentrations (topoisomerase II is critical for cell replication, being responsible for the decatenation of daughter chromatids during mitosis). Compound $1.1Y^1a$ (KA_AumacroPr), on the other hand, acts as a catalytic inhibitor of both topoisomerase I and topoisomerase II.

The gold(III) chelates of the invention are novel in design and structure and their mode of synthesis is novel. The complexes are readily crystallized, easily purified, and have been fully characterized. The complexes exhibit a highly specific mode of action (all of the compounds target topoisomerase II and some also target topoisomerase I). The most active compound shows good activity (mean GI_{50} = 7 μM; mean IC_{50} = 20 μM) against multiple cancer cell lines over the full NCI-60 screen. The mechanism of action has been proven to be dependent on the presence of the gold(III) ion since the metal-free complexes are inactive.

In preferred embodiments of the invention, Y may represent two hydrogen atoms or Y^1. For example, Y may be Y^1, and Z^{19} and Z^{24} may be N. In another preferred embodiment Z^{20}-Z^{23} may be C.

The groups R-R^5 may be selected from H, C_1-C_3 alkyl, O-C_1-C_3 alkyl, hydroxyl and halogen. In particular the C_1-C_3 alkyl group may be a methyl group, the O-C_1-C_3 alkyl group may be an O-ethyl group and the halogen may be chlorine.

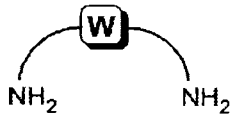
In other preferred embodiments W may be selected from W^1, W^2, W^3 or W^4. The groups R^6-R^{27} may then be selected from H, C_1-C_3 alkyl, O-C_1-C_3 alkyl and halogen. The C_1-C_3 alkyl group may be a methyl group, the O-C_1-C_3 alkyl may be an O-ethyl group and the halogen may be chlorine.

More preferred compounds are compounds selected from:
2,2'-{propane-1,3-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) chloride,
2,2'-{(2,2-dimethylpropane-1,3-diyl)bis[nitrilo(*E*)methylylidene]} bis(pyrrol-1-ido)gold(III) chloride,
2,2'-{(2-hydroxypropane-1,3-diyl)bis[nitrilo(*E*) methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(2-ethoxypropane-1,3-diyl)bis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(2-chloropropane-1,3-diyl)bis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{ethane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(2*S*)-propane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(1*R*,2*R*)-cyclohexane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(1*S*,2*S*)-cyclohexane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{cyclohexane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V)

2,2'-{(4-methylbenzene-1,2-diyl)bis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) nitrate(V),
4,4'-{propane-1,3-diyl)bis[nitrilo(*E*)methylylidene]}bis(5-methylimidazol-1-ide)gold(III) hexafluorophosphate(V),
4,4'-{(2,2-dimethylpropane-1,3-diyl)bis[nitrilo(*E*)methylylidene]}bis(5-methylimidazol-1-ide)gold(III) hexaflurophosphate(V),
{12,13-dihydro-14H-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V),
{12,14-dihydro-13,13-dimethyl-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V),
{12,13,14,15-tetrahydro-6,9:18,21-diepimino[1,6]diazacycloctadecino[12,13-b]quinoxalinato}gold(III) hexafluorophosphate(V), and
{13-chloro-12,14-dihydro-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V).

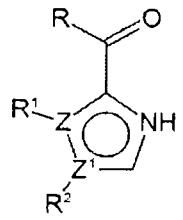
The invention extends further to a pharmaceutical composition comprising at least one compound as hereinbefore described.

The invention extends to a method of preparing a compound of Formula (I), which includes the steps of condensing a diamine of the general formula A

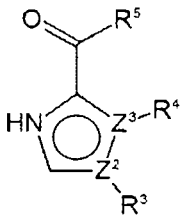


A

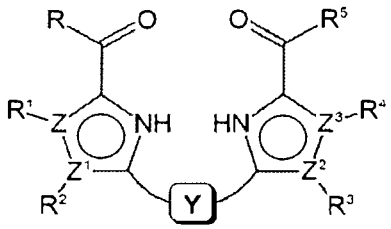
simultaneously or consecutively with a carbonyl compound selected from compounds of the general formula B, C and D



B

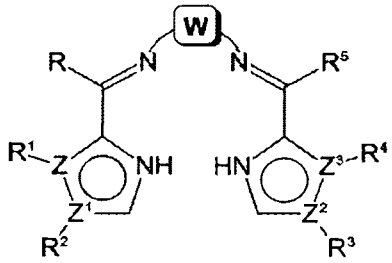


C

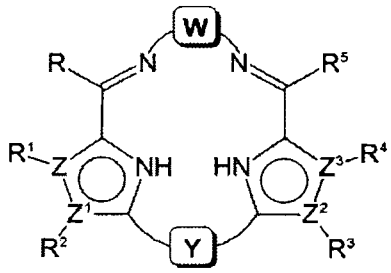


D

to produce a diimine Schiff base of the general formula E or F



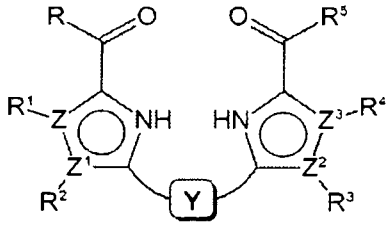
E



F

and reacting the diimine of general formula E or F with a tetraalkylammonium tetrahaloaurate(III) to produce the gold(III) compound of the general Formula (I) in which W, Y, R, Z and X are as hereinbefore described.

The invention extends further to a method of preparing a compound of general Formula (I), which includes the step of reacting a carbonyl compound of the general formula D



D

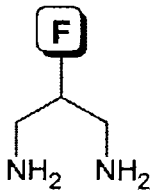
with a tetraalkylammonium tetrahaloaurate(III) and a diamine to produce the compound of general Formula (I) in which W, Y, R, Z and X are as hereinbefore described. The

tetraalkylammonium tetrahaloaurate(III) may be tetrabutylammonium tetrachloroaurate(III). The butyl group may be a *t*-butyl group.

The method may include reacting the diamine with the tetraalkylammonium tetrahaloaurate (III) in the presence of a salt selected from halides, hexafluorophosphates, nitrates, and triflates to produce the corresponding compound of Formula (I) in which X^- is the corresponding anion. In particular, the salt may be a tetraalkylammonium hexafluorophosphate such as tetra-*t*-butylammonium hexafluorophosphate.

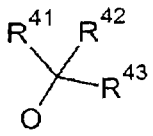
Where the compound of Formula (I) is a chloride the method may include the further step of reacting the compound of Formula (I) in which X^- is chloride with a salt selected from halides other than chloride, hexafluorophosphates, nitrates, and triflates to produce a compound of Formula (I) in which X^- is the anion of the said salt.

The invention extends to a method of preparing a 2-substituted 1,3-diamine intermediate of the general formula A^1



A^1

or its dihydrochloride salt, in which F is selected from F^1 or halogen,



F^1

in which

R^{41}-R^{43} are independently selected, H, halogen, Z_5 or Z_6 aryl, C_1-C_{12} alkyl, C_1-C_6 alkylamine, C_1-C_6 amide, carboxyl, C_1-C_6 ester or OR^{40},

R^{40} is as hereinbefore described, or

suitable pairs of adjacent R groups (R^{41}-R^{43}) optionally together form part of a C_5 or C_6 aryl ring, or

F is R^{44}, and

R^{44} is independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl, C_1-C_6 ester, poly(-C_2O-), amine, C_1-C_6 alkylamine, and C_1-C_6 amide or a Z_5 or Z_6 ring, and

Z_5 and Z_6 are as hereinbefore described,

the method including the steps of converting the hydroxyl group of 2,2,12,12-*t*-methyl-3,11-dioxo-4,10-dioxa-5,9-diazatridecan-7-ol to the group F.

The invention extends to bis(pyrrole-imine) ligands selected from:
2-ethoxy-*N*,*N*'-bis[(*E*)-1*H*-pyrrol-2-ylmethylidene]propane-1,3-diamine, and
2-chloro-*N*,*N*'-bis[(*E*)-1*H*-pyrrol-2-ylmethylidene]propane-1,3-diamine.

The invention extends further to a method for the preparation of tetrabutylammonium tetrachloroaurate, $[Bu_4N][AuCl_4]$, the method including the step of extracting $[Bu_4N][AuCl_4]$ from a mixture using an organic solvent-extraction purification step to produce an acid-free, crystalline $[Bu_4N][AuCl_4]$. The method may include reacting an aqueous solution of $H[AuCl_4]$ and $[Bu_4N][HSO_4]$ to produce the mixture and extracting the $[Bu_4N][AuCl_4]$ from the mixture with the organic solvent.

The invention is now illustrated, by way of example, with reference to the following examples.

Scheme 1 *Auranofin*

Scheme 5a *Partially labeled thermal ellipsoid diagram of the X-ray crystal structure of MA_AuPr. Ellipsoids are rendered as 50% probability surfaces; H atoms are of an arbitrary radius.*

Scheme 5b *Partially labeled thermal ellipsoid diagram of the X-ray crystal structure of KA_AumacroPr. Ellipsoids are rendered as 50% probability surfaces; H atoms are of an arbitrary radius.*

Scheme 5c *Partially labeled thermal ellipsoid diagram of the X-ray crystal structure of A_AuMeImPr. Ellipsoids are rendered as 30% probability surfaces; H atoms are of an arbitrary radius.*

Scheme 6a *Single-dose screening results for MA_AuPr over 60 human cancer cell lines. A negative growth percent is favorable and shows up as a positive bar on the graph.*

Scheme 6b *Single-dose screening results for KA_AumacroPr over 60 human cancer cell lines. A negative growth percent is favorable and shows up as a positive bar on the graph.*

Scheme 6c *Single-dose screening results for KA_AuMeImPr over 60 human cancer cell lines. A negative growth percent is favorable and shows up as a positive bar on the graph.*

Scheme 8a *Dose-response curves for three commercial anticancer drugs (cisplatin, mitomycin, camptothecin) and three Au(III) chelates. The more abrupt the curve, the harder the dose-response function.*

Scheme 8b *Dose-response curves (HeLa cells, pH 7.0, 37 °C) for three macrocyclic Au(III) chelates. IC_{50} values for the complexes against HeLa cells obtained from the least squares data fits (graph) are given in the 3rd column of the table.*

Scheme 9 *Plot of $-\log(GI_{50}/M)$ for MA_AuPr versus the equivalent data for cisplatin.*

Scheme 10a *Comparison of $-\log(GI_{50})$ values for MA_AuPr with commercially available anticancer drugs for selected human cancer cell lines.*

Scheme 10b *Comparison of $-\log(GI_{50})$ values for MA_AuPr and MA_AuDM with commercially available anticancer drugs for selected human cancer cell lines.*

Scheme 11 *Comparison of the activity profiles of commercial drugs with a known mechanism of action and the two Au(III) chelates MA_AuPr and MA_AuDM. (Group average method, Minkowski distance.)*

Scheme 12 *EB gel showing the poisoning at low concentrations (0.5 μM) and catalytic inhibition at higher concentrations (50 μM) of topoisomerase II activity on supercoiled plasmid DNA substrate by MA_AuPr.*

Scheme 13 *EB gel showing the inactivity of MA_AuPr against topoisomerase I compared to the chemotherapeutic agent CPT (camptothecin), which is specifically a topoisomerase I poison.*

Scheme 14 *EB gel showing the inactivity of MA_H2PrLig (the metal-free ligand) against topoisomerase II compared to the chemotherapeutic agent VP-16 (etoposide), which is specifically a topoisomerase II poison. There is evidence of weak DNA-cleavage induction in the presence of topoisomerase II from the free ligand at 500 μM concentration.*

Scheme 15 *EB gel showing the diminished activity of MA_PdPr (the Pd^{2+} analogue of MA_AuPr) against topoisomerase II compared to the chemotherapeutic agent VP-16 (etoposide), which is specifically a topoisomerase II poison. There is evidence of DNA-cleavage induction in the presence of topoisomerase II at 50 μM concentration (a 100-fold weaker effect than the gold(III) complex).*

Scheme 16 *Top: agarose gel electrophoresis topoisomerase II (topo II) DNA cleavage assay (66 ng kinetoplast DNA, 4 U topo II) as a function of the concentration of KA_AumacroPr (complex $1.1Y^1a$). Lanes 1–4 contain catenated DNA (no topo II), decatenated DNA (topo II present), decatenated DNA (solvent control), and linear DNA, respectively. The lane marked VP-16 contained DNA, topo II, and etoposide (VP-16). Band labels: I, catenated DNA; II, open-circular (OC) DNA; III, linear DNA; IV, closed-covalently circular (CCC) DNA. Lanes 5–13 included compound $1.1Y^1a$ from 5 nM to 500 nM in 10-fold concentration increments, respectively. Bottom: standard dose-response function fit of the experimental titration data (top gel) with (solid line) and without (dashed line) a Hill coefficient. The maximum ESD from triplicate measurements is shown (15%).*

Scheme 17 *Inhibition of human topoisomerase I by KA_AumacroPr as determined by supercoiled plasmid DNA relaxation assay (agarose gel electrophoresis).*

Lanes 2–12 have 5U of topoisomerase I. The enzyme fully relaxes supercoiled (SC) DNA in lanes 3–8 for KA_AumacroPr concentrations ranging from 0–50 nM. At concentrations from 500 nM–500 μM, topoisomerase I exhibits abnormal and incomplete substrate relaxation.

Scheme 18 *Titration of MA_AuPr (1.1a) with calf-thymus DNA in aqueous pH 7 phosphate buffer at 37 °C. The data indicate that compound 1.1a is a DNA intercalator.*

Scheme 23 *Graph of 3LL tumor growth in black mice (mean data for 6 subjects) as a function of time and type of anticancer drug. MA_AuPr was administered at a dose of 20 μmol/kg twice weekly and cisplatin at a dose of 26 μmol/kg once weekly. Untreated mice were the control.*

Scheme 24 *Mouse survival data as a function of metallodrug dose for MA_AuPr. The graph plots the survival of five groups of four mice on drug concentrations ranging from 1 to 30 μmol/kg for the displayed injection protocols.*

Example 1

In vitro anti-cancer tests

The gold(III) complexes of this invention were screened by the National Cancer Institute (NCI, USA) against their panel of 60 different human cancer cell lines. These screens initially entail a one-dose test for the compound at a high concentration (10 μM; e.g. Schemes 6a-6c). Compounds with a good cytotoxicity profile in the one-dose screen are then subjected to a five-dose screen for the full panel of sixty human cancer cell lines (the so-called 5-dose NCI-60 screen). In the full five-dose screen, the compound concentration is varied in five doses from 10^{-8} M to 10^{-4} M in order to establish a dose-response function of percentage cell growth versus the concentration of the test agent. The latter data permits determination of several key parameters indicative of a compound's cytotoxicity, namely, the GI_{50}, IC_{50}, and LC_{50} values for the test agent (these are the concentrations at which 50% growth inhibition, total growth inhibition, and 50% cell death occur, respectively). These data from 5-dose NCI-60

screens are summarized in Scheme 7 for selected chelates of this invention (by way of illustration). Similar data will shortly be available for compounds 1.1Y^1b and 1.5Y^1a as these derivatives are in 5-dose screens currently at the NCI.

The results of one-dose NCI-60 screens are noteworthy and merit some discussion as they quickly indicate activity profiles, cell-line specificity, and general cytotoxicity for the test agents across multiple human cancer cell lines. Schemes 6a, 6b, and 6c set out the one-dose screening results for MA_AuPr (Scheme 6a), KA_AumacroPr (Scheme 6b), and KA_AuMeImPr (Scheme 6c) obtained by the NCI. These three compounds are the parent derivatives that are representative of the three new types of gold(III) Schiff base chelate relevant to this invention. All other compounds synthesized as part of this invention have been similarly analyzed.

The preliminary cell screening data indicated that the three classes of compounds are inherently more toxic towards some cancer cell lines than others. This suggests that the compounds of the invention are not merely general poisons, but in fact agents with some tumor specificity and specific cellular mechanisms of action. From Schemes 6a–6c, leukemia, breast, and colon cancer cell lines are inherently more susceptible to the cytotoxic action of MA_AuPr. Breast and leukemia cell lines were, as a group, the most sensitive to KA_AuMeImPr while the macrocyclic derivative KA_AumacroPr showed good cytotoxicity for the majority of the cell lines constituting the groups: (i) non-small lung cancer, (ii) central nervous system cancer, (iii) renal carcinoma, and (iv) breast cancer.

Complexes 1.1a, 1.1b, and 1.1Y^1b were selected by the NCI for a five-dose screen against the full panel of 60 different human cancer cell lines to establish IC_{50} values and other parameters.

Complex 1.1c (with a hydroxyl group in the propyl bridge, MA_AuOH) was not sufficiently active in cell cultures to warrant a five-dose screen. The Applicant is of the opinion that cancer cells may have an active defense mechanism against 1.1c, e.g., an efflux pump or derivatization to an inactive form. The hydroxyl group is clearly implicated in the inactivity of the compound because 1.1a which lacks the hydroxyl group is highly active. A summary of the average cytotoxicity data over 60 human

cancer cell lines for 1.1a–1.1c and comparison with selected commercial and patented cytotoxic agents is shown in Scheme 7. Dose-response curves for three commercial anticancer drugs (cisplatin, mitomycin, camptothecin) and three Au(III) chelates are shown in Scheme 8a. The more abrupt the curve, the harder the dose-response function. Scheme 8b shows dose-response curves obtained with HeLa cells incubated with the macrocyclic gold(III) complexes $1.1Y^1a$, $1.1Y^1b$, and $1.5Y^1a$ at 37 °C. The data indicate that the complex with the butyl chain as the bridging group W (complex $1.5Y^1a$) has very good cytotoxicity with a sub-micromolar IC_{50} value of 370 nM; complexes $1.1Y^1a$ and $1.1Y^1b$ were also cytotoxic and had IC_{50} values of ca. 3 μM.

Drug	GI_{50} (μM)	TGI or IC_{50} (μM)	LC_{50} (μM)
MA_AuOH (*)	> 100	>100	>100
MA_AuDM (*)	12	31	72
MA_AuPr (*)	7(1)	20(3)	49(5)
cis-$[PtCl_2(NH_3)_2]$	2	27	>100
$[Au^{III}(terpy)Cl]Cl_2$	0.13	11	73
Mitomycin	0.71	6.5	18
Camptothecin	0.04	0.89	33

(*): This work.

Summary of the average cytotoxicity data over 60 human cancer cell lines for 1.1a-c and comparison with selected commercial and patented cytotoxic agents

Scheme 7

The mean cytotoxicity data summarized in Scheme 7 were compiled over 60 human cancer cell lines from the NCI database. The experimental parameters GI_{50}, IC_{50}, and LC_{50}, are mean concentrations at which 50% growth inhibition, 100% (total) growth inhibition, and 50% cell death occur, respectively. The data show that MA_AuPr is somewhat more cytotoxic than cisplatin and carboplatin when comparing the IC_{50} and LC_{50} values. The dose-response curves for the bis(pyrrolide-imine) chelates of the invention are steeper, or harder, than those of all the compounds compared in Scheme 7. Of the other drugs shown, only mitomycin (a powerful organic DNA alkylating and cross-linking agent) exhibits a comparably steep mean dose-response function.

The important features to note from the data in Scheme 7 and Schemes 8a and 8b are the following: (i) MA_AuPr has a lower LC_{50} value than the other Pt(II) and Au(III) compounds and a comparable LC_{50} value to camptothecin (a potent topoisomerase I poison). (ii) MA_AuPr has a better IC_{50} value than cisplatin and carboplatin. The hard dose-response function of MA_AuPr means that the therapeutic dose *in vitro* has a narrow window. Thus, 50% growth inhibition, on average, requires a relatively high concentration of the compound (7 μM). However, only a 7-fold increase in concentration to 49 μM effects a 50% cell kill (again on average, and over the full 60 cell lines). In contrast, a potent drug such as camptothecin requires an 825-fold increase in concentration (from 40 nM to 33 μM) to achieve the same effect.

The three Au(III) macrocycles developed and tested to date (Scheme 8b) exhibit the best cytotoxicity of all the compounds examined (at least in the HeLa cell line) with softer dose-response profiles more akin to commercial natural product drugs like

camptothecin. In particular, the GI_{50} values for the three compounds $1.1Y^1a$, $1.1Y^1b$, and $1.5Y^1a$ are all around 100 nM. Complex $1.5Y^1a$ has a particularly attractive dose-response profile that is better than that of camptothecin (Scheme 8a) because the LC_{50} value is < 10 μM (i.e. about one-third of camptothecin's LC_{50} value).

Further, the *in vitro* data suggest that if general and organ-specific toxicity of MA_AuPr is not high in an animal model, i.e., micromolar concentrations of the compound are well-tolerated *in vivo*, then this new class of Au(III) compounds has a fundamental activity profile unlike any other compounds currently in use or in trials. Most importantly, this new class of compounds might be useful for completely clearing stubborn tumours or cisplatin-resistant tumours (complex $1.5Y^1a$ is clearly an extremely promising candidate for such a role). Small structural changes to the basic ligand structure (compare MA_AuPr with MA_AuDM and MA_AuOH) clearly dramatically alter the mean cytotoxicity profile of the compound. This suggests a strong link between structure and activity and that the synthesis and screening of other derivatives of the basic bis(pyrrolide-imine) chelate system are likely to enhance the cytotoxicity of the lead compound and afford GI_{50} and IC_{50} values in the same range as commercially viable drugs such as mitomycin or camptothecin.

Scheme 9 shows a plot of $-\log(GI_{50}/M)$ for MA_AuPr versus the equivalent data for cisplatin.

The plot in Scheme 9 shows that, on average, the chelate MA_AuPr exhibits 95% of the growth inhibition activity of cisplatin. The region marked A on the plot accounts for *ca.* 25% of the cancer cell lines tested and confirms that a sizeable fraction of cancer cell lines are either equivalently susceptible or significantly more susceptible to MA_AuPr than to cisplatin. The complex MA_AuDM shows a similar activity profile to that of MA_AuPr (with 91% of the activity of cisplatin on average and around 12% of the cell lines being more susceptible to this Au(III) drug than to cisplatin). These data demonstrate that the new class of bis(pyrrolide-imine) Au(III) chelates of the invention should compete favorably with cisplatin or, in fact, be better for around 25% of human cancers. We have yet to test the Au(III) macrocycles $1.1Y^1a$, $1.1Y^1b$, and $1.5Y^1a$ in the full 5-dose NCI-60 screens. However, complex $1.1Y^1b$ has just entered this phase of

the screening process and is expected to perform better than MA_AuPr if its performance in the HeLa cell line is an indicator of its more general cytotoxicity.

Scheme 10a shows a comparison of $-\log(GI_{50})$ values for MA_AuPr (the best performing open-chelate Au(III) complex of this invention) with two comparable commercially available anticancer drugs (cisplatin and mitomycin) for selected human cancer cell lines (LE, leukemia; LC, lung cancer; CO, colo-rectal cancer; RE, renal carcinoma; PR, prostate cancer; BR, breast cancer).

Scheme 10b compares the performance (specifically as the drug concentration at which 50% growth inhibition is observed) of two open-chelate gold(III) complexes of the invention with existing commercial anti-cancer drugs for selected human cancer cell lines. The average $-\log(GI_{50})$ values for all of the drugs over the cancer cell lines plotted are marked with an asterisk.

Schemes 10a and 10b show the following. Firstly MA_AuPr is more active than MA_AuDM and cisplatin for the cancer cell lines plotted. MA_AuPr also performs similarly to mitomycin for several important cancers (renal carcinoma and colon cancer) and is better than cisplatin, on average, for the selected leukemia, colon, and renal cancer cell lines. MA_AuPr is also significantly more active than 5-fluorouracil and carmustine [mean $-\log(GI_{50}) = 4.20$, data not shown]. MA_AuPr is less active than the topoisomerase poisons camptothecin (topo I) and daunorubicin (topo II). This is consistent with the fact that the compound is a dual-mode catalytic inhibitor and poison of topoisomerase II and has a slightly different mode of action with the enzyme. It is noteworthy that potent topoisomerase poisons are acutely toxic with some severe side-effects. This is often problematic because the damage caused to healthy cell DNA by these drugs is mutagenic and has been shown to result in the initiation of secondary cancer post-treatment (i.e. genotoxicity). The current strategy employed by oncologists is therefore to administer a potent topoisomerase poison (camptothecin or daunorubicin) *and* an independent topoisomerase catalytic inhibitor to diminish the damage caused by these highly cytotoxic topoisomerase poisons. There is thus an advantage to having a less cytotoxic dual-mode drug like MA_AuPr with a better balance between general and specific cytotoxicity. Indeed, this is why cisplatin, oxaliplatin, and carboplatin are widely used in first-line chemotherapy to treat the

majority of human cancers (all are notably less genotoxic and less cytotoxic than duanorubicin).

The *in vitro* cytotoxicities of the two non-macrocyclic gold(III) chelates of the invention shown in Schemes 10a and 10b are clearly comparable to or better than that of cisplatin. Inherent specificity for renal, colon, and some leukemia cell lines has also been observed. It is an advantage of the invention that gold is cheaper than platinum and this would confer a competitive edge to the compounds of the invention.

Mechanism of action

From the data presented above, it is clear that the compound MA_AuPr is an effective cytotoxic agent that is suitably active against multiple human cancer cell lines. Identification of the cellular target of the compound and elucidation of its biological mechanism of action are critical to the optimization of lead compounds into successful chemotherapeutic agents. There are three key parameters which define the cytotoxic activity of a compound against a given cancer cell line, namely its GI_{50}, IC_{50}, and LC_{50} values (see Scheme 8a). One drug tested over 60 cancer cell lines affords 180 experimental data that may be compared with the same parameters for all other compounds similarly tested against the NCI's panel of 60 human cancer cell lines. Only hierarchical cluster analysis offers a tractable statistical approach to establish functional relationships between drugs with a large data set. There are various ways in which to effect hierarchical cluster analysis of a large data set. Irrespective of the method chosen, one expects to delineate which drugs exhibit similar activity profiles over the full 60 cell line panel. Compounds most similar in behavior will converge in the statistical analysis to form a tight group or cluster. If a test agent has an unknown mechanism of action and is found to cluster or fall within a group of compounds whose mechanism of action has been previously and independently determined, then one can conclude, with reasonably high certainty, that the test agent is active against the same cellular target as the majority of the compounds within a particular cluster.

Scheme 11 (below) shows a dendrogram obtained via hierarchical cluster analysis of the GI_{50}, IC_{50}, and LC_{50} values for a range of commercial anti-cancer drugs with known mechanisms of action. The Au(III) compounds of the invention were included in

the analysis and are highlighted in red. It is clear from the clusters shown that the activity of MA_AuPr correlates best with that of etoposide, one of the most widely used topoisomerase II poisons. The compound also appears on a branch with a direct, though distant, link to the drugs daunorubicin and cisplatin. Daunorubicin is a potent topoisomerase II poison, while cisplatin has been shown to be an effective catalytic inhibitor[25] of topoisomerase II (in addition to its role as a DNA cross-linker and guanine-N7 "alkylating" agent).

Topoisomerase II is an essential nuclear enzyme found in all living cells. Topoisomerase II participates in various DNA metabolic processes, such as transcription, DNA replication, chromosome condensation, and de-condensation, and is essential at the time of chromosome segregation after cell division.[26] This enzyme transiently creates a protein-concealed double-strand break in one DNA molecule through which a second double-stranded DNA molecule can be transported prior to religation of the DNA.[26] There are two classes of compounds that act against topoisomerase II—poisons and catalytic inhibitors. The former compounds stabilize the ternary drug-enzyme-DNA cleavage complex and favor an increase in the number of DNA double strand breaks; these are highly damaging to cancer cells and lead to apoptosis (programmed cell death).[27] The latter compounds (catalytic inhibitors) are either competitive inhibitors (block DNA binding), non-specific inhibitors (react with topoisomerase II sulfhydryl groups, e.g., cisplatin,[25] thereby altering the proper function of the enzyme), or inhibitors that block the ATPase domain of the enzyme (effectively curtailing the ATP-dependent DNA strand passage step in the cycle). Highly successful, though highly toxic, commercial anticancer compounds active against topoisomerase II include the drugs etoposide, teniposide, doxorubicin, daunorubicin, and idarubicin.[26] There are, however, difficulties associated with the use of these drugs in chemotherapy due to their high general toxicity. The cardiac toxicity of the compounds is generally high and catalytic inhibitors of topoisomerase II (such as dexrazoxane, ICRF-187) are administered along with a topoisomerase poison to temper the toxicity of the poison,[28] or to prevent tissue damage (necrosis) when extravasation of a topoisomerase poison occurs during chemotherapy.[29] There is also good evidence to suggest that topoisomerase poisons are themselves carcinogenic, such that the development of post-treatment (secondary) cancer occurs in some patients. [30]

The compound MA_AuPr clearly targets topoisomerase II if the statistical analysis of the NCI data for a range of drugs shown in Scheme 11 is correct. MA_AuPr was therefore assayed for its action against topoisomerase II *in vitro* using TopoGEN's standard protocol over a wide range of test agent concentrations (0.005 to 500 μM) in order to obtain direct experimental proof for the apparent cellular target of the compound to ensure that a fundamental understanding of the mechanism of action of this new class of Au(III) compounds exists. These experiments were performed by the company TopoGEN and at the University of Central Florida. The DNA cleavage experiments were performed *in vitro* using purified topoisomerase I and II enzymes and supercoiled plasmid DNA as the substrate. The controls that were used in the experiment were linear marker DNA as well as reactions without the gold(III) complex and high concentrations of VP16. The compound VP16 (etoposide) is a commercially available DNA intercalator chemotherapeutic agent, widely used in the treatment of lung and testicular cancers as well as lymphomas. The choice of VP16 as a control is based on the fact that it is a poor topoisomerase II inhibitor, but is a powerful topoisomerase II poison which arrests the enzyme's cycle at the ternary drug-enzyme-DNA cleavage complex stage, leading to observation of linear DNA fragments upon SDS denaturation of the enzyme (i.e., work-up). Comparison of the VP16 results with the results of MA_AuPr would therefore give a good indication of whether the gold(III) chelate is an inhibitor or a poison. The results of the ethidium bromide (EB) gel analysis are shown in Scheme 12.

Lane 1 of the gel (Scheme 12) is the control experiment with only supercoiled plasmid DNA present. The control contains no topoisomerase II and so the DNA supercoiled structure cannot be relaxed, as the topoisomerase II enzyme would usually do. The gel shows that the complex MA_AuPr begins to effectively poison topoisomerase II at a concentration of 0.5 μM (lane 5 of the gel), as evidenced by the formation, trapping, and detection of linear DNA cleavage products at this concentration of the test agent. At a higher concentration of the test agent (50 μM), both supercoiled plasmid DNA and linear cleavage products are observed. This shows that MA_AuPr exhibits dual action at this concentration in that it functions both as a topoisomerase II poison (forming linear DNA) and as a topoisomerase II catalytic inhibitor (preventing relaxation of the supercoiled plasmid DNA substrate). At very high concentrations (>500 μM), MA_AuPr behaves exclusively as a catalytic inhibitor of the enzyme.

The formation of a low concentration of linear DNA (lane 5 of the gel) demonstrates that the compound MA_AuPr has the ability to interrupt the second step of the cleavage/ligation cycle, in particular preventing religation of the double-stranded DNA. This conclusion is based on the fact that the cleavage/ligation cycle leads to formation of trapped intermediates, which resolve as linear DNA in the gels. In summation, the test compound MA_AuPr is therefore both a poison and a catalytic topoisomerase II inhibitor.

This result is particularly interesting since, in the treatment of brain cancers in mice, combinations of topoisomerase II inhibitors and poisons are often used because the efficacy of the combined treatment is greater than the sum of the parts and a catalytic inhibitor modulates the acute toxicity of the poison. Therefore, a drug that demonstrates both inhibition and poisoning of the enzyme is potentially a novel and useful chemotherapeutic agent. [25]

MA_AuPr was also tested to determine if the compound was a topoisomerase I poison or inhibitor since the compound appears to be a topoisomerase II-specific agent and not a DNA intercalator with multiple enzyme targets. The results are shown in the EB gel in Scheme 13. The gel electrophoresis experiment shows that the gold(III) chelate is not a topoisomerase I poison. This conclusion is based on comparison of the migration of the DNA with various concentrations of the gold(III) chelate with the lane containing CPT (camptothecin, a topoisomerase-I specific poison) and linear DNA as a reference or marker. This result shows that the gold(III) chelate specifically poisons topoisomerase II and not topoisomerase I.

The role of gold(III) in the efficacy of the compound was determined by modifying the structure of MA_AuPr by replacing the Au(III) cation with Pd(II) to afford MA_PdPr (the isoelectronic square planar coordination complex of known structure and geometry[31]) and carrying out the DNA relaxation assay with topoisomerase II as before. The metal-free ligand (MA_H2PrLig) was tested under identical conditions to confirm that the mechanism of action is related to the intact structure of the metal chelate. The results are shown in Schemes 14 and 15.

The data confirm firstly that the free ligand is not a good topoisomerase II poison. Secondly, The efficacy of the Au(III) chelate is *100 times higher* than that of the isoelectronic Pd(II) chelate. This result is expected and is consistent with the electrophilic character of the Au(III) ion, which is known to favor electrostatic interactions with aromatic groups or anions perpendicular to the square planar coordination group (i.e., the vacant axial interaction sites at the metal center). Compound 1a is also positively charged, whereas the Pd(II) chelate is neutral and thus likely to exhibit diminished electrostatic attraction for the phosphate backbone of double-stranded DNA.

The topo II inhibition assay for the Au(III) macrocycle KA_AumacroPr is shown above in Scheme 16. In contrast to MA_AuPr, this complex functions as a pure catalytic inhibitor of topo II since no trapped linear DNA cleavage products are evident that would signal behavior of the complex as a topo II poison. The enzyme inhibition is characterized by an IC_{50} of 4.8 μM, which is in excellent agreement with the cell cytotoxicity IC_{50} value measured for this compound against HeLa cells (Scheme 8b).

As indicated by the DNA unwinding assay in Scheme 17, the test agent KA_AumacroPr interferes with the normal operation of human topoisomerase I. Specifically, abnormal relaxation products are generated from supercoiled plasmid DNA. This is consistent with strong intercalative binding of KA_AumacroPr to the plasmid DNA probably before and after the action of topoisomerase I, and consequently inhibition of its normal turnover cycle. Collectively the data in Schemes 16 and 17 show that the macrocyclic Au(III) complex $1.1Y^1b$ functions as a catalytic inhibitor of human topoisomerase I. Similar data were obtained for complexes $1.1Y^1a$ and $1.5Y^1a$.

For a drug to act as a topoisomerase II poison, two molecular recognition events must occur. Firstly, the drug must bind to DNA via intercalation between base pairs and secondly, the drug must interact with topoisomerase II in such a way that religation of the DNA after formation the topoisomerase II-DNA covalent complex (the catalytic intermediate) is impossible. The enzyme is poisoned at this point and the cycle irreversibly disrupted by the drug. Scheme 18 shows titration data for the titration of complex 1.1a with calf-thymus DNA (ctDNA).

The hypochroism of the absorption band of the complex at 383 nm was monitored as a function of added ctDNA. The data were fitted to equation (1)[32] to determine the affinity constant by non-linear regression:

$$(\varepsilon_a - \varepsilon_f)/(\varepsilon_b - \varepsilon_f) = (b - (b^2 - 2K_a{}^2Ct[DNA]/s)^{1/2})/2K_aCt \quad (1a)$$

$$b = 1 + K_aCt + K_a[DNA]/2s \quad (1b)$$

where [DNA] is the concentration of DNA base pairs, ε_a is the extinction coefficient (A_{abs}/[M]) observed for the 383-nm MLCT absorption band of MA_AuPr at a given DNA concentration, ε_f and ε_b are the extinction coefficient for the free Au(III) complex and the extinction coefficient for the Au(III) complex in the fully bound form, respectively. K_a is the equilibrium binding constant in M^{-1}, Ct is the total Au(III) complex concentration, and *s* is the binding site size.

From Scheme 18, it is clear that compound 1.1a binds to ctDNA with a high affinity constant. Moreover, since the MLCT (metal-to-ligand-charge-transfer) band of the complex at 383 nm decreased upon DNA binding (hypochroism), the mode of interaction is likely to be intercalation, as occurs with Ru(II) complexes with known DNA-intercalating bidentate ligands.

Complex	K_a (calf thymus DNA) / M^{-1}	Cytotoxicity#
1.1a (MA_AuPr)	$2.05(2) \times 10^5$	active
1.1b (MA_AuDM)	$1.63(3) \times 10^5$	active
1.1c (MA_AuOH)	$1.43(3) \times 10^5$	*in vitro* only
1.1d (MA_AuOEt)	$1.01(4) \times 10^6$	active
1.1e (MA_AuCl)	$3.91(7) \times 10^5$	active
1.1Y[1]a (KA_AumacroPr)	$2.8(2) \times 10^6$	active
1.1Y[1]b (KA_AumacroDM)	$1.49(8) \times 10^6$	active
1.5Y[1]a (KA_AumacroBu)	$1.20(9) \times 10^6$	active

Conditions:
MA series of complexes in pH 7.0 phosphate buffer at 37 °C.
KA series of complexes in pH 7.0 15% DMSO-TRIS buffer at 25 °C.
Active: mean IC_{50} value in low µM range in the NCI-60 cytotoxicity screen or in an independent cytotoxicity screen. *In vitro*: the compound is a proven topo II poison *in vitro* (cell-free enzyme assay).

Summary of selected calf thymus DNA binding constants for open- and macrocyclic Au(III) chelates.

Scheme 19

Scheme 19 summarizes the DNA affinity constants for the compounds. The affinity constants are high (10^5 to 10^6 M^{-1}) and the data clearly show, in unison with Scheme 18, that both the non-macrocyclic and macrocyclic Au(III) complexes are DNA intercalators. Consequently, the compounds are capable of disrupting the topoisomerase I or II DNA religation step and/or its ability to bind DNA (competitive inhibition). In short, the compounds of this invention act as poisons and/or inhibitors of the human topoisomerase I and/or II enzyme *in vitro*.

Toxicology

Key to the design of compounds for cancer chemotherapy is an early assessment of their toxicology profiles. Compounds have to be well-tolerated in live subjects, easily metabolized or excreted, well-transported across cell membranes, and have favorable plasma stability to be worthy of detailed pre-clinical animal model studies.

Test	Key Indicator	Comment
Microsomal clearance	$t_{1/2}$ < 10 min	Highly metabolized; low liver toxicity expected
Plasma half-life	$t_{1/2}$ < 20 min	Highly metabolized
Plasma protein binding	No binding – drug undetected	Unstable in plasma; requires encapsulation for transport
Genotoxicity	Negative	Non-mutagenic
Cytotoxicity (Hep-G2)	Strong positive	Good cytotoxicity expected (consistent with NCI-60 screens of drug)
Caco-2	Not an efflux transporter substrate	Favorable intestinal uptake expected

Summary of key in vitro ADME-Tox (absorption, distribution, metabolism, toxicology) data for MA_AuPr.

Scheme 20

The most promising non-macrocyclic Au(III) complex, MA_AuPr, was selected for *in vitro* ADME-Tox profiling to gauge the potential of the compound for pre-clinical animal toxicology testing and further development towards phase I human trials. The data are summarized in Scheme 20, which reveals a number of positive attributes for the compound. First, the compound is not genotoxic (i.e. mutagenic). This means the invented compounds have a clear advantage over topo II poisons such as daunorubicin and its derivatives which are known to be genotoxic but are in clinical use. Second, the compound is rapidly metabolized by liver cytochrome P450 enzymes and hepatotoxicity is not anticipated. Third, the Hep-G2 cytotoxicity assay confirmed the expected good cytotoxicity displayed in the NCI-60 screen of the compound. Fourth, the Caco-2 transport data clearly demonstrate that the test agent is not an efflux transporter substrate and has the ability to freely pass across a monolayer of Caco-2 cells (a model for the human small intestine wall or mucosa) without much preference for direction. The Caco-2 data are especially important as many drugs fail due to poor membrane transport/absorption. The transport rates for MA_AuPr are summarized in Scheme 21.

Cpd.	Test Conc. (uM)	Assay Duration (h)	mean A→B P_{app} (10^{-6} cm s^{-1})	mean B→A P_{app} (10^{-6} cm s^{-1})	Efflux Ratio
Ranitidine	10	2	0.7	2.3	3.3
Warfarin	10	2	37.0	8.0	0.2
MA_AuPr	10	2	4.0	9.0	1.2

Summary of Caco-2 transport for MA_AuPr, ranitidine (a substrate for efflux transporter proteins), and warfarin (a non-substrate for efflux transporters).

Scheme 21

The only possibly concerning ADME-Tox result shown in Scheme 20 is that the test compound did not bind to plasma protein and was, in fact, not identified in a structurally intact form by LC-MS in the protein-free fraction (i.e. the molecular ion peak

for MA_AuPr was not detected in the mass spectrum). The $t_{1/2}$ of MA_AuPr in plasma was < 20 min. This suggests fast conversion of the compound to another species in the presence of plasma constituents and could suggest covalent interaction with proteins or metal ion aquation/hydrolysis possibly by enzyme action. Experiments in our lab with compound 1.2a (MA_AuEt, in which W = W^2, R and R^1–R^4 are H, Y = 2H, and Z and Z^1 = C) have shown that water may displace a pyrrole ring from the Au(III) ion to form a Au(III)–OH species and protonated pyrrole ring. MA_AuPr did not show hydrolysis in phosphate buffered aqueous solutions presumably because the 6-membered chelate ring leads to a more stable chelate for Au(III). This is why binding to DNA of the intact chelate occurs (Schemes 12 and 18). However, it is noteworthy that hydrolysis of a Au(III)–$N_{pyrrole}$ bond is a reaction that may be catalyzed by enzymes in plasma and could account for the plasma instability of MA_AuPr. By way of comparison, the plasma half-life of cisplatin measures 0.88 h or ca. 53 min, while that of its mono(aqua) complex is 0.26 h (16 min).[33] The plasma stability of MA_AuPr is thus very similar to that of the mono(aqua) cisplatin derivative (cisplatin is one of the most successful anticancer drugs in the history of cancer chemotherapy).

The Applicant is of the firm opinion that encapsulation of the non-macrocyclic Au(III) compounds belonging to Formula (I) in γ-cyclodextrin or other water-soluble encapsulating agents such as curcubit-[8]-uril will permit increased plasma half-lives for these compounds. Encapsulation for metallo-drug transport and stabilization is well-established in the literature,[34] and has been shown to enhance the redox and plasma stability of cisplatin analogues.[34] It should be noted that enhanced plasma stability for the macrocyclic Au(III) complexes belonging to Formula (I) is anticipated because hydrolysis of the Au–$N_{pyrrole}$ bonds in the macrocycle is quite unlikely. Experiments investigating this concept further are currently underway in our laboratory.

	MA_AuPr				Chlorpromazine (control)			
Cell Health Parameter	MEC (μM)	AC_{50} (μM)	MEC	AC_{50}	MEC (μM)	AC_{50} (μM)	MEC	AC_{50}
Cell Loss	<0.23	7.4		x	100	7.8		
Nuclear Area	6.2	17			>11	100		
DNA structure	>19	N/A			11	196		
Membrane permeability	2.1	16	x		11	30		
Mitochondrial mass	2.1	41	x		3.7	5.4	x	x
Mitochondrial membrane potential	6.2	>500	x		3.7	50	x	
Cytochrome C release	19	33			11	16		

MEC: Minimum effective concentration that significantly crosses vehicle control threshold.

N/D: Not determined due to lowest concentration tested is the returned MEC.

AC_{50}: The concentration at which 50% maximum effect is observed for each cell health parameter.

N/A: The response was not significantly above control to determine an AC_{50} value.

First Signal (x): The cell health feature which responds at the lowest observed dose.

Summary of cell health parameters for HepG2 human hepatocellular carcinoma cells exposed to serial dilutions of MA_AuPr and chlorpromazine (control).

Scheme 22

The data for MA_AuPr in Scheme 22 are consistent with a cytotoxic compound capable of inducing apoptosis (programmed cell death) and, indeed, a compound that performs better than the control drug. The lowest MEC response data indicate that the compound MA_AuPr has resulted in an increase in membrane permeability (indicating general cell death), an increase in mitochondrial mass (indicating an adaptive response to cellular energy demands), and an increase in mitochondrial potential (implying adaption to cellular energy requirements). Other cell health parameters which respond are a loss of total cells per well (indicating toxicity due to necrosis, apoptosis or a reduction in cellular proliferation), an increase in nuclear area (indicating necrosis or G2 cell cycle arrest), an increase in cytochrome c release (implying activation of a signalling cascade leading to apoptosis). The latter is particularly relevant as we may rule out cell death by necrosis in the case of MA_AuPr. The mechanism of action of the compound thus leads to cell cycle arrest in the G2 phase and the induction of apoptosis (highly desirable for an anticancer drug). The lowest AC_{50} response indicates that the compound MA_AuPr has resulted in a loss of total cells per well (indicating toxicity due

to necrosis, apoptosis or a reduction in cellular proliferation). Since the compound induces cytochrome c release, cytotoxicity involves apoptosis.

The plasma stability and cytotoxicity of a test drug may be examined more extensively in an animal model (*in vivo*).

Scheme 23 shows a graph of 3LL tumor growth (measured by caliper methods at the University of Strasbourg, France) in black mice over a 20-day period at the indicated doses. (The 3LL cell line is a solid Lewis lung carcinoma cell line of the mouse.) The compound MA_AuPr, despite its modest plasma stability *in vitro* (Scheme 20) and poor performance against human lung carcinoma cell lines in the NCI-60 screen (Scheme 6a), clearly slows down the growth rate of 3LL tumors in black mice by about 33% relative to the control after 20 days. In comparison to cisplatin, which reduces the growth rate of 3LL tumors by 76% in 20 days and is a highly effective drug against lung carcinoma cell lines, MA_AuPr has about 43% of the in vivo performance of cisplatin *for this particular cancer cell line*. We note that the gold(III) chelates of this invention out-perform cisplatin for several colorectal carcinoma cell lines, renal carcinomas, and breast cancer cell lines (Scheme 10), so that the data presented in Scheme 23 may be taken as a lower limit of the compound's *in vivo* cytotoxicity. The value of the experimental data shown in Scheme 23 clearly lies in the fact that it demonstrates that MA_AuPr has sufficient plasma stability in live animals to exert a positive cytotoxic effect leading to reduced tumor growth rates, even for a class of tumors for which the compound is expected to perform poorly.

The results are most encouraging and suggest that xenografts of human tumor cell lines susceptible to MA_AuPr (e.g. colon carcinoma cell lines) in mouse model subjects are likely to prove illuminating and worth the cost. Furthermore, the Applicant anticipates that the most cytotoxic macrocyclic Au(III) complexes, e.g., compound 1.5Y^{1}a, may have good plasma half-lives due to their enhanced redox stability and resistance to hydrolysis such that better time-dependent tumor growth profiles are quite likely for the macrocyclic members of Formula (I) of the invention.

Scheme 24 shows a set of survival data for five groups of four mice receiving from 1 to 30 μmol/kg doses of MA_AuPr. A single dose of the compound was administered

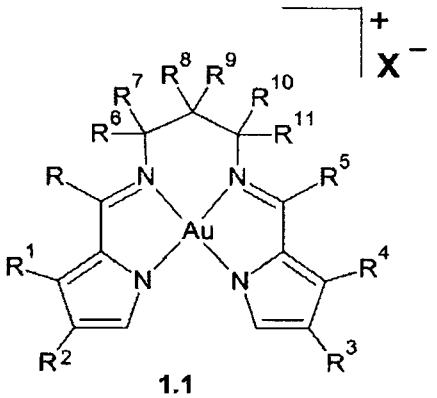
by injection over the first week followed by two injections per week per mouse for a total period of 50 days. All of the mice remained healthy and showed no abnormal weight changes over the timeframe of the experiment (mouse mass data not shown, but available as a time dependent plot). The results demonstrate that MA_AuPr has an acute toxicity > 30 μmol/kg/week and a chronic toxicity > 60 μmol/kg/week. This is fully consistent with the ADME-Tox data (Scheme 20) which showed that the compound is highly metabolized by liver microsomes.

In conclusion, the ADME-Tox and *in vivo* toxicology data for MA_AuPr are complementary and collectively indicate that:

- MA_AuPr is a cytotoxic metal complex (a topoisomerase II poison and inhibitor) with a mean *in vitro* IC_{50} value in the low μM range.
- MA_AuPr is not genotoxic.
- MA_AuPr induces apoptosis in cancer cells such as HepG2.
- MA_AuPr is not a substrate for the efflux transporters in a Caco-2 cell monolayer and exhibits facile bidirectional transfer across this mucosal membrane mimic.
- MA_AuPr is readily metabolized by liver microsomes.
- MA_AuPr has a short plasma half life ($t_{1/2}$ < 20 min) which is similar to the mono(aqua) derivative of cisplatin, $[PtCl(NH_3)_2(OH_2)]^+$.
- MA_AuPr is cytotoxic in a live animal setting (mice) and demonstrates the ability to reduce tumor growth rates for mouse lung carcinoma cells (despite having poor cytotoxicity in general for lung tumor cell lines).
- MA_AuPr is non-toxic to healthy black mice exhibiting acute and chronic toxicity values > 30 μmol/kg/week and > 60 μmol/kg/week, respectively.

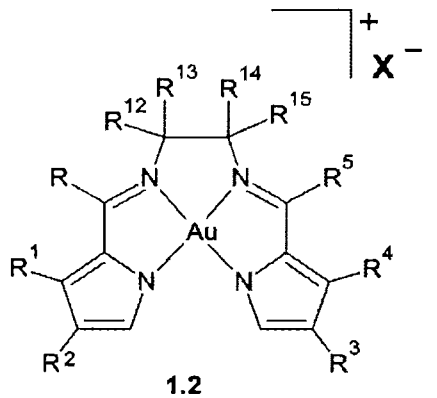
Example 2

Synthesis of MA_AuPr and other open-chelate derivatives



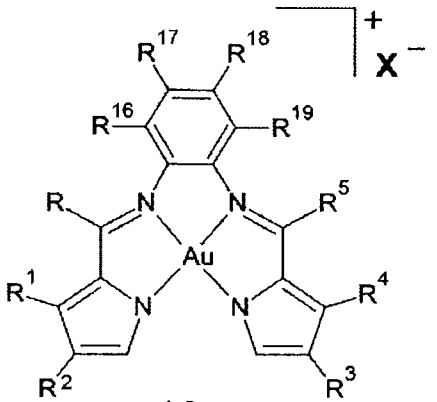
1.1

1.1a R = H, R^n = H
1.1b R-R^7 = H, R^8 = R^9 = CH_3, R^{10}-R^{11} = H
1.1c R-R^8 = H, R^9 = OH, R^{10}-R^{11} = H
1.1d R-R^8 = H, R^9 = OCH_2CH_3, R^{10}-R^{11} = H
1.1e R-R^8 = H, R^9 = Cl, R^{10}-R^{11} = H



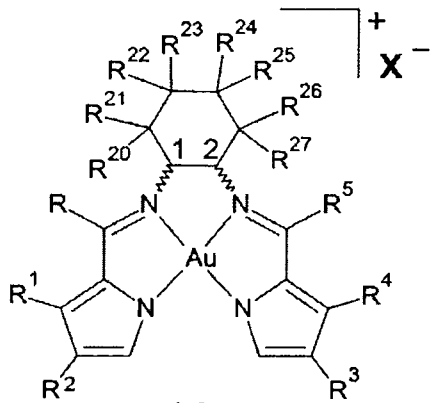
1.2

1.2a R = H, R^n = H
1.2b R-R^5 = H, R^{12}-R^{14} = H, R^{15} = CH_3



1.3

1.3a R = H, R^n = H
1.3b R-R^5 = H, R^{16} = H, R^{17} = CH_3, R^{18}-R^{19} = H



1.4

1.4a R = H, R^n = H, racemic
1.4b R = H, R^n = H, 1*S*, 2*S* enantiomer
1.4c R = H, R^n = H, 1*R*, 2*R* enantiomer

Open chelate Au(III) compound library synthesized and fully characterized using the methodology outlined for MA_AuPr. The anion X^- is typically chloride or PF_6^-.

Scheme 25

Generic description of materials for the synthesis of bis(pyrrolide-imine) and bis(imidazolato-imine) gold(III) chelates

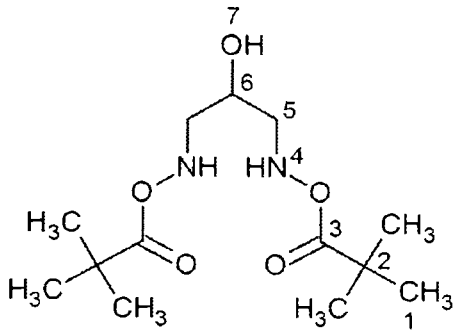
The general synthetic procedure for the synthesis of all non-macrocyclic ligands in this invention involves the condensation of two equivalents of 1*H*-pyrrole-2-carbaldehyde or 5-methyl-1*H*-imidazole-4-carbaldehyde with an appropriate 1,2- or 1,3-diaminoalkane linker unit, which forms a diiminoalkane bridge in the Schiff base condensation product. The bis(imine) compounds produced from such condensation reactions are then purified and reacted with a gold(III) salt in a suitable solvent system to form a relatively planar chelate of gold(III).

The synthetic procedure for macrocyclic gold(III) chelates required, in most cases, the initial reaction of 2,3-bis(5'-formylpyrrol-2'-yl)quinoxaline with a gold(III) salt to form an intermediate metal chelate in which the formyl oxygen atoms and deprotonated pyrrole nitrogen atoms function in unison as a tetradentate chelating ligand and most likely form a gold(III) chelate with a AuN_2O_2 coordination group. This intermediate is not isolated but condensed *in situ* with a 1,3- or 1,4-diaminoalkane linker unit, which, through the formation of a pair Au-bound imine groups and concomitant loss of two molar equivalents of water, cyclizes the ligand to form the product Au(III) macrocycle as a monocationic complex.

Commercially available diaminoalkanes were purchased from Aldrich and used without further purification. Commercially unavailable 1,3-diamines such as 2-ethoxy-1,3-diaminopropane and 2-chloro-1,3-diaminopropane were synthesized by *t*-boc protection of the two amino groups of 1,3-diamino-2-hydroxypropane followed by reaction of the hydroxy group and subsequent deprotection of the amino groups. Thus, although the compounds 2-ethoxy-1,3-diaminopropane and 2-chloro-1,3-diamino-propane are themselves not novel, with several synthetic approcahes available from the literature,[35,36] the method we have employed to make them (as dihydrochloride salts) from *t*-boc-protected 1,3-diamino-2-hydroxypropane and to use them in subsequent condensation reactions to form diimines is novel.

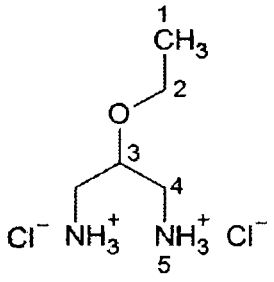
Synthetic details for making key synthons for subsequent preparation of the chelating ligands described herein are given below.

Synthesis of 2,2,12,12-*t*-methyl-3,11-dioxo-4,10-dioxa-5,9-diazatridecan-7-ol (*N,N'*-di-*t*-boc-2-hydroxy-1,3-diaminopropane)



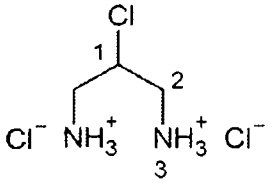
Sodium hydrogencarbonate (8.3 g, 99 mmol) was dissolved in 1:1 acetonitrile:water mixture (190 mL) and the solution cooled to 4 °C in an ice bath. 1,3-diamino-2-hydroxypropane (2.5 g, 27 mmol) and di-tert-butyldicarbonate (12.8 g, 59 mmol) were dissolved in the same solvent system (65 mL). This mixture was then added to the chilled sodium hydrogencarbonate solution and stirred on ice for two hours. The reaction was then heated to room temperature and stirred overnight. The acetonitrile was removed by rotary evaporation and the protected amine extracted into dichloromethane (3 x 75 mL portions). The organic portions were combined, dried over sodium carbonate, and evaporated to dryness by rotary evaporation.[37] The resulting oil was re-crystallised from diethylether/hexane,[38] giving colourless crystals (7.2 g, 91% yield). The compound was characterised by ^1H and ^{13}C NMR and FT-IR spectroscopy. IR (cm^{-1}): 3316m br ν(OH and NH), 2971m and 2930m ν(CH_3 and CH), 1681s ν(C=O). ^1H NMR (400 MHz, $CDCl_3$, 298 K) [δ, ppm]: 1.45 (s, 18H, H-1), 3.20 (m, 4H, H-5), 3.75 (m, 2H, H-6 and H-7), 5.20 (s br, 2H, H-4). ^{13}C NMR (100 MHz, $CDCl_3$, 298K) [δ, ppm]: 28.55 (C-1), 43.72 (C-2), 71.07 (C-5), 79.87 (C-6), 157.24 (C-3).

Synthesis of 2-ethoxy-1,3-diaminopropane dihydrochloride



N,N'-di-*t*-boc-2-hydroxy-1,3-diaminopropane (2.0 g, 6.9 mmol) and $[Bu_4N][HSO_4]$ (0.44 g, 1.3 mmol) were dissolved in toluene (7.5 mL). To this 50 % aqueous NaOH (7.5 mL) and ethyl iodide (1.67 mL, 20.7 mmol) were added. The resulting biphasic solution was heated to 100 °C for 18 hours. The solution was diluted with water and the alkylated compound extracted into ethylacetate (75 mL); this solution was washed with brine and then water and dried over anhydrous Na_2CO_3. The solvent was then removed by rotary evaporation and the resulting oil purified by column chromatography on silica gel using 1:4 ethylacetate:hexane as the eluent.[39] The solvent in the column fractions containing the alkylated product was removed by rotary evaporation and the resulting oil was dissolved in methanolic HCl (1.25 M, 30 mL) and stirred overnight. 2-ethoxy-1,3-diaminopropane dihydrochloride precipitated as an oil from the methanol solution with the addition of diethylether. The oil was separated from the methanol by centrifugation and dried over P_2O_5 to give the hydrochloride salt as a white powder (0.70 g, 53% yield). The powder was characterised by ^{1}H NMR. ^{1}H NMR (400 MHz, D_2O, 298 K) [δ, ppm]: 1.24 (t, 3H, H-1), 3.14 (dd, 2H, $^3J_1$ = 7.13 Hz, $^3J_2$ = 14.2 Hz, H-4), 3.35 (dd, 2H, $^3J_1$ = 4.3 Hz, $^3J_2$ = 13.0 Hz, H-4), 3.69 (q, 2H, H-2), 4.03 (m, 1H, H-3).

Synthesis of 2-chloro-1,3-diaminopropane dihydrochloride



N,N'-di-*t*-boc-2-hydroxy-1,3-diaminopropane (1.0 g, 3.5 mmol) and triphenylphosphine (1.5 g, 5.72 mmol) were dissolved in chloroform (15 mL) and carbon tetrachloride (35 mL). This solution was refluxed for 5 hours, before the solvents were removed under reduced pressure by rotary evaporation. The resulting oil was dissolved in diethylether to precipitate the $OPPh_3$ and the resulting solution centrifuged to remove the insoluble $OPPh_3$. The diethyl ether was removed by rotary evaporation and the resulting oil dissolved in methanolic HCl (1.25 M, 30 mL) and stirred overnight. The 2-chloro-1,3-diaminopropane dihydrochloride was precipitated as a white powder by the addition of dichloromethane. The powder was stored over P_2O_5 (0.304 g, 49% yield). The complex was characterised by ^1H and ^{13}C NMR spectroscopy. ^1H NMR (400 MHz, D_2O, 298 K) [δ, ppm]: 3.34 (dd, 2H, $^3J_1$ = 3.8 Hz, $^3J_2$ = 14.7 Hz, H-2), 3.57 (dd, 2H, $^3J_1$ = 3.3 Hz, $^3J_2$ = 13.9 Hz, H-2), 4.58 (m, 1H, H-1). ^{13}C NMR (100 MHz, D_2O, 298K) [δ, ppm]: 42.95 (C-2), 54.94 (C-1).

General synthesis of simple bis(pyrrole-imine) and bis(imidazole-imine) ligands

1*H*-Pyrrole-2-carbaldehyde (30 mmol) or 5-methyl-1*H*-imidazole-4-carbaldehyde (30 mmol) and a 1,2- or 1,3-diaminoalkane derivative (15 mmol) were refluxed in ethanol (30 mL) for two hours. During refluxing the reaction mixture changed from colourless to a clear, bright orange. Solvent was then removed by rotary evaporation, leaving a viscous orange-coloured oil. The oil was then dissolved in dichloromethane prior to adding hexane to the solution, which was left to re-crystallise overnight. This typically yields the crystalline bis(Schiff base) product in around 70-90% yield. The crystalline product can be shown to be clean by thin layer chromatography or ^1H NMR spectroscopy. Single crystals suitable for X-ray crystallography may also be obtained from the re-crystallisation process. The procedure and full characterization for *N,N'*-bis[(1*E*)-1*H*-pyrrol-2-ylmethylene]propane-1,3-diamine have, for example, been reported elsewhere.[14]

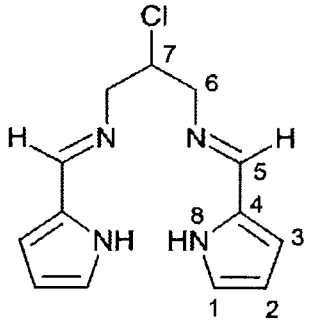
General synthesis of new bis(pyrrole-imine) ligands from 1,3-diaminopropane dihydrochloride salts

The general strategy when condensing dihydrochloride salts of the diamine linker group with two molar equivalents of 1*H*-pyrrole-2-carbaldehyde was to carry out the

reaction under solvent-free conditions to avoid incompatible solubility of the two reagents and to obviate the use of organic bases for deprotonation of the diamine reagent's ammonium groups. A typical solid-state reaction is described below.

Excess sodium carbonate (ca. 4 mmol) and a relevant 2-substituted 1,3-diaminopropane dihydrochloride derivative (ca. 2 mmol) were ground in an agate pestle and mortar for 1 minute. To the resulting white paste, 1*H*-pyrrole-2-carbaldehyde (ca. 4 mmol) was added and the mixture ground together for a further 10 min. Water was then added to the paste, followed by acetone, to dissolve the ligand. The solvent solution was collected and the acetone allowed to evaporate, yielding the ligand as a pale yellow powder. The powder was purified by re-crystallisation from 1:30:50 ethanol:THF:hexane. Typical isolated yields were of the order of 60-70%. The product ligands were analysed by ^{1}H NMR, ^{13}C NMR, UV/visible and IR spectroscopy. In some cases, crystals suitable for a structure determination by X-ray diffraction were obtained during the re-crystallisation step. Synthetic methods and characterization data for several novel ligands prepared in this way are described below.

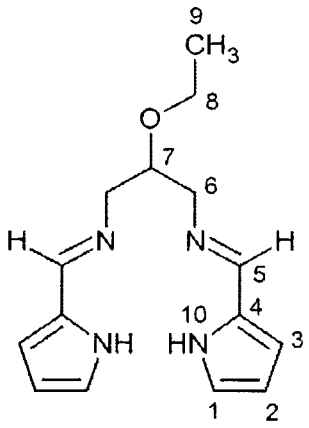
Synthesis of 2-chloro-*N*-[(1*E*)-1*H*-pyrrol-2-ylmethylene]-*N'*-[(1*Z*)-1*H*-pyrrol-2-ylmethylene]propane-1,3-diamine



Sodium carbonate (0.448 g, 4.24 mmol) and 2-chloro-1,3-diaminopropane dihydrochloride (0.350 g, 1.93 mmol) were ground in an agate pestle and mortar for 1 minute. To the resulting white paste, 1*H*-pyrrole-2-carbaldehyde (0.365 g, 3.93 mmol) was added and the mixture ground together for a further 10 min. Water was then added to the paste, followed by acetone, to dissolve the ligand. The solvent solution was collected and the acetone allowed to evaporate, yielding the ligand as a pale yellow powder. The powder was re-crystallised from 1:30:50 ethanol:THF:hexane (0.290 g,

62% yield). The novel ligand was further characterized by ^{1}H NMR, ^{13}C NMR, UV/visible and IR spectroscopy. UV/vis (ethanol) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 292; 3.81 × 10^4. IR (cm^{-1}): 3183w δ(NH, pyrrole), 2942m br ν(CH, imine), 2838m ν(CH, H-CCl), 1643s br ν(C=N), 743 (C-Cl stretch). ^{1}H NMR (400 MHz, DMSO-d_6, 298 K) [δ, ppm]: 3.74 (dd, $^{3}J_1$ = 7.2 Hz, $^{3}J_2$ = 5.3 Hz, 2H, H-6), 4.01 (dd, $^{3}J_1$ = 7.88 Hz, $^{3}J_2$ = 5.3 Hz, 2H, H-6), 4.45 (m, 1H, H-7) 6.13 (t, 2H, H-2), 6.50 (dd, $^{3}J_1$ = 3.7 Hz, $^{3}J_2$ = 1.3 Hz, 2H, H-3), 6.90 (s br, 2H, H-1), 8.11 (s, 2H, H-5), 11.37 (s br, 2H, CD_3OD exchangeable, H-8). ^{13}C NMR (100 MHz, DMSO-d_6, 298 K) [δ, ppm]: 63.57 (C-6), 64.88 (C-7), 109.47 (C-2), 114.53 (C-3), 122.96 (C-1), 129.98 (C-4), 154.43 (C-5).

Synthesis of 2-ethoxy-*N*,*N*'-bis[(1*E*)-1*H*-pyrrol-2-ylmethylene]propane-1,3-diamine



Sodium carbonate (0.366 g, 3.45 mmol) and 2-ethoxy-1,3-diaminopropane dihydrochloride (0.300 g, 1.57 mmol) were ground together in an agate pestle and mortar for 5 min. To the resulting white paste, 1*H*-pyrrole-2-carbaldehyde (0.299 g, 3.14 mmol) was added and the mixture ground for a further 10 min. The crude ligand was dissolved in dichloromethane (40 mL) and washed with water (3 x 25 mL) portions. The organic layer was dried over anhydrous sodium carbonate. To the dichloromethane solution, aliquots of ethanol (1 mL) and hexane (50 mL) were added to re-crystallise the ligand. Crystals suitable for singe crystal X-ray diffraction were obtained from the re-crystallisation (0.280 g, 65% yield). The novel ligand was further characterized by ^{1}H NMR, ^{13}C NMR, UV/visible and IR spectroscopy and X-ray diffraction. UV/vis (ethanol) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 290; 3.48 × 10^4. IR (cm^{-1}): 3158w δ(NH, pyrrole), 2975m br ν(CH, imine), 2901m ν(CH, H-$COCH_2$), 2838m ν(CH, CH_3) 1631s br ν(C=N), 734 (C-O stretch). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) [δ, ppm]: 1.08 (t, 3H, H-9), 3.49-3.65 (m, 4H,

H-6), 3.65-3.80 (m, 3H, H-8), 6.21 (t, 2H, H-2), 6.46 (dd, $^3J_1$ = 3.7 Hz, $^3J_2$ = 1.3 Hz, 2H, pyrrole H-3), 6.86 (s br, 2H, H-1), 8.03 (s, 2H, H-5), 9.53 (s, 2H, CD_3OD exchangeable, H-10). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) [δ, ppm]: 15.62 (C-9), 62.64 (C-6), 65.82 (C-8), 79.31 (C-7), 109.66 (C-2), 114.34 (C-3), 122.02 (C-1), 130.26 (C-4), 153.68 (C5).

Synthesis of tert-butylamonium tetrachloroaurate(III)

There are several methods in the literature for making $[Bu_4N][AuCl_4]$. We have developed a modified version of a typical method which involves precipitation of $[Bu_4N][AuCl_4]$ after the addition of $[Bu_4N]Cl$ to a solution of $H[AuCl_4]$.[40] More specifically, we found it necessary to add a solvent-extraction step to the preparative method to obtain an acid-free product suitable for subsequent metallation reactions of the potentially hydrolysable Schiff base ligands described in this invention.

Hydrogen tetrachloroaurate(III) (0.406 g, 0.98 mmol) was dissolved in deionised water (15 mL). To this solution *tert*-butylamonium hydrogen sulphate (340 mg, 1.01 mmol) was added, forming a lipophillic gold(III) salt, which immediately precipitated from the aqueous solution as a bright yellow powder:

$$H[AuCl_4](aq) + [Bu_4N][HSO_4](aq) \rightarrow [Bu_4N][AuCl_4](s) + H_2SO_4(aq)$$

The $[Bu_4N][AuCl_4]$ was then extracted from the sulphuric acid into chloroform. The organic solution was dried over magnesium sulphate before the chloroform was removed by rotary evaporation, leaving a bright yellow, crystalline solid (0.570 g, 97.2% yield). The crystalline solid was dried under vacuum and stored under nitrogen.

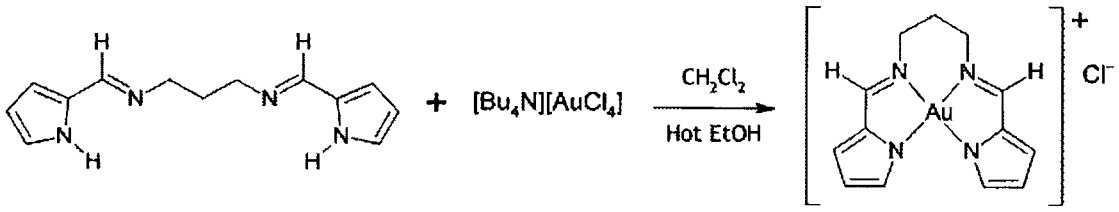
General metallation of simple bis(pyrrole-imine) and bis(imidazole-imine) ligands

In a typical reaction carried out under an inert atmosphere, $[Bu_4N][AuCl_4]$ (100 mg, 0.172 mmol) was added to a dry 100 mL round-bottom flask and dissolved in 20 mL of dry dichloromethane. Five molar equivalents of free base ligand (0.860 mmol) were dissolved in 15 mL of dry ethanol. The ethanolic solution was then heated and the gold(III) solution was added via cannula transfer to the hot ethanol solution and the mixture stirred under nitrogen. The solution rapidly turned a deep red colour and the

product precipitated from the solution as a pale yellow powder after approximately 45 minutes. The precipitate was collected by centrifugation. This crude material was re-crystallized by slow liquid diffusion of a methanol solution of the complex into diethylether. The re-crystallized product may be isolated in 60-70% yield and analysed by X-ray crystallography as well as LCMS, NMR, IR and UV/visible spectroscopy.

Specific synthetic procedure for compound 1.1a

The synthetic scheme (Scheme 26 below) and structures of the reagents and products are shown below for MA_AuPr. The method is general for all of the non-macrocyclic bis(pyrrolide-imine) structures listed in Formula (I).



Scheme 26

The following reaction was carried out under inert atmosphere conditions. To a dry 100 mL round-bottomed flask, $[Bu_4N][AuCl_4]$ (100 mg, 0.172 mmol) was added and dissolved in 20 mL dry dichloromethane. Five molar equivalents of free base ligand (196 mg, 0.860 mmol) was dissolved in 15 mL of dry ethanol (the ligand was synthesized as previously described[14]). The ethanolic solution was then heated and the gold(III) solution was added via cannula transfer to the hot ethanol solution and the mixture stirred under nitrogen. The solution rapidly turned a deep red color and the product precipitated from the solution as a pale yellow powder after approximately 45 minutes. The precipitate was now air stable and was collected by centrifugation. This crude material was re-crystallized by slow liquid diffusion of a methanol solution into diethylether. The re-crystallized product (52.8 mg, 0.148 mmol, 67% yield) was shown to be MA_AuPr by X-ray crystallography as well as NMR, IR and UV/visible spectroscopy.

It was found that use of a smaller excess of ligand resulted in the desired chelate. The counterion of this chelate was not, however, the desired chloride ion but rather a linear gold(I) chloride, $[AuCl_2]^-$. The presence of this undesirable anion was confirmed by X-ray crystallography. The developed method with the addition of the gold(III) solution to the excess ligand, dissolved in hot ethanol consistently produced the desired chelate, with the desired anion.

The salt $[Bu_4N][AuCl_4]$ was found to be more satisfactory than the more conventional $[Na][AuCl_4]$ as the source of gold(III) ions for two reasons. First, the use of $[Na][AuCl_4]$ resulted in the formation of $[AuCl_2]^-$ anions, regardless of the concentration of the ligand solution. Second, the salt $[Bu_4N][AuCl_4]$ is soluble in non-polar solvents, unlike $[Na][AuCl_4]$ which is only soluble in polar solvents. This therefore means that the chelation reaction can be carried out in non-polar solvents. This is ideal since the starting materials are soluble in non-polar solvents, while the gold(III) chelate is not. The gold(III) chelate therefore precipitates out of solution relatively pure. This synthetic method was therefore found to require no additional purification steps, the final crystallization was sufficient to generate a high purity material.

Characterization data for compound 1.1a

2,2'-{propane-1,3-diylbis[nitrilo(E)methylylidene]}bis(pyrrol-1-ido)gold(III) chloride: M/Z^+ = 423.0885 M^+ (calc. = 423.0884). UV/vis (methanol) [λ_{max}, nm; ε, $mol^{-1}\ dm^3\ cm^{-1}$]: 288; $1.47x10^4$, 382; $1.05x10^4$. IR (KBr pellet, cm^{-1}): 3090m br ν(CH, imine), 3010m ν(CH, $CH_2CH_2CH_2$), 2930m ν(CH, CH_2-N=CH), 1590s br ν(C=N). ^1H NMR (400 MHz, CD_3OD, 298 K) [δ, ppm]: 2.28 (q, 2H, $CH_2CH_2CH_2$), 3.78 (t, 4H, CH_2-N=CH), 6.49 (dd, $^3J_1$ = 2.5 Hz, $^3J_2$ = 2.5 Hz, 2H, pyrrole β-H), 7.05 (d, 2H, pyrrole γ-H), 7.58 (d br, 2H, pyrrole α-H), 8.22 (s, 2H, imine). ^{13}C NMR (100 MHz, CD_3OD, 298 K) [δ, ppm]: 32.53 ($CH_2CH_2CH_2$), 52.95 ($CH=NCH_2$), 113.96 (pyrrole β-*C*), 124.39 (pyrrole γ-*C*), 138.32 (pyrrole *C* NH-*C*-C=N), 139.25 (pyrrole α-*C*), 164.55 (imine *C*).

Characterization data for compound 1.1b

2,2'-{(2,2-dimethylpropane-1,3-diyl)bis[nitrilo(E)methyl- ylidene]} bis(pyrrol-1-ido)gold(III) chloride: M/Z$^+$ = 451.1196 M$^+$ (calc. = 451.1197). UV/vis (ethanol) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 290; 1.48x10^4, 381; 1.11x10^4. IR (KBr pellet, cm^{-1}): 3176w δ(NH, pyrrole), 3125m br ν(CH, imine), 2970m ν(CH, terminal CH_3), 2854m ν(CH_2, alkyl), 1631s br ν(C=N). ^{1}H NMR (400 MHz, CD_3OD, 298 K) [δ, ppm]: 0.98 (s, 6H, terminal CH_3), 3.43 (s, 4H, alkyl CH_2), 6.26 (dd, $^3J_1$ = 3.7 Hz, $^3J_2$ = 1.3 Hz, 2H, pyrrole β-*H*), 6.45 (t, 2H, pyrrole γ-*H*), 6.91 (s br, 2H, pyrrole α-H), 8.02 (s, 2H, imine). ^{13}C NMR (100 MHz, CD_3OD, 298 K) [δ, ppm]: 22.18 (CH_3), 39.03 ($C(CH_3)_2$), 61.70 (CH=NCH_2), 112.84.69 (pyrrole β-*C*), 123.33 (pyrrole γ-*C*), 137.57 (Pyrrole *C* NH-*C*-C=N), 137.95 (pyrrole α-*C*) 163.98 (imine *C*).

Characterization data for compound 1.1c

2,2'-{(2-hydroxypropane-1,3-diyl)bis[nitrilo(E) methyl- ylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V): M/Z$^+$ = 439.0834 M$^+$ (calc. = 439.0833). UV/vis (methanol) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 282; 1.57x10^4, 379; 1.15x10^4. IR (KBr pellet, cm^{-1}): 3431m br δ(OH), 3110m br ν(CH, imine), 2985m ν(CH, H-COH), 2946m ν(CH, CH_2-N=CH), 1592s br ν(C=N), 1104w (C-O stretch). ^{1}H NMR (400 MHz, D_2O, 298 K) [δ, ppm]: 3.35 (s ,1H, *H*OCH), 3.77 (s, 2H, CH_2-N=CH, 6.36 (dd, $^3J_1$ = 2.1 Hz, $^3J_2$ = 1.8 Hz pyrrole β-H), 6.89 (s br, 2H, pyrrole γ-H) 7.24 (s, 2H, pyrrole α-H), 8.02 (s, 2H, imine). ^{13}C NMR (100 MHz, D_2O, 298 K) [δ, ppm]: 54.95 ($CH_2CHOHCH_2$), 69.02 ($CH_2CHOHCH_2$), 100.03 (pyrrole β-*C*), 113.07 (pyrrole γ-*C*), 124.00 (pyrrole *C* NH-*C*-C=N), 137.08 (pyrrole α-*C*), 164.62 (imine *C*).

Characterization data for compound 1.1d

2,2'-{(2-ethoxypropane-1,3-diyl)bis[nitrilo(E)methylylidene]}bis (pyrrol-1-ido)gold(III) hexafluorophosphate(V): M/Z$^+$ = 467.1148 M$^+$ (calc. = 467.1146). UV/vis (acetonitrile) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 288; 1.43x10^4, 379.5; 1.10x10^4. IR (cm^{-1}): 2909m br ν(CH, imine), 2880m ν(CH, H-COC), 1581s br ν(C=N), 1045s ν(C-O) 834w ν(PF_6). ^{1}H NMR (400 MHz, CD_3CN, 298 K) [δ, ppm]: 1.16 (t, 3H, CH_3), 3.61 (q, 2H,

OCH_2CH_3), 3.80 (d, 2H, CH_2-N=CH), 3.95 (dd, $^3J_1$ = 9.6 Hz, $^3J_2$ = 5.8 Hz, 2H, CH_2-N=CH), 4.31 (t ,1H, OC*H*), 6.53 (dd, $^3J_1$ = 2.1 Hz, $^3J_2$ = 1.8 Hz pyrrole β-H), 7.10 (s br, 2H, pyrrole γ-H) 7.54 (s, 2H, pyrrole α-H), 8.12 (s, 2H, imine). ^{13}C NMR (100 MHz, CD_3CN, 298 K) [δ, ppm]: 14.50 (CH_3), 29.99 (OCH_2CH_3) 53.28 and 64.20 ($CH_2CHClCH_2$), 75.49 (CH), 112.85 (pyrrole γ-*C*), 123.59 (pyrrole *C* NH-*C*-C=N), 137.65 (pyrrole α-*C*), 164.36 (imine *C*).

Characterization data for compound 1.1e

2,2'-{(2-chloropropane-1,3-diyl)bis[nitrilo(E)methylylidene]}bis (pyrrol-1-ido)gold(III) hexafluorophosphate(V): M/Z$^+$ = 457.0497 M$^+$ (calc. = 457.0494). UV/vis (acetonitrile) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 289; 1.54x10^4, 381.5; 1.22x10^4. IR (cm^{-1}): 3141m br ν(CH, imine), 3046m ν(CH, H-CCl), 1581s br ν(C=N), 822w ν(PF_6), 741s ν(C-Cl). ^{1}H NMR (400 MHz, CD_3CN, 298 K) [δ, ppm]: 3.96 (dd, $^3J_1$ = 10.00 Hz, $^3J_2$ = 4.85 Hz, 2H, CH_2-N=CH), 4.15 (d, 2H, CH_2-N=CH), 5.00 (t ,1H, ClC*H*), 6.56 (dd, $^3J_1$ = 2.1 Hz, $^3J_2$ = 1.8 Hz pyrrole β-H), 7.16 (s br, 2H, pyrrole γ-H) 7.57 (s, 2H, pyrrole α-H), 8.11 (s, 2H, imine). ^{13}C NMR (100 MHz, CD_3CN, 298 K) [δ, ppm]: 55.86 ($CH_2CHClCH_2$), 58.00 ($CH_2CHClCH_2$), 100.03 (pyrrole β-*C*), 113.28 (pyrrole γ-*C*), 124.52 (pyrrole *C* NH-*C*-C=N), 137.59 (pyrrole α-*C*), 164.65 (imine *C*).

Characterization data for compound 1.2a

2,2'-{ethane-1,2-diylbis[nitrilo(E)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V): M/Z$^+$ = 409.0728 M$^+$ (calc. = 409.0729). UV/vis (acetonitrile) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 292; 1.45x10^4, 385; 1.07x10^4. IR (KBr pellet, cm^{-1}): 3127m br ν(CH, imine), 3053m ν(CH, CH_2CH_2), 2866m ν(CH, CH_2-N=CH), 1575s br ν(C=N). ^{1}H NMR (400 MHz, CD_3OD, 298 K) [δ, ppm]: 4.40 (s, 4H, CH_2-N=CH), 6.50 (dd, $^3J_1$ = 2.14 Hz, $^3J_2$ = 1.3 Hz, 2H, pyrrole β-*H*), 7.08 (s, 2H, pyrrole α-*H*), 7.47 (t, 2H, pyrrole γ-*H*), 7.86 (s, 2H, imine). ^{13}C NMR (100 MHz, CD_3CN, 298 K) [δ, ppm]: 62.49 (CH_2CH_2), 112.89 (pyrrole β-*C*), 125.67 (pyrrole γ-*C*), 137.99 (pyrrole α-*C*), 138.84 (Pyrrole *C* NH-*C*-C=N), 161.44 (imine *C*). ^{31}P NMR (162 MHz, CD_3CN, 298 K) [δ, ppm]: -144.62 (PF_6). ^{19}F NMR (376 MHz, CD_3CN, 298 K) [δ, ppm]: -73.82, -71.95 (PF_6).

Characterization data for compound 1.2b

2,2'-{(2S)-propane-1,2-diylbis[nitrilo(E)methylylidene]} bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V): M/Z$^+$ = 423.0883 M$^+$ (calc. = 423.0884) . UV/vis (acetonitrile) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 293.5; 1.42x10^4, 385; 1.08x10^4. IR (KBr pellet, cm^{-1}): 3125w br ν(CH, imine),1552s br ν(C=N), 830s (PF_6). ^{1}H NMR (400 MHz, CD_3OD, 298 K) [δ, ppm]: 1.62 (d, 3H, C*H*$_3$) 4.21 (dd, $^3J_1$ = 7.88 Hz, $^3J_2$ = 6.5 Hz, 1H, C*H*$_2$), 4.48 (dd, $^3J_1$ = 8.58 Hz, $^3J_2$ = 5.81 Hz, 1H, C*H*$_2$) 4.85 (m, 1H, C*H*CH$_3$), 6.50 (dd, $^3J_1$ = 2.14 Hz, $^3J_2$ = 1.3 Hz, 2H, pyrrole β-*H*), 7.08 (s, 2H, pyrrole α-*H*), 7.47 (t, 2H, pyrrole γ-*H*), 7.84 (s, 1H, imine), 7.88 (s,1H, imine). ^{13}C NMR (100 MHz, CD_3CN, 298 K) [δ, ppm]: 16.18 (*C*H$_3$), 68.07 (*C*H$_2$), 113.03 (pyrrole β-*C*), 125.58 (pyrrole γ-*C*), 140.00 (pyrrole α-*C*), 143.11 (Pyrrole *C* NH-*C*-C=N), 159.68 (imine *C*), 161.36 (imine *C*). ^{31}P NMR (162 MHz, CD_3CN, 298 K) [δ, ppm]: -144.27 (PF_6). ^{19}F NMR (376 MHz, CD_3CN, 298 K) [δ, ppm]: -73.87, -71.99 (PF_6).

Characterization data for compound 1.3b

2,2'-{(4-methyl-1,2-phenylene)bis[nitrilo(E)methylylidene]}bis(pyrrol-1-ido)gold(III) nitrate(V): M/Z$^+$ = 471.0887 M$^+$ (calc. = 471.0889). UV/vis (ethanol) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 296; 2.00x10^4, 323; 4.03x10^4, 374.5; 1.58x10^4, 457; 1.43x10^4. IR (cm^{-1}): 3097m br ν(CH, imine), 2983m ν(aromatic C-H), 1553s br ν(C=N). ^{1}H NMR (400 MHz, $CDCl_3$, 298 K) [δ, ppm]: 2.40 (s, 3H, C*H*$_3$) 6.62-8.0 (m, 9H, aromatic C-*H*), 8.84 (s, 2H, imine). ^{13}C NMR (100 MHz, $CDCl_3$, 298 K) [δ, ppm]: 21.78 (*C*H3), 115.26 (pyrrole α-*C*), 118.04 (pyrrole β-*C*), 120.35 (CH$_3$*C*CHCN), 120.98 (*C*HCHCN) 124.68 (pyrrole γ-*C*), 127.25 (CH*C*HCN) 131.23 (pyrrole *C* NH-*C*-C=N), 143.76 (CH$_3$*C*), 145.4 (Ph *C*), 153.33 (imine *C*).

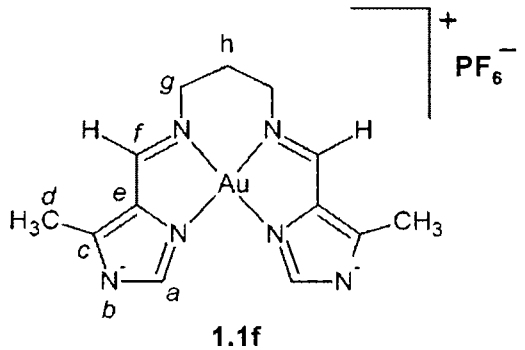
Characterization data for compound 1.4c

2,2'-{(1R,2R)-cyclohexane-1,2-diylbis[nitrilo(E)methylylid en]}bis(pyrrol-1-ido)gold(III)hexafluorophosphate(V): M/Z$^+$ = 463.1195 M$^+$ (calc. = 463.1197). UV/vis (acetonitrile) [λ_{max}, nm; ε, mol^{-1} dm^3 cm^{-1}]: 294; 1.54x10^4, 380.5; 1.22x10^4. IR (cm^{-1}): 2955m br ν(CH, imine), 2867m ν(CH, CH$_2$C*H*$_2$), 1564s br ν(C=N), 821s ν(PF_6). ^{1}H NMR

(400MHz, DMSO, 298 K) [δ, ppm]: 1.31 and 1.65 (t, 2H, CH_2CH), 1.78 and 2.61 (d, 2H, CH_2CH_2CH), 4.32 (d, 2H, CH) 6.47 (dd, $^3J_1$ = 2.14 Hz, $^3J_2$ = 1.3 Hz, 2H, pyrrole β-*H*), 7.07 (t, 2H, pyrrole α-*H*), 7.78 (s br, 2H, pyrrole γ-*H*), 8.37 (s, 2H, imine). ^{13}C NMR (100 MHz, DMSO, 298 K) [δ, ppm]: 24.40 ($CHCH_2CH_2CH_2$), 29.08 ($CHCH_2CH_2CH_2$), 76.86 ($CHCH_2CH_2CH_2$), 113.02 (pyrrole α-*C*), 125.20 (pyrrole β-*C*), 140.00 (pyrrole γ-*C*), 143.38 (Pyrrole *C* NH-*C*-C=N), 158.92 (imine *C*).

Synthesis of bis(imidazolato-imine) chelates

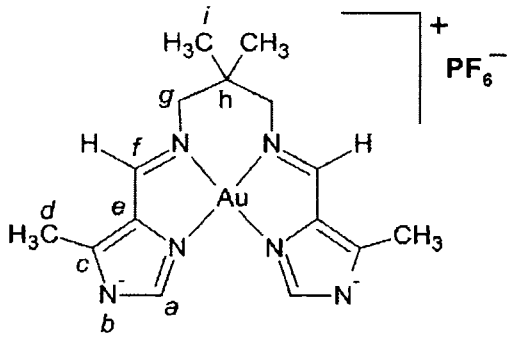
Procedure for compound 1.1f



1.1f

A solution of *tert*-butylammonium tetrachloroaurate (100 mg, 0.172 mmol) and *tert*-butylammonium hexafluorophosphate(V) (400 mg, 0.103 mmol) in dichloromethane (20 ml) was added to *N,N'*-bis[(1*E*)-(5-methyl-1*H*-imidazol-4-yl)methylene]propane-1,3-diamine (246 mg. 0.860 mmol) in ethanol (10 mL). A yellow precipitate immediately formed. The solution was stirred at room temperature for 1 hour. The yellow precipitate of *4,4'-{propane-1,3-diylbis[nitrilo(E)methylylidene]}bis(5-methylimidazol-1-ide)gold(III) hexafluorophosphate(V)* (complex 1.1f) was filtered and dried (81 mg, 79%). ^1H NMR: (500 MHz, DMSO-d_6) δ 2.22 (br, 2H, ***h***), 2.52 (s, 6H, ***d***), 3.74 (br, 4H, ***g***), 8.41 (s, 2H, ***a***), 8.83 (s, 2H, ***f***). ^{13}C NMR: (125 MHz, DMSO-d_6) δ 14.5 (***d***), 30.5 (***h***), 51.9 (***g***), 134.5 (***c***), 147.6 (***a***), 152.7 (***e***), 162.0 (***f***). IR (cm^{-1}): 1595(s), 1359(m), 1298(m), 1256(m), 1201(m), 1157(m), 971(w), 820(vs), 641 (m), 555(s), 482(m), 431 (m); MS: m/z 453.1099 $(M+Na)^+$.

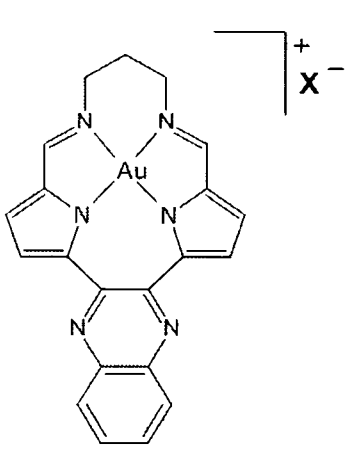
Procedure for compound 1.1g



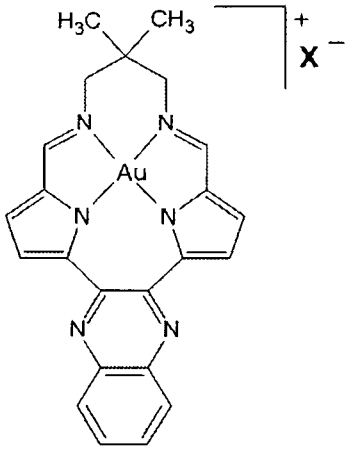
1.1g

A solution of *tert*-butylammonium tetrachloroaurate (100 mg, 0.172 mmol) and *tert*-butylhexafluorophosphate(V) (400 mg, 0.103 mmol) in dichloromethane (20 mL) was added to a 2,2-dimethyl-*N*,*N*'-bis[(1*E*)-(5-methyl-1*H*-imidazol-4-yl)methylene]propane-1,3-diamine (178 mg, 0.688 mmol) in ethanol (5 mL). This resulted in the immediate formation of a yellow precipitate. The reaction mixture was stirred for one hour at room temperature. The yellow precipitate of *4,4'-{(2,2-dimethylpropane-1,3-diyl)bis-[nitrilo(E)methylylidene]}bis(5-methylimidazol-1-ide)gold(III)* hexaflurophosphate(V) (complex 1.1g) was filtered and dried (89 mg, 83%). ^{1}H NMR: (500 MHz, DMSO-d_6) δ 1.08 (s, 6H, ***i***), 2.53 (s, 6H, ***d***), 3.47 (s, 4H, ***g***), 8.45 (s, 2H, ***a***), 8.80 (s, 2H, ***f***). ^{13}C NMR: (125 MHz, DMSO-d_6) δ 14.5 (***d***), 30.5 (***h***), 51.9 (***g***), 134.5 (***c***), 147.6 (***a***), 152.7 (***e***), 162.0 (***f***). IR (cm^{-1}): 1593(s), 1381(m), 1359(m), 1277(m), 1206(m), 922(vs), 642(w), 557(vs), 438(s). MS: m/z 481.1420 (M^+).

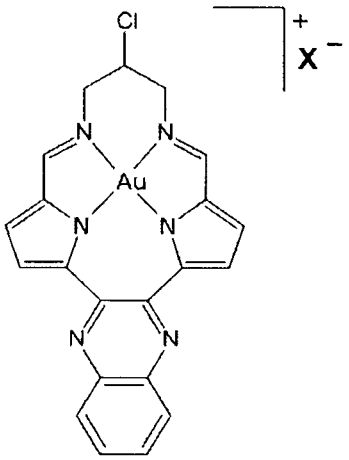
Synthesis of KA_AumacroPr and related Au(III) macrocycles



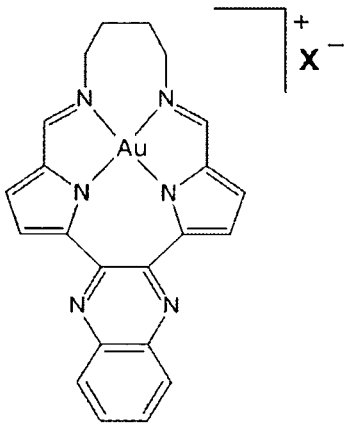
1.1Y¹a



1.1Y¹b



1.1Y¹e



1.5Y¹a

Macrocyclic Au(III) compound library synthesized and characterized using the methodology outlined for KA_AumacroPr and KA_AumacroDM. The anion X^- is typically PF_6^-, but may also be an anion such as triflate.

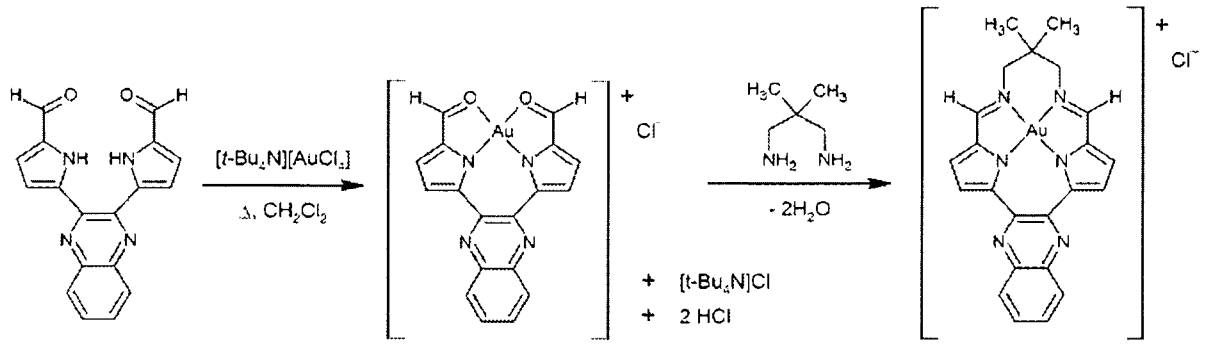
Scheme 26

Only the macrocyclic ligand for 1.1Y[1]a (i.e. that with a propyl bridge linking the two imine units) could be metallated by straightforward reaction of the macrocycle with a Au(III) salt using the method described for compound 1.1a. Complexes 1.1Y[1]b and 1.5Y[1]a had to be synthesized by a novel metal-templated reaction in which closure of the macrocycle through the formation of the bis(imine) links with the relevant diamine nucleophile occurs about the Au(III)-bound 2,3-bis(5'-formylpyrrol-2'-yl)quinoxaline moiety (i.e. metal-templated cyclization).

Procedure for compound 1.1Y[1]a

The free ligand was synthesized following the literature method.[41] A solution of *tert*-butylammonium tetrachloroaurate(III) (80 mg, 0.138 mmols) and *tert*-butylammonium hexafluorophosphate(V) (160 mg, 0.414 mmols) in dichloromethane (15 mL) was added dropwise to the free ligand, 12,13-dihydro-14*H*-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino [12,13-b]quinoxaline (99 mg, 0.275 mmols) in dichloromethane (20 mL). The solution was refluxed for 16 hours. Over this time a precipitate formed which was filtered, washed with dichloromethane and dried to afford a brick red powder of *{12,13-dihydro-14H-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V)* (44 mg, 37%). Crystals suitable for single crystal X-ray diffraction were grown by vapor diffusion of diethylether into a benzonitrile solution of the product. ^{1}H NMR (400 MHz, DMSO-d_6): δ 2.42 (br, 2H, =N-CH$_2$-C*H*$_2$), 3.94 (br, 4H, =N-C*H*$_2$-CH$_2$), 7.25 (d, $^3J_{HH}$= 4.4 Hz, 2H, *3*-pyrrole), 7.81 (d, $^3J_{HH}$= 4.4 Hz, 2H, *4*-pyrrole), 7.94-7.96 (dd, $^4J_{HH}$=3.3 Hz, $^3J_{HH}$=3.1 Hz, 2H, *6,7*-quinoxaline), 8.05-8.07 (dd, $^4J_{HH}$=3.3 Hz, $^3J_{HH}$=3.1 Hz, 2H, *8,5*-quinoxaline), 8.73 (s, 2H, -C*H*=N); ^{13}C (100 MHz, DMSO-d_6): δ 33.81, 51.27, 118.76, 122.46, 128.48, 131.69, 135.53, 138.99, 139.35, 147.54, 163.05; IR (cm^{-1}): 2955 (br), 1649 (m), 1572 (w), 1472 (w), 1400 (m), 1294 (m),1115 (m), 1068 (w), 832 (s), 760 (s), 664 (w), 497 (s), 424 (m); UV-vis (CH_3CN) λ_{max} [nm] (ε/M^{-1} cm^{-1}): 246 (23 346), 309 (30 077), 346 (18 001), 373 (15 237), 455 (12 041);); MS: m/z 549.1104 (M$^+$).

Procedure for compound 1.1Y[1]b



5,5'-quinoxaline-2,3-diylbis(1*H*-pyrrole-2-carbaldehyde)

postulated intermediate (not isolated)

Initial macrocyclic reaction product prior to conversion to PF_6^- salt

Metal-templated synthesis of the chloride salts of macrocyclic Au(III) compounds such as KA_AumacroDM and KA_AumacroBu. The chloride ion is then exchanged with PF_6^- for crystallization.

Scheme 27

2,3-Bis(5'-formylpyrrol-2'-yl)quinoxaline, alternatively named 5,5'-quinoxaline-2,3-diylbis(1*H*-pyrrole-2-carbaldehyde), was synthesized by the literature method.[41] A solution of 2,3-bis(5'-formylpyrrol-2'-yl)quinoxaline (54 mg, 0.172 mmols) in dichloromethane (10 mL) was added dropwise to *tert*-butylammonium tetrachloroaurate(III) (100 mg, 0.172 mmols) in dichloromethane (20 mL). The solution was allowed to reflux for 90 min before the addition 1,3-diamino-2,2-dimethylpropane (18 mg, 0.172 mmols) whereupon a yellow solid immediately precipitates out of solution. The reaction mixture was refluxed for a further 30 min and after this time triethylamine (35 mg, 0.344 mmols) was added after which the precipitate turned orange. The reaction mixture was refluxed for 1 hour before the orange precipitate was isolated and dried. This precipitate was dissolved in methanol and a saturated solution of ammonium hexafluorophosphate(V) was added to precipitate out the hexafluorophosphate salt of the gold complex. The precipitate was filtered and dried to afford an orange powder of *{12,14-dihydro-13,13-dimethyl-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V)* (45 mg, 36%). ^{1}H NMR (500 MHz, DMSO-d_6): δ 1.19 (s, 6H, CH_3), 3.72 (s, 4H, =N-CH_2-C(CH$_3$)$_2$), 7.44 (d, $^3J_{HH}$= 4.4 Hz,

2H, 3-pyrrole), 7.97-7.99 (dd, $^4J_{HH}$=3.3 Hz, $^3J_{HH}$=3.1 Hz, 2H, *6,7*-quinoxaline), 7.99 (d, $^3J_{HH}$= 4.4 Hz, 2H, *4*-pyrrole), 8.17-8.19 (dd, $^4J_{HH}$=3.3 Hz, $^3J_{HH}$=3.1 Hz, 2H, *8,5*-quinoxaline), 8.83 (s, 2H, -C*H*=N); ^{13}C (125 MHz, DMSO-d_6): δ 23.09, 43.05, 61.57, 119.35, 123.39, 129.08, 132.31, 136.73, 139.67, 140.03, 148.43, 164.56; IR (cm^{-1}): 1569 (m), 1471 (w), 1405 (m),1339 (w), 1238 (w), 1107 (m), 835 (s), 557 (m), 433 (m); UV-vis (CH_3CN) λ_{max} [nm] (ε/M^{-1} cm^{-1}): 230 (17 642), 249 (14 463), 309 (16 131), 348 (8 795), 375 (8 680), 458 (6 640), 481 (6 360); MS: m/z 577.1416 (M$^+$).

Procedure for compound 1.5Y^{1}a

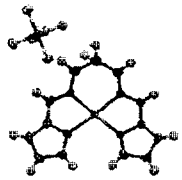
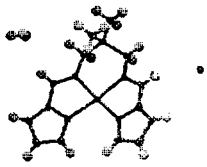
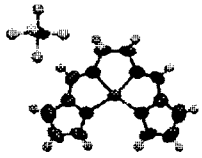
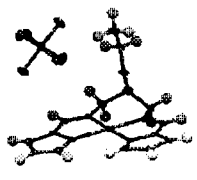
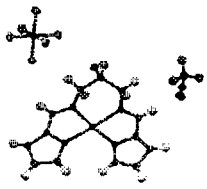
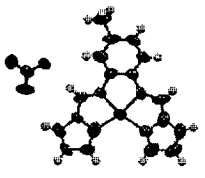
This complex was prepared by the same method used for the synthesis of 1.1Y^{1}b but with 1,4-diaminobutane (15.2 mg, 0.172 mmols) as the macrocycle-closing diamine to give a brown powder of compound 1.5Y^{1}a, *{12,13,14,15-tetrahydro-6,9:18,21-diepimino[1,6]diazacyclooctadecino[12,13-b]quinoxalinato}gold(III) hexafluorophosphate(V)* (20 mg, 16%). ^{1}H NMR (500 MHz, DMSO-d_6): δ 2.04 (br, 4H, =N-CH_2-C*H*$_2$), 4.31 (br, 4H, =N-C*H*$_2$-CH_2), 7.45 (d, $^3J_{HH}$= 4.4 Hz, 2H, 3-pyrrole), 7.95-7.97 (dd, $^4J_{HH}$=3.3 Hz, $^3J_{HH}$=3.1 Hz, 2H, *6,7*-quinoxaoline), 8.06 (d, $^3J_{HH}$= 4.4 Hz, 2H, *4*-pyrrole), 8.17-8.18 (dd, $^4J_{HH}$=3.3 Hz, $^3J_{HH}$=3.1 Hz, 2H, *8,5*-quinoxaline), 8.74 (s, 2H, -C*H*=N); ^{13}C (125 MHz, DMSO-d_6): δ 23.68, 55.41, 118.92, 122.26, 128.52, 131.69, 135.69, 139.64, 139.72, 147.92, 164.83; IR (cm^{-1}): 2964 (w), 1590 (m), 1400 (m), 1354 (m), 1100 (m), 1059 (m), 829 (s), 555 (s), 446 (w); UV-vis (CH_3CN) λ_{max} [nm] (ε/M^{-1} cm^{-1}): 244 (16 439), 306 (19 364), 347 (13 712), 370 (13 425), 449 (9 825); MS: m/z 563.1265 (M$^+$).

Compound 1.1Y^{1}e, *{13-chloro-12,14-dihydro-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V)*, was similarly synthesized.

Table 2 shows a summary of X-Ray data of some of the gold(III) chelates of the invention.

Table 2

Summary of X-Ray data of some of the gold(III) chelates of the invention

Crystal Data			
Formula	$C_{13}H_{14}AuF_6N_4OP$	$C_{15}H_{19}AuClN_4O_{0.5}$	$C_{12}H_{12}AuF_6N_4P$
Compound number	MA_AuOH (**1.1c**)	MA_AuDM (**1.1b**)	MA_AuEn (**1.2a**)
Cell Setting	Monoclinic	Monoclinic	Orthorhombic
Space Group	$P2_1/n$	$P2_1/c$	Pbcn
Formula Weight	584.22	495.76	554.2
a / Å	7.6496(2)	13.5985(3)	10.0520(5)
b / Å	11.8256(4)	11.9234(3)	20.1960(5)
c / Å	18.8218(6)	19.7476(5)	8.2450(5)
α / °; β/°; γ/°	90; 101.181(3); 90	90; 97.299(2); 90	90; 90; 90
T / K	131(2)	140(2)	298(2)
Z	4	4	4
V / Å^3	1670.32(9)	3175.94(13)	1673.82(14)
Density (g cm^{-3})	2.323	2.074	2.20
F(000)	1104	1896	1039.7
μ (mm^{-1})	8.977	9.435	8.948
Crystal Dim. (mm^3)	0.05 x 0.10 x 0.40	0.45 x 0.45 x 0.45	0.07 x 0.1 x 0.40
Radiation M_o K_α (Å)	0.71073		
Total data collected	17500	31771	16589
Unique Data	3297	6250	1665
R_{int}	0.0302	0.0741	0.068
Refinement Method	Full-matrix least-squares on F^2		
Final *R* indices [I>2sigma(I)]	R_1 = 0.0206 wR_2 = 0.0399	R_1 = 0.0424 wR_2 = 0.121	R_1 = 0.050 wR_2 = 0.140
Final *R* indices [all data]	R_1 = 0.0286 wR_2 = 0.0413	R_1 = 0.0479 wR_2 = 0.1238	R_1 = 0.072 wR_2 = 0.154
Crystal Data			
Formula	$C_{15}H_{17}AuF_6N_4OP$	$C_{15}H_{16}AuClF_6N_5P$	$C_{17}H_{14}AuF_6N_5O$
Compound number	MA_AuOEt (**1.1d**)	MA_AuCl (**1.1e**)	MA_AuTol (**1.3b**)
Cell Setting	Monoclinic	Monoclinic	Monoclinic
Space Group	$P2_1/n$	$P2_1/n$	$P2_1/n$

Formula Weight	611.3	643.7	533.3
a / Å	8.2220(5)	11.3580(3)	17.7717(12)
b / Å	10.5390(5)	12.5390(5)	8.9015(7)
c / Å	21.1170(5)	13.9730(4)	22.696(16)
α / °; β/°; γ/°	90; 95.430(5); 90	90; 106.490(5); 90	90; 102.530(7); 90
T / K	100(2)	100(2)	298(2)
Z	4	4	8
V / Å^3	1821.61(17)	1908.16(32)	3504.89(56)
Density (g cm^{-3})	2.229	2.24	2.02
F(000)	1164	1223.7	2031.3
μ (mm^{-1})	8.237	8.003	8.422
Crystal Dim. (mm^3)	0.10 x 0.10 x 0.60	0.07 x 0.10 x 0.60	0.02 x 0.15 x 0.50
Radiation M_o K_α (Å)	0.71073		
Total data collected	12681	18903	10005
Unique Data	3607	6137	5945
R_{int}	0.0542	0.041	0.061
Refinement Method	Full-matrix least-squares on F^2		
Final R indices [I>2sigma(I)]	R_1 = 0.0536 wR_2 = 0.1516	R_1 = 0.040 wR_2 = 0.101	R_1 = 0.079 wR_2 = 0.179
Final R indices [all data]	R_1 = 0.0598 wR_2 = 0.1546	R_1 = 0.051 wR_2 = 0.105	R_1 = 0.133 wR_2 = 0.194

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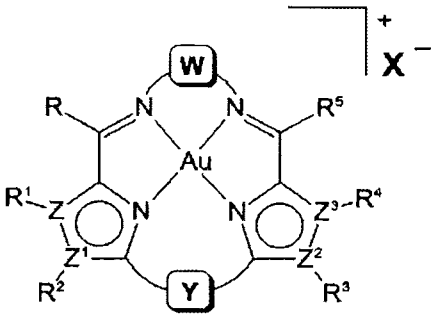
CLAIMS

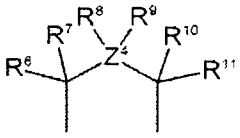
1. A compound selected from compounds of the Formula (I),



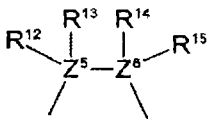
(I)

in which

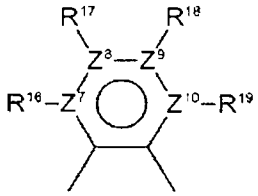
W is independently selected from W^1, W^2, W^3, W^4, W^5,



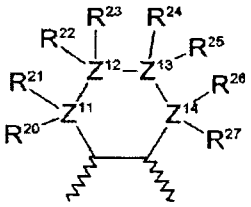
W^1



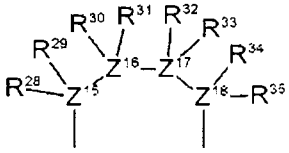
W^2



W^3



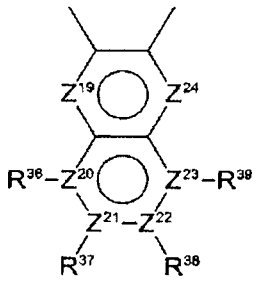
W^4



W^5

or W represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl or C_1-C_6 amide in which the amide is optionally part of a linking chain, and the Z^n–$Z^{n'}$ bonds (n = 4–17; n' = n + 1) are optionally of any whole or partial bond order,

Y is Y^1



Y^1

or Y represents a pair of substituents independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl,

or Y is optionally a bridging structure that may comprise one or more C_1-C_6 amide, C_1-C_6 ether, or C_1-C_6 ester groups,

R–R^{39} are independently selected from no substituent, a lone pair of electrons, H, halogen, C_5-C_6 aryl, C_1-C_{12} alkyl, amine, C_1-C_6 alkylamine, C_1-C_6 amide, nitro, cyano, carboxyl, C_1-C_6 ester, phosphane, thiol, C_1-C_6 thioether, OR^{40}, and suitable pairs of adjacent R groups (R–R^{39}) may optionally together form part of a C_5 or C_6 aryl ring, a Z_5 or Z_6 ring,

R^{40} is independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl, C_1-C_6 ester, poly(-C_2O-), amine, and C_1-C_6 alkylamine,

Z–Z^{24} are independently selected from C, N, P, O, and S, and

X^- is a pharmaceutically acceptable anion.

2. A compound as claimed in claim 1, in which the anion is selected from from halide, hexafluorophosphate, nitrate, and triflate.

3. A compound as claimed in claim 1 or claim 2, in which Y represents two hydrogen atoms or Y^1.

4. A compound as claimed in claim 3, in which Y is Y^1 and Z^{19} and Z^{24} are N.
5. A compound as claimed in claim 4, in which Z^{20}-Z^{23} are C.

6. A compound as claimed in any one of the preceding claims, in which R-R^5 are selected from H, C_1-C_3 alkyl, O-C_1-C_3 alkyl, hydroxyl and halogen.

7. A compound as claimed in claim 6, in which C_1-C_3 alkyl is methyl, O-C_1-C_3 alkyl is O-ethyl, and halogen is chlorine.

8. A compound as claimed in any of the preceding claims in which W is selected from W^1, W^2, W^3 W^4 or W^5.

9. A compound as claimed in claim 8, in which R^6-R^{35} are selected from H, C_1-C_3 alkyl, O-C_1-C_3 alkyl and halogen.

10. A compound as claimed in claim 9, in which C_1-C_3 alkyl is methyl, O-C_1-C_3 alkyl is O-ethyl and halogen is chlorine.

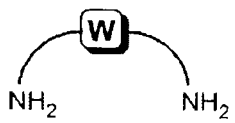
11. A gold(III) compound selected from:
2,2'-{propane-1,3-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) chloride,
2,2'-{(2,2-dimethylpropane-1,3-diyl)bis[nitrilo(*E*)methylylidene]} bis(pyrrol-1-ido)gold(III) chloride,
2,2'-{(2-hydroxypropane-1,3-diyl)bis[nitrilo(*E*) methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(2-ethoxypropane-1,3-diyl)bis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(2-chloropropane-1,3-diyl)bis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{ethane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(2*S*)-propane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),

2,2'-{(1*R*,2*R*)-cyclohexane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{(1*S*,2*S*)-cyclohexane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V),
2,2'-{cyclohexane-1,2-diylbis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) hexafluorophosphate(V)
2,2'-{(4-methylbenzene-1,2-diyl)bis[nitrilo(*E*)methylylidene]}bis(pyrrol-1-ido)gold(III) nitrate(V),
4,4'-{propane-1,3-diyl)bis[nitrilo(*E*)methylylidene]}bis(5-methylimidazol-1-ide)gold(III) hexafluorophosphate(V),
4,4'-{(2,2-dimethylpropane-1,3-diyl)bis[nitrilo(*E*)methylylidene]}bis(5-methylimidazol-1-ide)gold(III) hexaflurophosphate(V),
{12,13-dihydro-14H-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V),
{12,14-dihydro-13,13-dimethyl-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V),
{12,13,14,15-tetrahydro-6,9:18,21-diepimino[1,6]diazacyclooctadecino[12,13-b]quinoxalinato}gold(III) hexafluorophosphate(V), and
{13-chloro-12,14-dihydro-6,9:17,20-diepimino[1,6]diazacyclo-heptadecino[12,13-β]quinoxalinato}gold(III) hexafluorophosphate(V).

12. A compound as claimed in any one of claims 1-11 inclusive for the treatment of cancer.

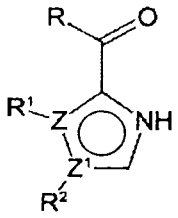
13. A pharmaceutical composition comprising at least one compound as claimed in any one of claims 1-11 inclusive.

14. A method of preparing a compound of Formula (I) as claimed in claim 1, which includes the steps of condensing a diamine of the general formula A

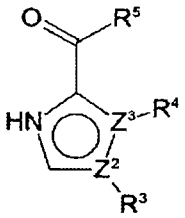


A

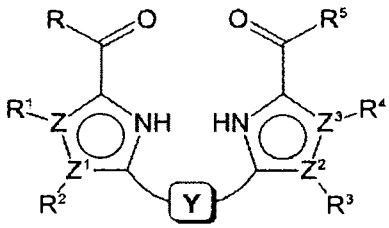
simultaneously or consecutively with a carbonyl compound selected from compounds of the general formula B, C and D



B

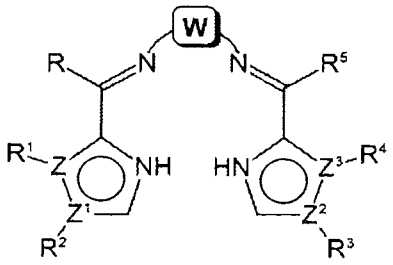


C

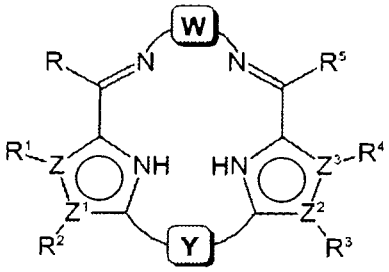


D

to produce a diimine Schiff base of the general formula E or F



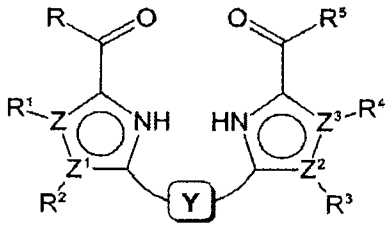
E



F

and reacting the diimine of general formula E or F with a tetraalkylammonium tetrahaloaurate(III) to produce the gold(III) compound of the general Formula (I) in which W, Y, R, Z and X are as described in claim1.

15. A method of preparing a compound of general Formula (I) as claimed in claim 1, which includes the step of reacting a carbonyl compound of the general formula D



D

with a tetraalkylammonium tetrahaloaurate(III) and, consecutively or simultaneously, a diamine to produce the compound of general Formula (I) in which W, Y, R, Z and X are as described in claim 1.

16. A method as claimed in claim 14 or claim 15, in which the tetraalkylammonium tetrahaloaurate(III) is tetrabutylammonium tetrachloroaurate(III).

17. A method as claimed in claim 16, in which the tetraalkylammonium tetrahaloaurate(III) is tetra-*t*-butylammonium tetrachloroaurate(III).

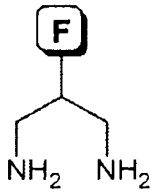
18. A method as claimed in any one of claims 15 to 17 inclusive, in which reacting with the tetraalkylammonium tetrahaloaurate(III) is carried out in the presence of a salt selected from halides, hexafluorophosphates, nitrates, and triflates.

19. A method as claimed in claim 18, in which the salt is a tetraalkylammonium hexafluorophosphate.

20. A method as claimed in claim 19, in which the salt is tetra-*t*-butylammonium hexafluorophosphate.

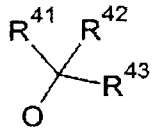
21. A method as claimed in any one of claims 15 to 17 inclusive, in which the compound of Formula (I) is a chloride and the method includes the further step of reacting the compound of Formula (I) in which X^- is chloride with a salt selected from halides other than chloride, hexafluorophosphates, nitrates, and triflates to produce a compound of Formula (I) in which X^- is the anion of the said salt.

22. A method of preparing a 2-substituted 1,3-diamine intermediate of the general formula A^1



A^1

or its dihydrochloride salt, in which
F is selected from F^1 or halogen,



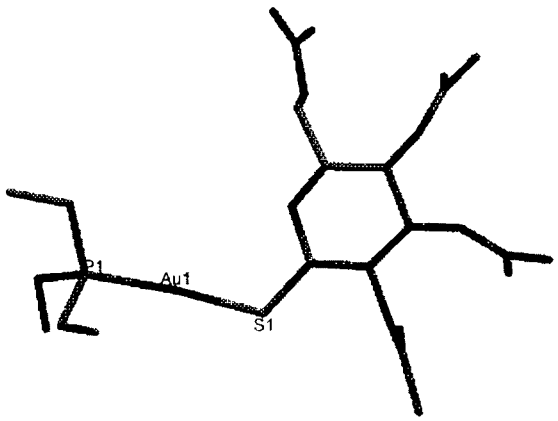
F^1

R^{41}-R^{43} are independently selected from H, halogen, Z_5 or Z_6 aryl, C_1-C_{12} alkyl, C_1-C_6 alkylamine, C_1-C_6 amide, carboxyl, C_1-C_6 ester and OR^{40},
R^{40} is as defined in claim 1, or
pairs of adjacent R groups (R^{41}-R^{43}) together form part of a C_5 or C_6 aryl ring, or
F is R^{44}, and
R^{44} is independently selected from H, C_1-C_6 alkyl, Z_5 or Z_6 aryl, C_1-C_6 ester, poly(-C_2O-), amine, C_1-C_6 alkylamine, and C_1-C_6 amide or a Z_5 or Z_6 ring, and
Z_5 and Z_6 are as defined in caim 1,
the method including the steps of converting the hydroxyl group of 2,2,12,12-*t*-methyl-3,11-dioxo-4,10-dioxa-5,9-diazatridecan-7-ol to the group F.

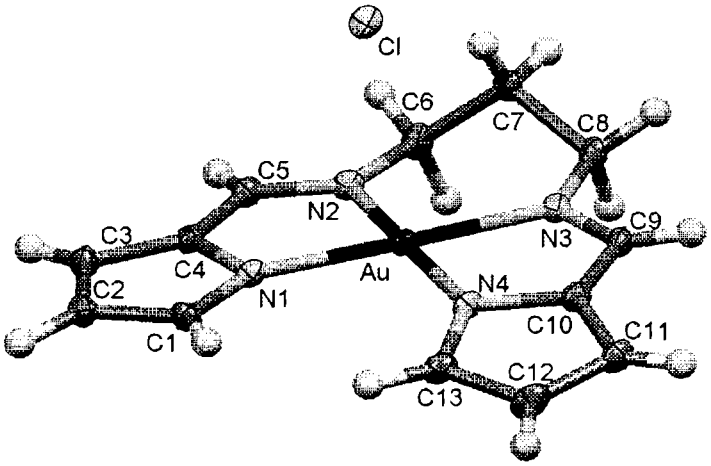
23. A bis(pyrrole-imine) ligand selected from:
2-ethoxy-*N*,*N*'-bis[(*E*)-1*H*-pyrrol-2-ylmethylidene]propane-1,3-diamine, and
2-chloro-*N*,*N*'-bis[(*E*)-1*H*-pyrrol-2-ylmethylidene]propane-1,3-diamine.

24. A method for the preparation of tetrabutylammonium tetrachloroaurate, $[Bu_4N][AuCl_4]$, the method including the step of extracting $[Bu_4N][AuCl_4]$ from a mixture using an organic solvent-extraction purification step to produce an acid-free, crystalline $[Bu_4N][AuCl_4]$.

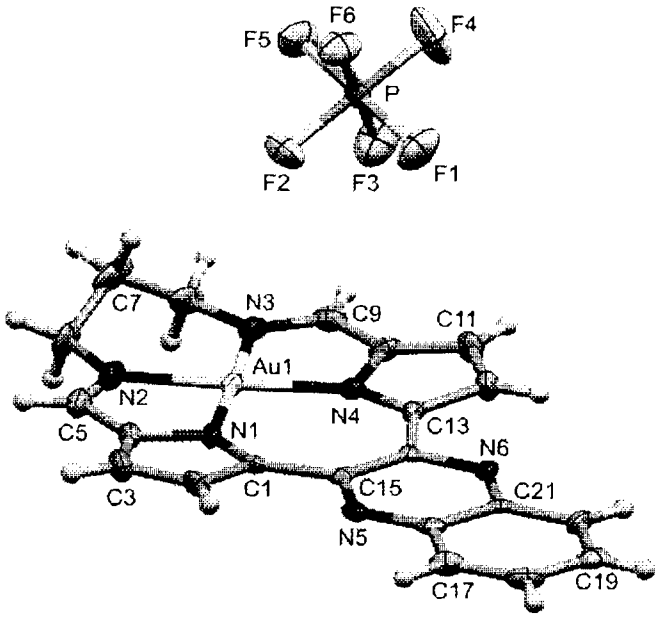
25. A method as claimed in claim 24, which includes reacting an aqueous solution of $H[AuCl_4]$ and $[Bu_4N][HSO_4]$ to produce the mixture and extracting the $[Bu_4N][AuCl_4]$ from the mixture with the organic solvent.



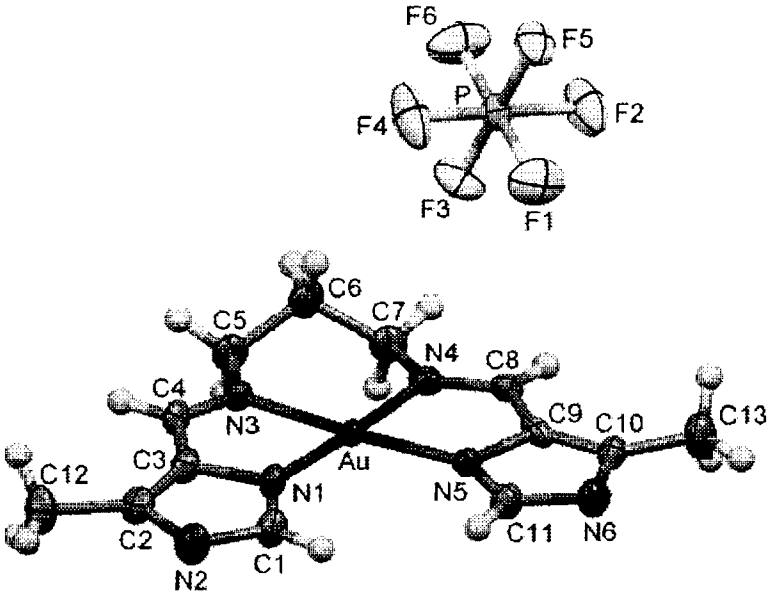
Scheme 1



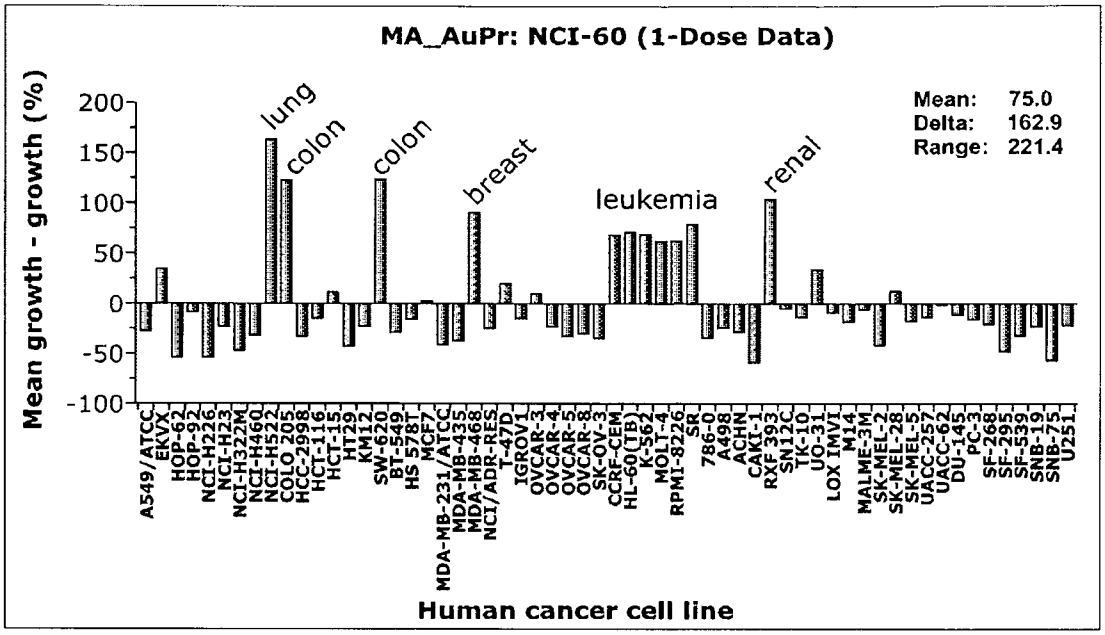
Scheme 5a



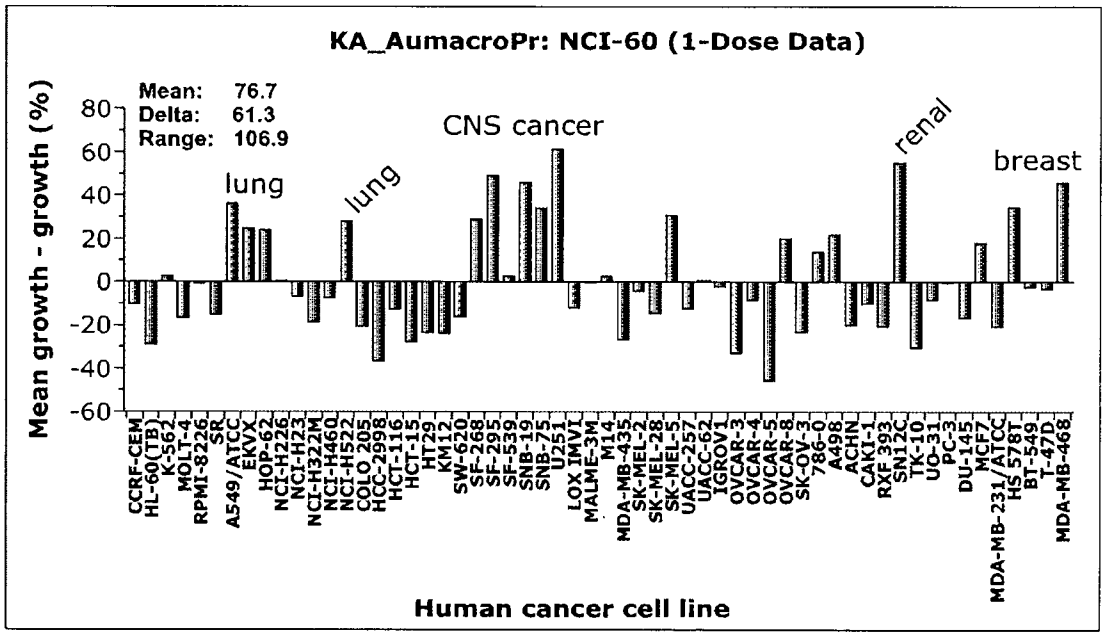
Scheme 5b



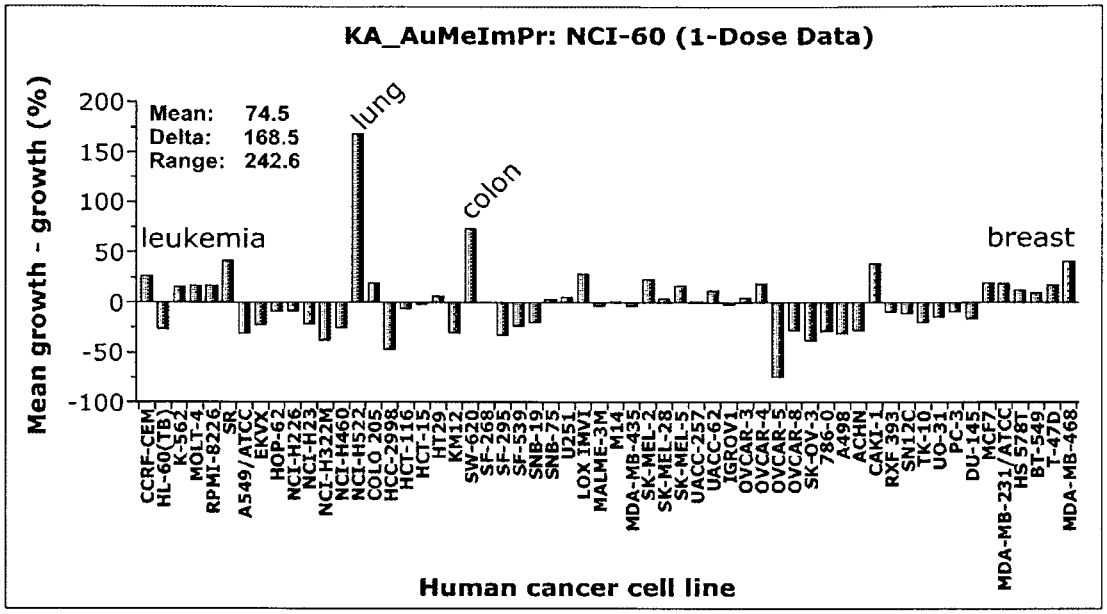
Scheme 5c



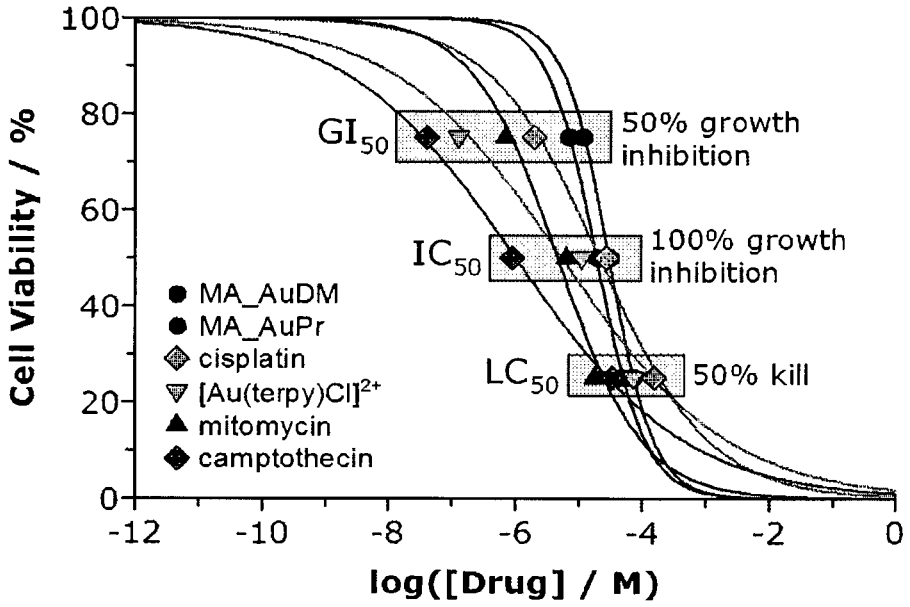
Scheme 6a



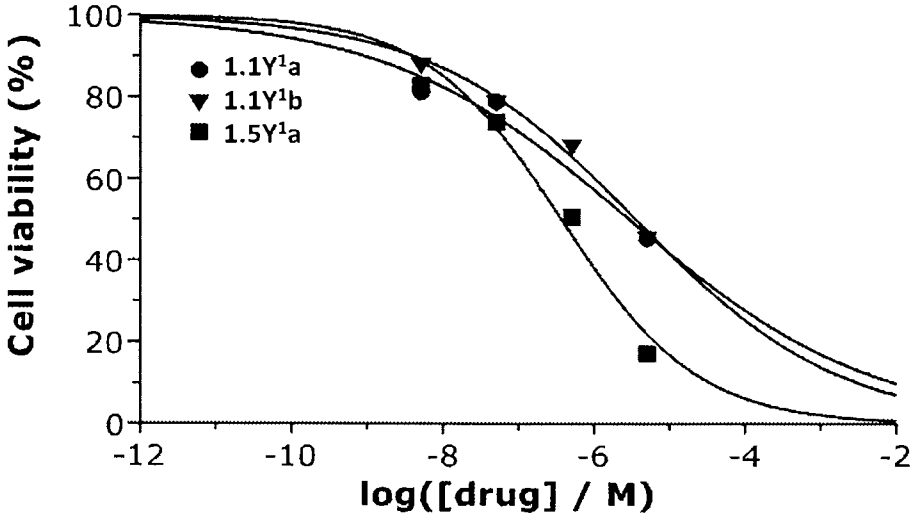
Scheme 6b



Scheme 6c

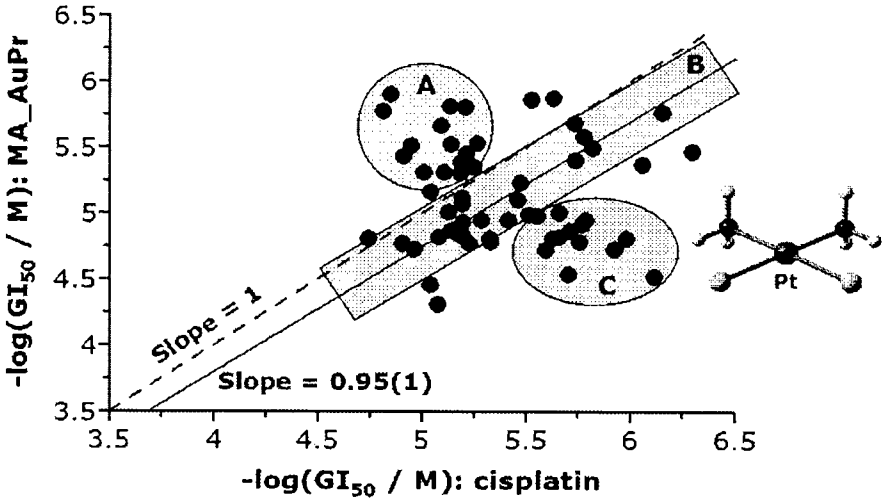


Scheme 8a

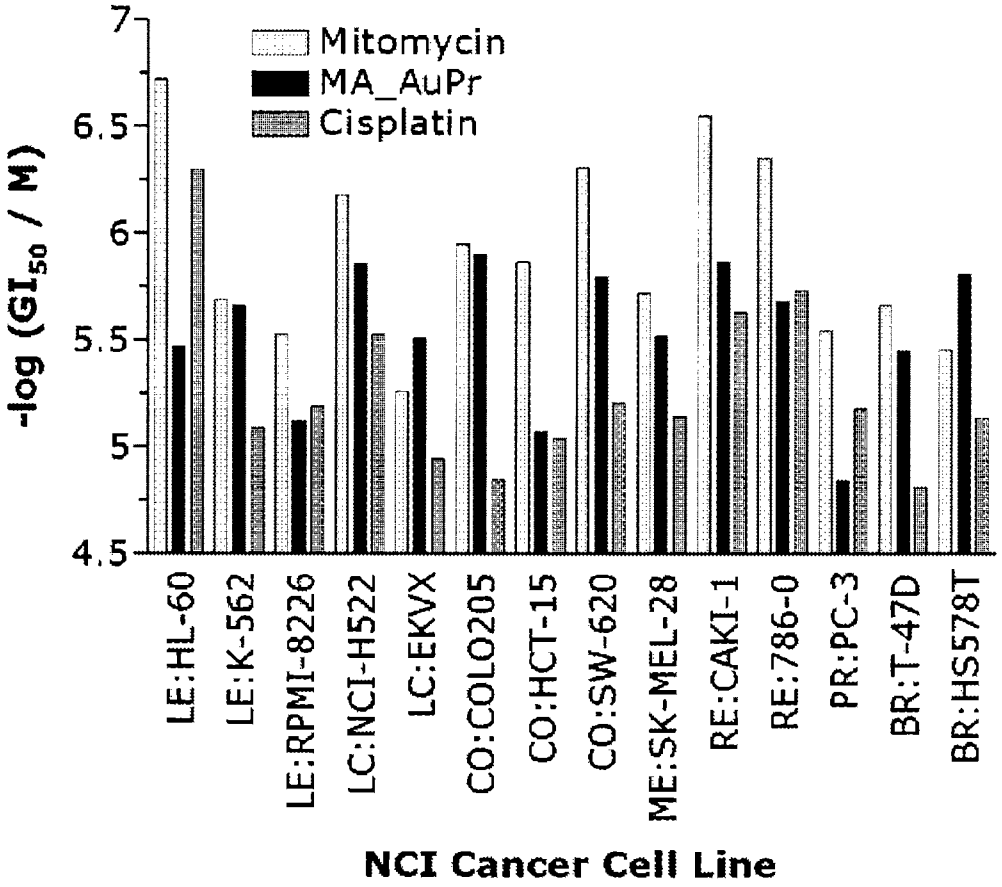


Compound	"W" group	IC_{50} / uM (HeLa Cells)	Hill Coeff.
1.1Y¹a (KA_AumacroPr)	$CH_2CH_2CH_2$	3.0(2.5)	0.27(6)
1.5Y¹a (KA_AumacroBu)	$CH_2(CH_2)_2CH_2$	0.37(27)	0.48(9)
1.1Y¹b (KA_AumacroDM)	$CH_2C(CH_3)_2CH_2$	3.6(1.1)	0.32(3)

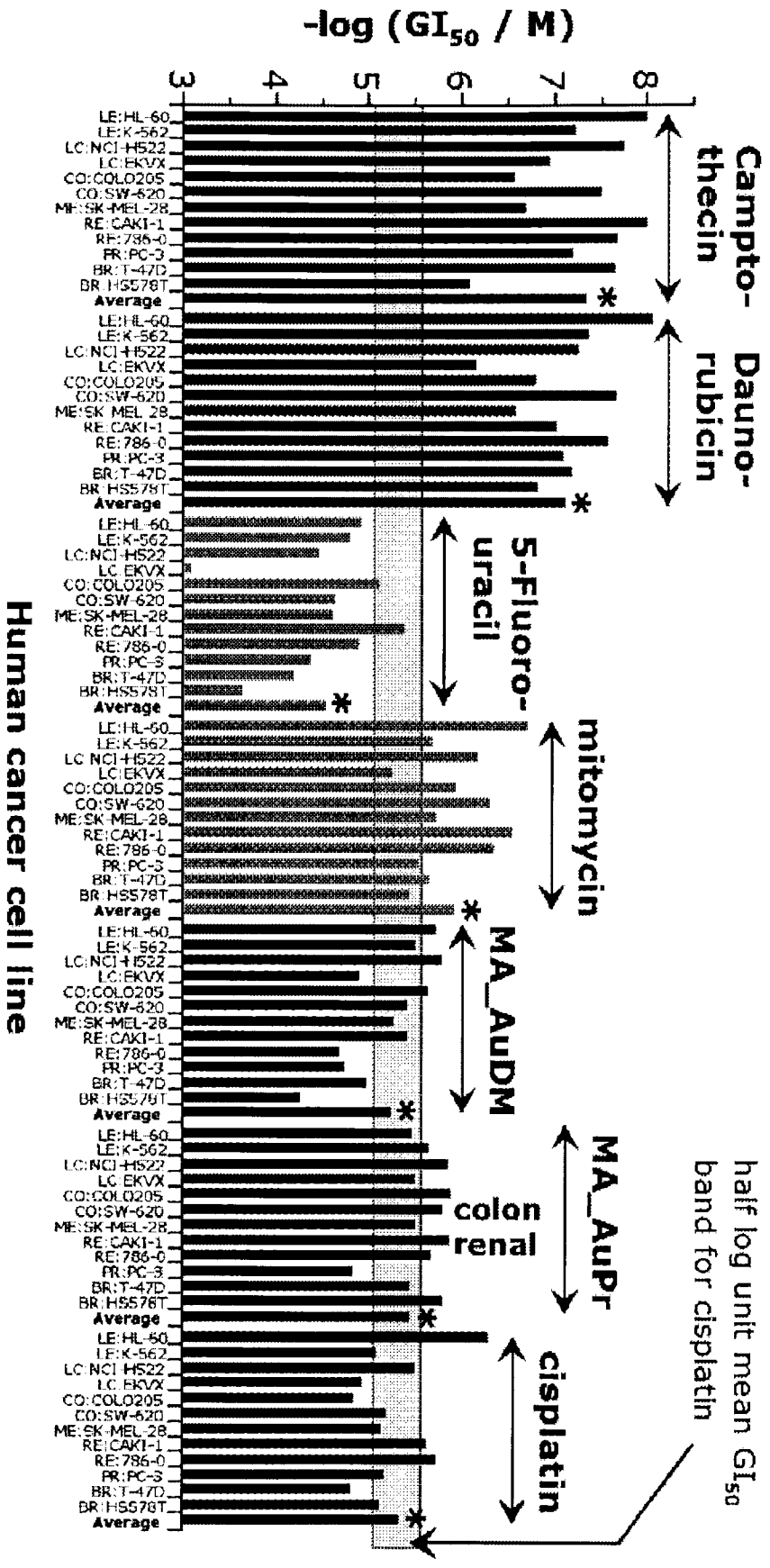
Scheme 8b



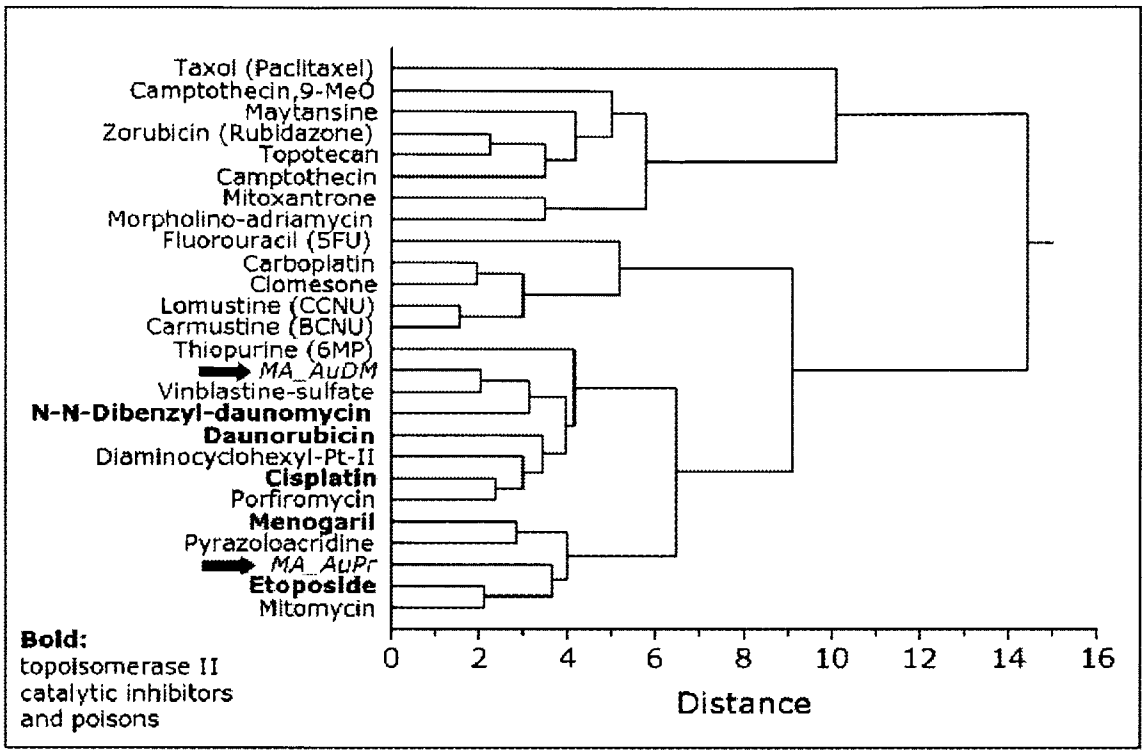
Scheme 9


Mitomycin
MA_AuPr
Cisplatin
-log (GI50 / M)
7
6.5
6
5.5
5
4.5
LE:HL-60
LE:K-562
LE:RPMI-8226
LC:NCI-H522
LC:EKVX
CO:COLO205
CO:HCT-15
CO:SW-620
ME:SK-MEL-28
RE:CAKI-1
RE:786-0
PR:PC-3
BR:T-47D
BR:HS578T
NCI Cancer Cell Line

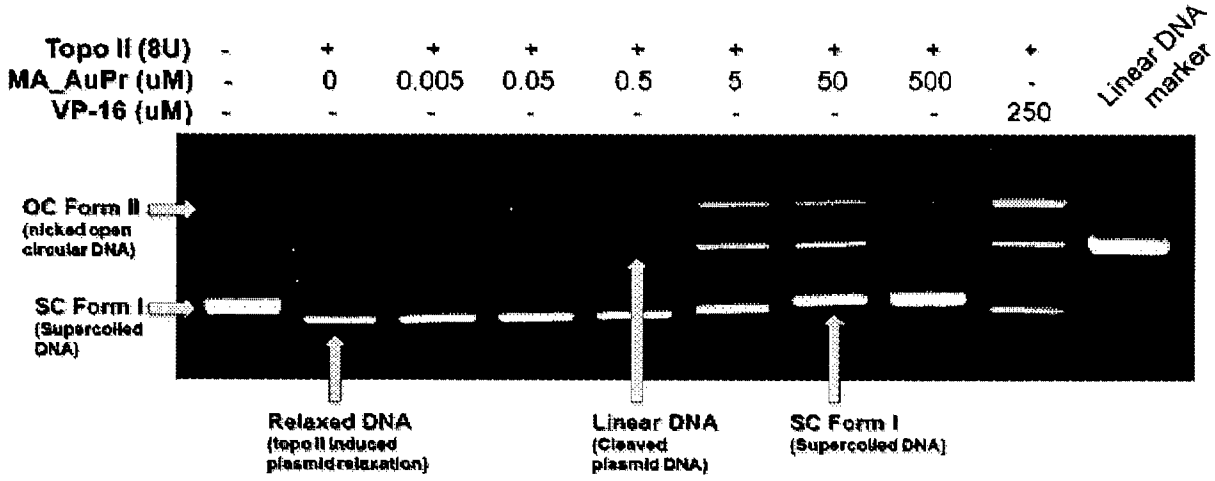
Scheme 10a


-log (GI50 / M)
3
4
5
6
7
8
Human cancer cell line
LE:HL-60
LE:K-562
LC:NCI-H522
LC:EKVX
CO:COLO205
CO:SW-620
ME:SK-MEL-28
RE:CAKI-1
RE:786-0
PR:PC-3
BR:T-47D
BR:HS578T
Average
Campto-thecin
Dauno-rubicin
5-Fluoro-uracil
mitomycin
MA_AuDM
MA_AuPr
colon renal
cisplatin
half log unit mean GI50 band for cisplatin

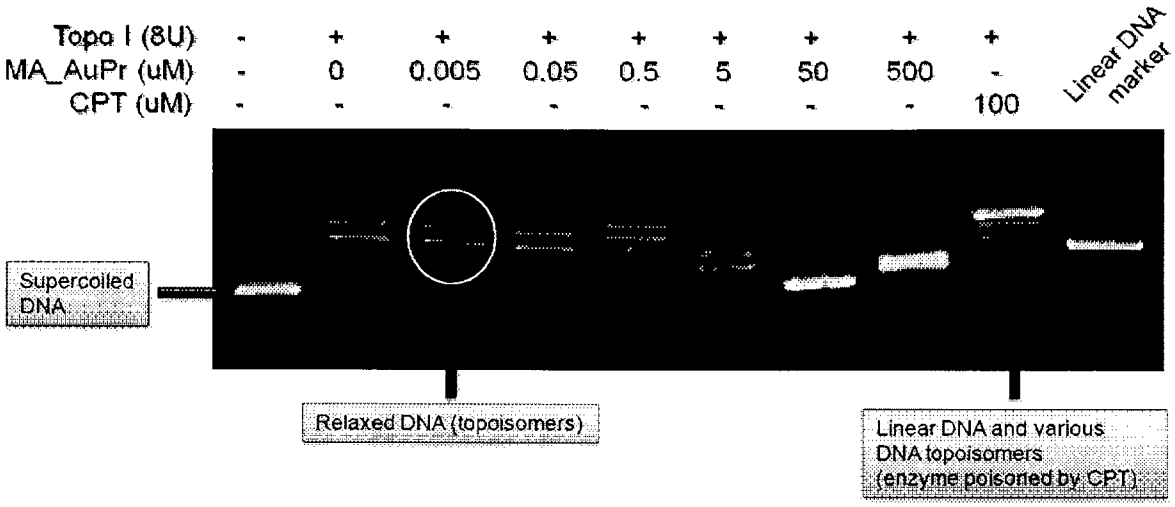
Scheme 10b



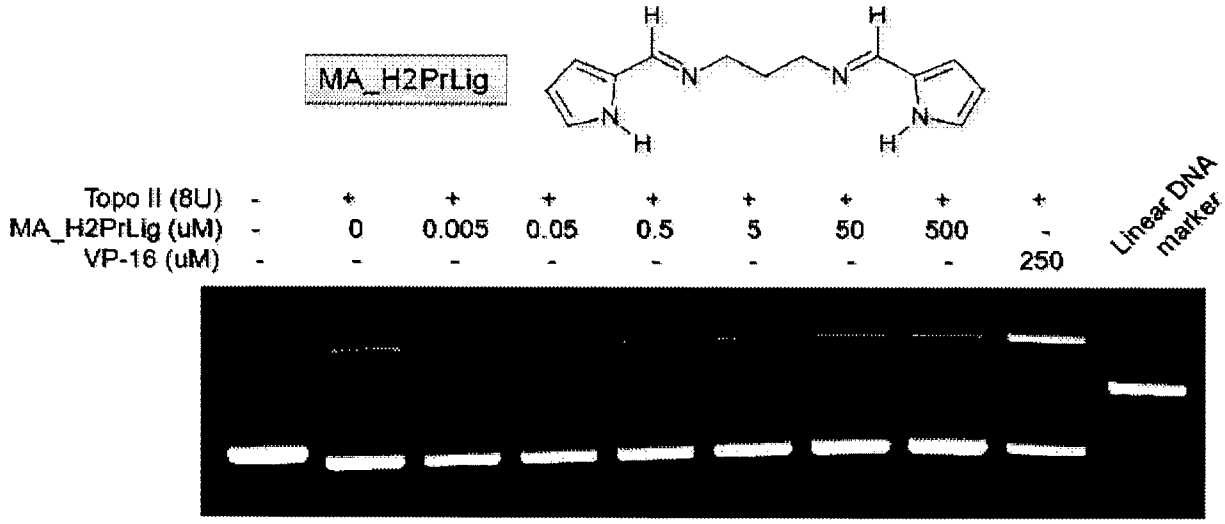
Scheme 11



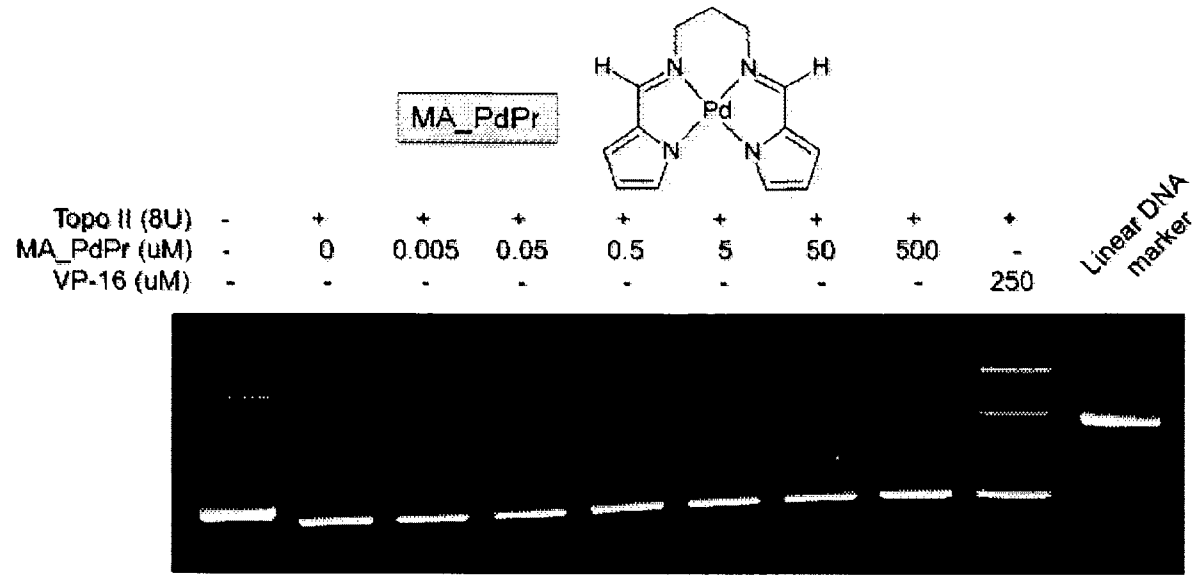
Scheme 12



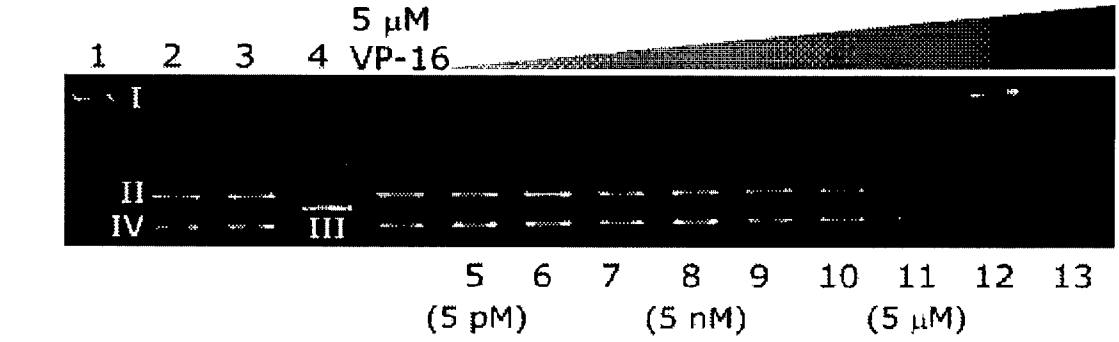
Scheme 13

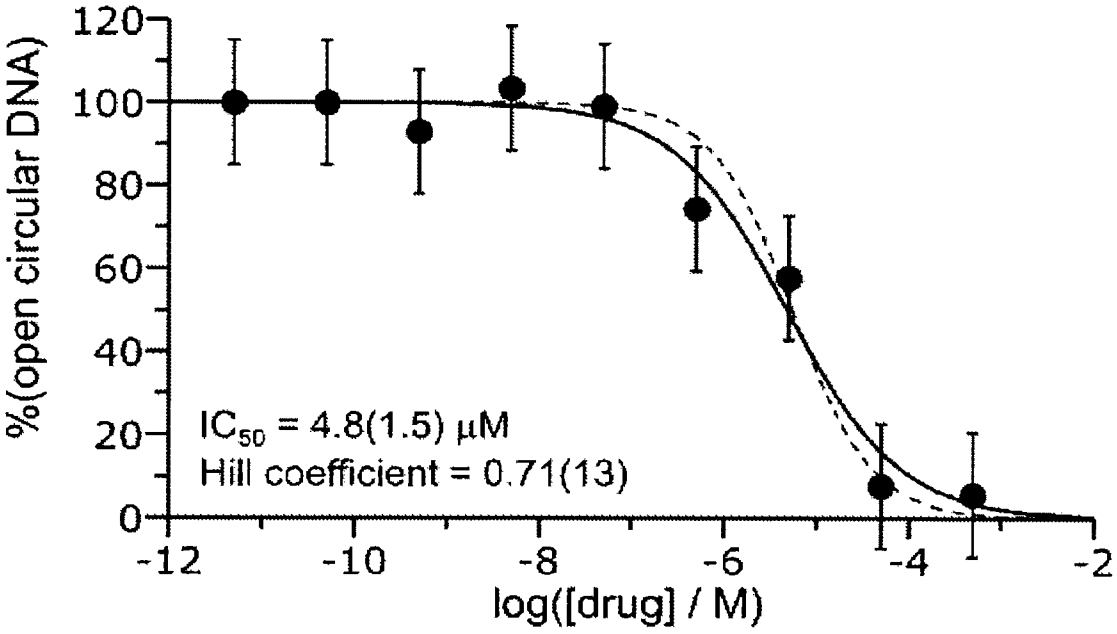


Scheme 14

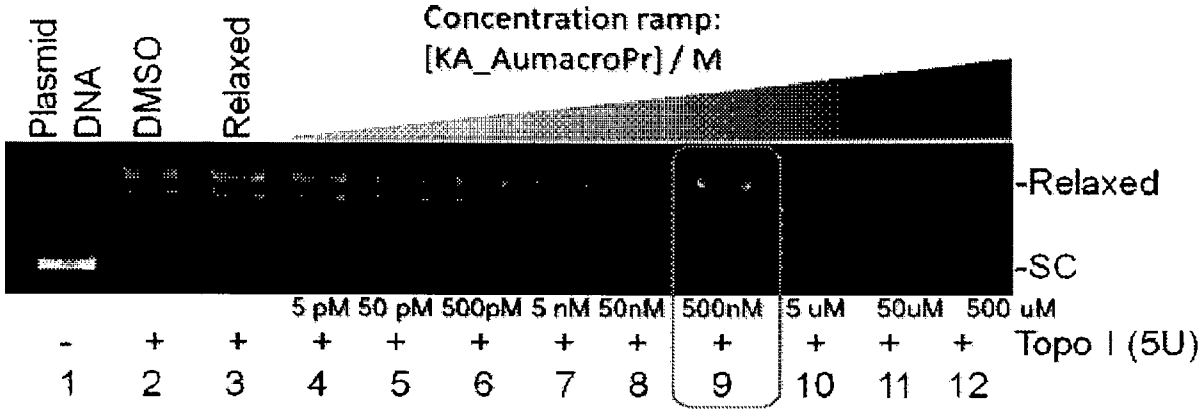


Scheme 15

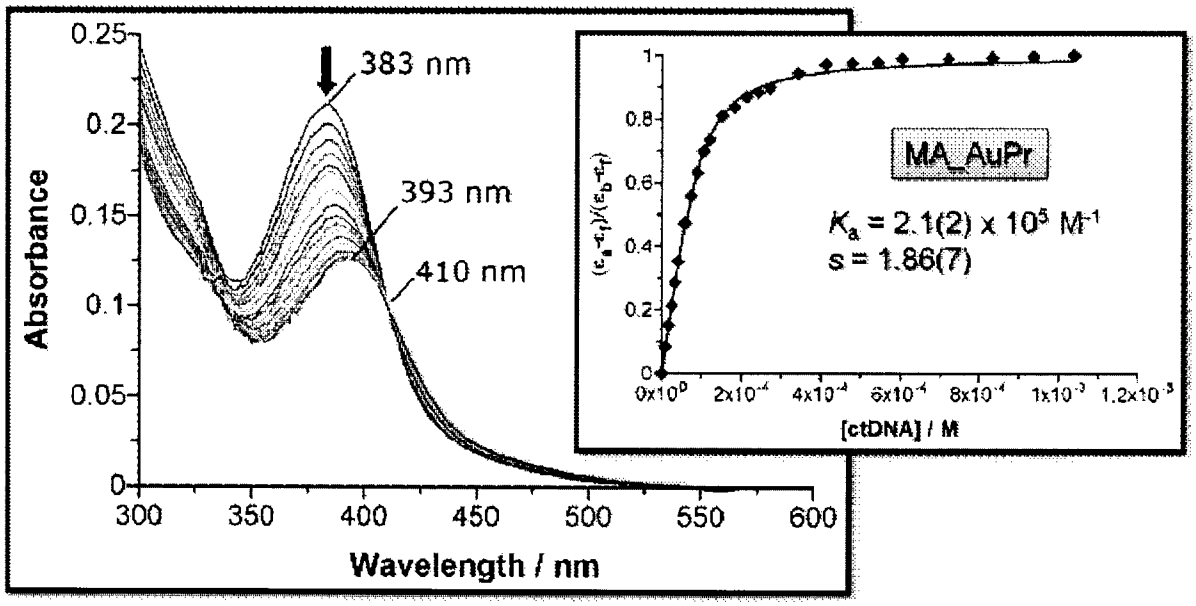




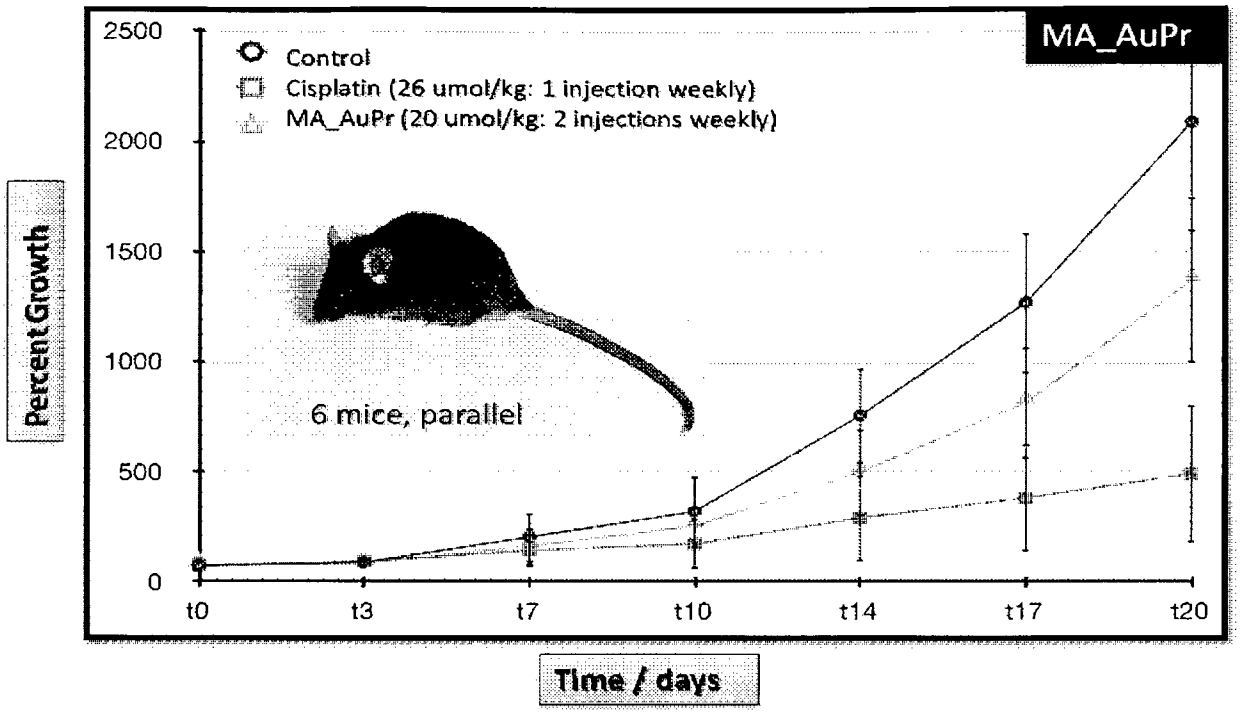
Scheme 16



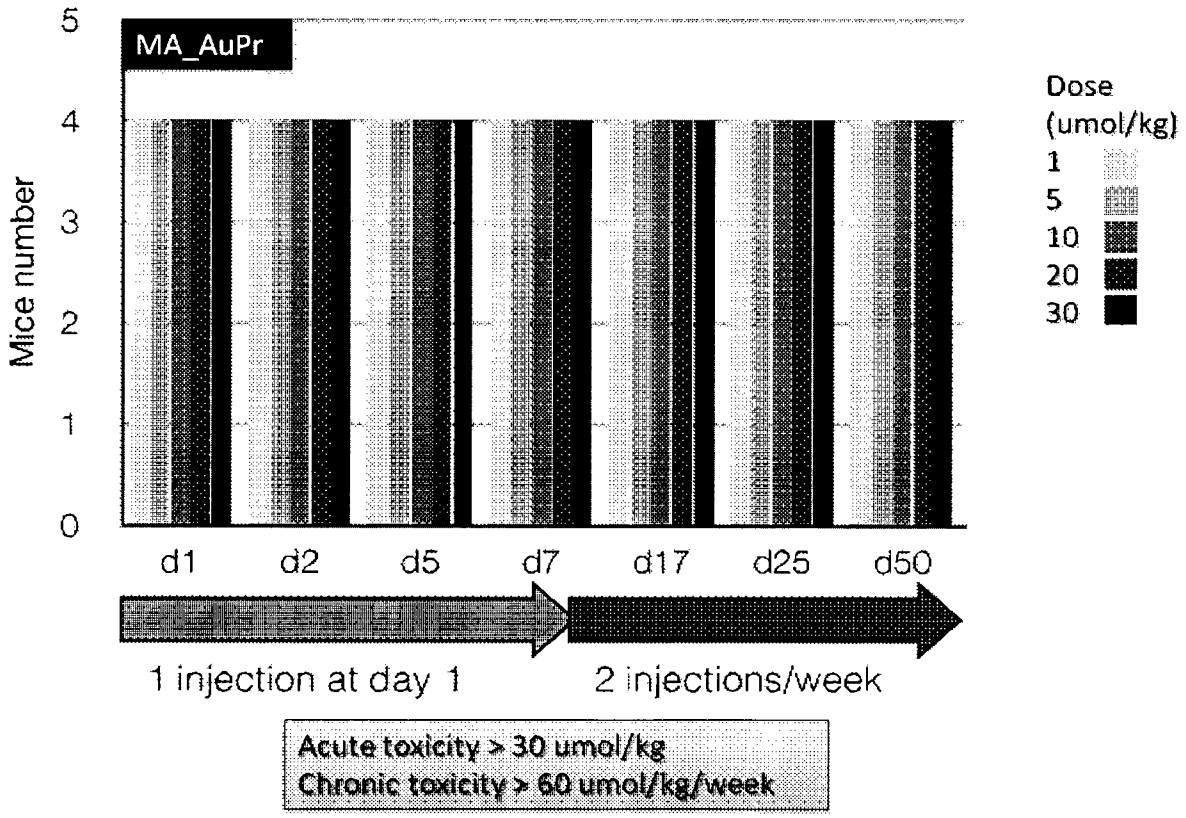
Scheme 17



Scheme 18



Scheme 23



Scheme 24

APPENDIX A: *CRYSTOLLOGRAPHIC DATA TABLES OF LIGANDS*

A.1: Crystallographic Data Tables for H_2L2

Table A.1.1 Crystal data and structure refinement details for H_2L2

Identification code	H_2L2	
Empirical formula	$C_{23}\ H_{22}\ N_6$	
Formula weight	382.47	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P $2_1/c$	
Unit cell dimensions	a = 9.170(5) Å	α = 90°.
	b = 11.244(5) Å	β= 96.718(5)°.
	c = 18.720(6) Å	γ = 90°.
Volume	1916.9(14) $Å^3$	
Z	4	
Density (calculated)	1.325 Mg/m^3	
Absorption coefficient	0.083 mm^{-1}	
F(000)	808	
Crystal size	0.50 x 0.30 x 0.05 mm^3	
Theta range for data collection	2.84 to 26.01°	
Index ranges	-11<=h<=11, -11<=k<=13, -22<=l<=23	
Reflections collected	13312	
Independent reflections	3693 [R(int) = 0.1083]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9959 and 0.9599	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3693 / 2 / 272	
Goodness-of-fit on F^2	0.865	
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1130	
R indices (all data)	R1 = 0.1261, wR2 = 0.1310	
Largest diff. peak and hole	0.515 and -0.276 $e.Å^{-3}$	

Table A.1.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for H_2L2. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(1)	8489(3)	1540(2)	773(1)	21(1)
C(2)	7106(3)	1871(2)	431(1)	25(1)
C(3)	6112(3)	1820(2)	942(1)	25(1)
C(4)	6924(3)	1480(2)	1590(1)	22(1)
C(5)	6467(3)	1310(2)	2291(1)	24(1)
C(6)	6924(3)	918(2)	3553(1)	29(1)
C(7)	7565(3)	-236(2)	3922(1)	25(1)
C(8)	9263(3)	-210(3)	4032(1)	27(1)
C(9)	11134(3)	-545(2)	3200(1)	25(1)
C(10)	11675(3)	-328(2)	2545(1)	23(1)
C(11)	13004(3)	-728(2)	2319(1)	28(1)
C(12)	13024(3)	-302(2)	1634(2)	27(1)
C(13)	11676(3)	343(2)	1454(1)	21(1)
C(14)	11265(3)	922(2)	746(1)	20(1)
C(15)	12209(3)	1369(2)	-323(1)	22(1)
C(16)	13412(3)	1384(2)	-726(1)	26(1)
C(17)	13228(3)	1846(3)	-1407(2)	30(1)
C(18)	11837(3)	2287(2)	-1713(2)	30(1)
C(19)	10653(3)	2264(2)	-1340(1)	26(1)
C(20)	10828(3)	1823(2)	-623(1)	20(1)
C(21)	9846(3)	1430(2)	438(1)	21(1)
C(22)	7005(3)	-1325(3)	3473(2)	33(1)
C(23)	7052(3)	-300(3)	4668(2)	35(1)
N(1)	8360(3)	1323(2)	1477(1)	22(1)
N(2)	7405(3)	1075(2)	2842(1)	25(1)
N(3)	9881(3)	-125(2)	3348(1)	27(1)
N(4)	10875(2)	334(2)	2008(1)	22(1)
N(5)	12397(2)	917(2)	361(1)	22(1)
N(6)	9673(2)	1863(2)	-232(1)	22(1)

Table A.1.3: IUCR CIF Check Report

Datablock: H_2L2

Bond precision: C-C = 0.0040 A Wavelength=0.71073

Cell: a=9.170(5) b=11.244(5) c=18.720(6)
alpha=90 beta=96.718(5) gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	1916.9(15)	1916.9(14)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C23 H22 N6	C23 H22 N6
Sum formula	C23 H22 N6	C23 H22 N6
Mr	382.47	382.47
Dx,g cm-3	1.325	1.325
Z	4	4
Mu (mm-1)	0.083	0.083
F000	808.0	808.0
F000'	808.24	
h,k,lmax	11,13,23	11,13,23
Nref	3768	3693
Tmin,Tmax	0.971,0.996	0.960,0.996
Tmin'	0.959	

Correction method= MULTI-SCAN

Data completeness= 0.980 Theta(max)= 26.010

R(reflections)= 0.0579(1933) wR2(reflections)= 0.1310(3693)

S = 0.865 Npar= 272

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level C

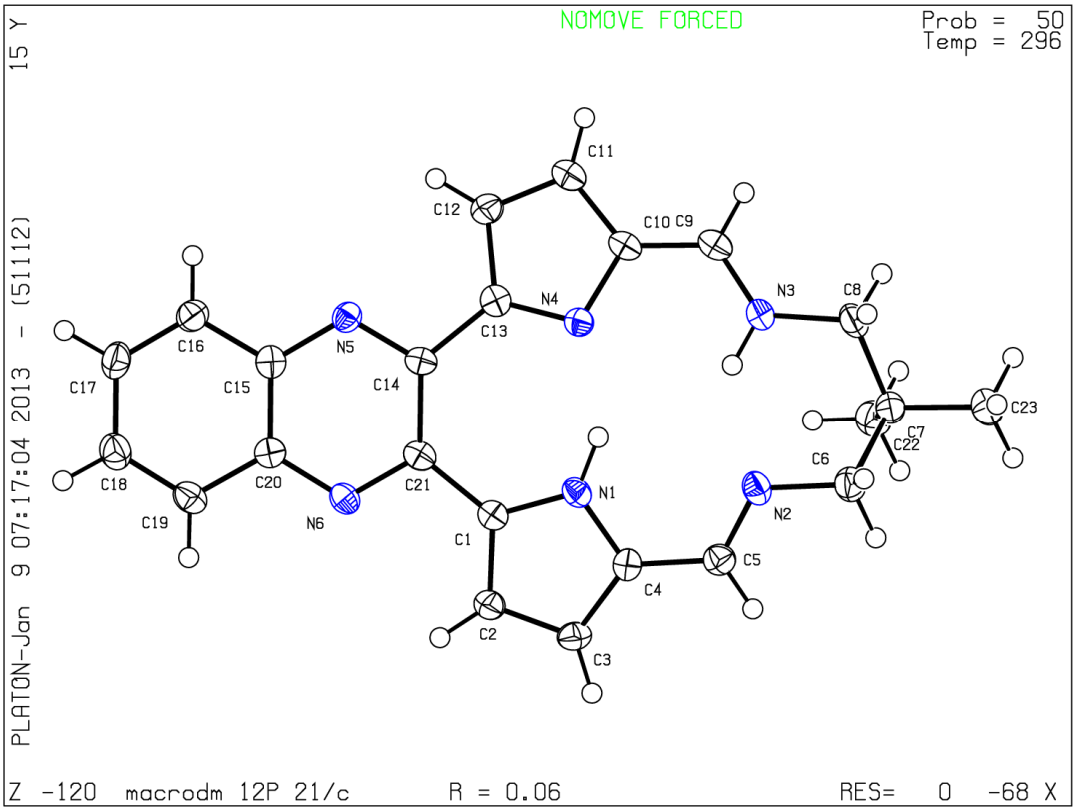
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 11.155
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.754
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 3
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 20
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 2
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 72

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock H_2L2 - ellipsoid plot



A.2: Crystallographic Data Tables for H_2L5

Table A.2.1 Crystal data and structure refinement details for H_2L5

Identification code	H_2L5	
Empirical formula	$C_{23}H_{22}N_6$	
Formula weight	382.47	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 31.645(5) Å	α= 90°.
	b = 7.749(4) Å	β= 123.596(5)°.
	c = 19.067(5) Å	γ = 90°.
Volume	3895(3) $Å^3$	
Z	8	
Density (calculated)	1.305 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	1616	
Crystal size	0.50 x 0.30 x 0.10 mm^3	
Theta range for data collection	2.84 to 26.04°.	
Index ranges	-38<=h<=38, -7<=k<=9, -23<=l<=23	
Reflections collected	13929	
Independent reflections	3841 [R(int) = 0.0384]	
Completeness to theta = 25.00°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9919 and 0.9605	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3841 / 2 / 272	
Goodness-of-fit on F^2	0.896	
Final R indices [I>2sigma(I)]	R1 = 0.0382, wR2 = 0.0853	
R indices (all data)	R1 = 0.0579, wR2 = 0.0893	
Largest diff. peak and hole	0.240 and -0.299 $e.Å^{-3}$	

Table A.2.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for H_2L5. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
N(001)	3208(1)	-813(2)	913(1)	23(1)
N(002)	2752(1)	209(2)	1646(1)	22(1)
N(003)	3867(1)	-661(1)	3675(1)	21(1)
N(004)	1813(1)	397(2)	81(1)	29(1)
N(005)	4348(1)	-1808(1)	2898(1)	22(1)
N(006)	2293(1)	-289(2)	-705(1)	30(1)
C(007)	3642(1)	-477(2)	2850(1)	19(1)
C(008)	3149(1)	405(2)	2458(1)	19(1)
C(009)	4571(1)	-1657(2)	5008(1)	24(1)
C(010)	3702(1)	-908(2)	1547(1)	21(1)
C(011)	5035(1)	-2438(2)	5484(1)	25(1)
C(012)	3891(1)	-1079(2)	2444(1)	19(1)
C(013)	4331(1)	-1411(2)	4134(1)	21(1)
C(014)	2733(1)	-366(2)	-601(1)	28(1)
C(015)	4010(1)	-845(2)	1220(1)	26(1)
C(016)	5279(1)	-2684(2)	6414(1)	33(1)
C(017)	4575(1)	-1986(2)	3742(1)	21(1)
C(018)	2992(1)	1461(2)	2868(1)	22(1)
C(019)	1879(1)	1208(2)	717(1)	27(1)
C(020)	2491(1)	1917(2)	2280(1)	24(1)
C(021)	1820(1)	132(2)	-1499(1)	33(1)
C(023)	5286(1)	-3008(2)	5090(1)	26(1)
C(024)	3190(1)	-656(2)	178(1)	25(1)
C(025)	2346(1)	1118(2)	1523(1)	23(1)
C(026)	3685(1)	-689(2)	362(1)	28(1)
C(027)	1352(1)	628(2)	-763(1)	34(1)
C(028)	1496(1)	1337(2)	-1351(1)	35(1)
C(029)	5058(1)	-2781(2)	4245(1)	25(1)
C(030)	5799(1)	-3856(2)	5611(1)	34(1)

Table A.2.3: IUCR CIF Check Report

Datablock: H_2L5

Bond precision: C-C = 0.0023 A Wavelength=0.71073

Cell: a=31.645(5) b=7.749(4) c=19.067(5)
alpha=90 beta=123.596(5) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	3895(2)	3895(3)
Space group	C 2/c	C2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C23 H22 N6	C23 H22 N6
Sum formula	C23 H22 N6	C23 H22 N6
Mr	382.47	382.47
Dx,g cm-3	1.304	1.305
Z	8	8
Mu (mm-1)	0.081	0.081
F000	1616.0	1616.0
F000'	1616.48	
h,k,lmax	38,9,23	38,9,23
Nref	3850	3841
Tmin,Tmax	0.971,0.992	0.961,0.992
Tmin'	0.960	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.040

R(reflections)= 0.0382(2654) wR2(reflections)= 0.0893(3841)

S = 0.896 Npar= 272

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level C

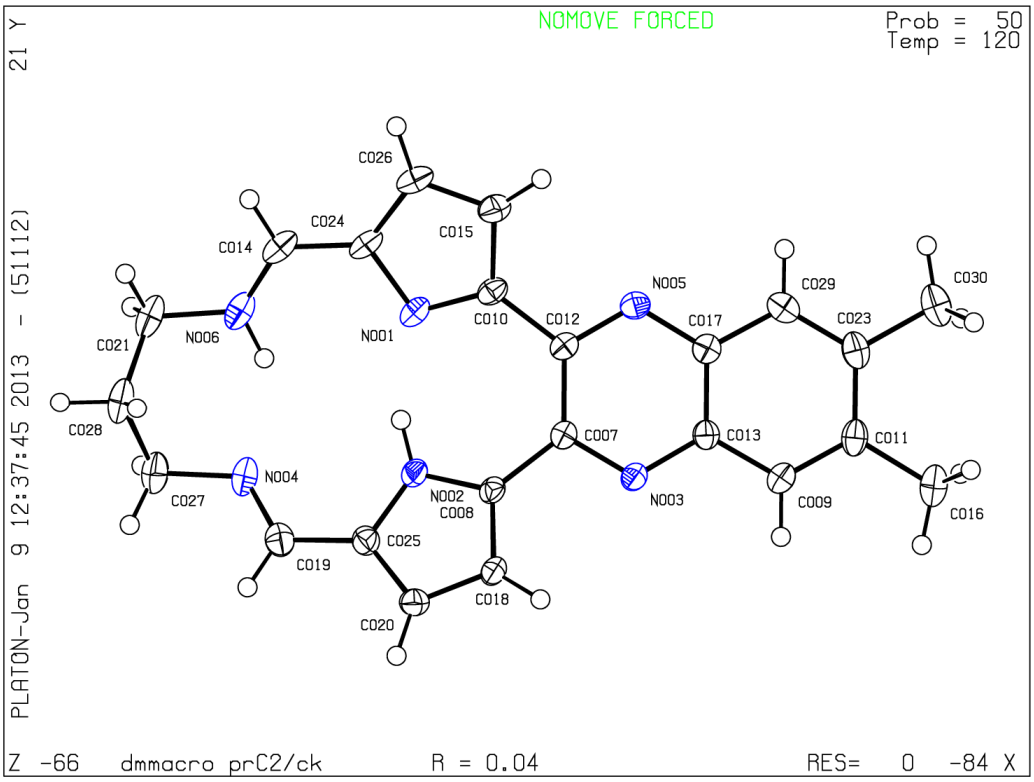
PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of . 31 A**3
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 5.813
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 5

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 49
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 2
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 4
PLAT961_ALERT_5_G Dataset Contains no Negative Intensities ..... !

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock H_2L5 - ellipsoid plot



A.3: Crystallographic Data Tables for H_2L6

Table A.3.1 Crystal data and structure refinement details for H_2L6

Identification code	H_2L6	
Empirical formula	$C_{22}\ H_{20}\ N_6\ O_{0.5}$	
Formula weight	376.44	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 2/c	
Unit cell dimensions	a = 31.219(5) Å	α= 90°.
	b = 7.724(4) Å	β= 125.403(5)°.
	c = 19.098(5) Å	γ= 90°.
Volume	3754(3) $Å^3$	
Z	8	
Density (calculated)	1.332 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	1584	
Crystal size	0.45 x 0.45 x 0.10 mm^3	
Theta range for data collection	3.20 to 26.03°.	
Index ranges	-38<=h<=37, -9<=k<=7, -23<=l<=23	
Reflections collected	13380	
Independent reflections	3700 [R(int) = 0.0387]	
Completeness to theta = 26.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9915 and 0.9627	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3700 / 3 / 281	
Goodness-of-fit on F^2	0.968	
Final R indices [I>2sigma(I)]	R1 = 0.0549, wR2 = 0.1532	
R indices (all data)	R1 = 0.0806, wR2 = 0.1624	
Largest diff. peak and hole	0.600 and -0.368 $e.Å^{-3}$	

Table A.3.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for H_2L6. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
N(5)	3966(1)	843(2)	8826(1)	36(1)
N(4)	2813(1)	-108(2)	6748(1)	33(1)
N(1)	3278(1)	790(2)	6020(1)	31(1)
N(6)	4460(1)	1858(2)	8054(1)	35(1)
N(3)	1829(1)	-308(3)	5154(2)	50(1)
C(007)	3732(1)	591(2)	7990(1)	30(1)
N(2)	2316(1)	304(2)	4375(1)	43(1)
C(009)	3792(1)	863(2)	6685(1)	30(1)
C(010)	3988(1)	1116(2)	7584(1)	30(1)
C(011)	4696(1)	2111(3)	8906(1)	36(1)
C(012)	4101(1)	709(3)	6363(2)	38(1)
C(013)	3224(1)	-290(3)	7578(1)	33(1)
C(014)	4448(1)	1599(3)	9297(2)	37(1)
C(015)	5193(1)	2924(3)	9414(2)	44(1)
C(016)	2398(1)	-1043(3)	6621(2)	40(1)
C(017)	3248(1)	568(3)	5280(1)	33(1)
C(018)	4696(1)	1899(3)	10183(2)	46(1)
C(019)	2765(1)	290(3)	4480(1)	39(1)
C(020)	3757(1)	517(3)	5485(2)	41(1)
C(021)	5427(1)	3212(3)	10270(2)	49(1)
C(022)	1913(1)	-1129(3)	5807(2)	47(1)
C(023)	5176(1)	2694(3)	10663(2)	49(1)
C(024)	3069(1)	-1347(3)	7997(2)	46(1)
C(025)	2555(1)	-1815(3)	7396(2)	52(1)
C(026)	5466(2)	3094(6)	11547(3)	44(1)
C(027)	1483(1)	-1278(3)	3700(2)	58(1)
C(028)	1823(1)	-109(3)	3557(2)	52(1)
C(029)	1352(1)	-505(4)	4284(2)	59(1)
C(030)	5923(2)	4070(7)	10879(3)	53(1)
O(1W)	5000	4147(4)	7500	68(1)

Table A.3.3: IUCR CIF Check Report

Datablock: H_2L6

Bond precision: C-C = 0.0041 A Wavelength=0.71073

Cell: a=31.219(5) b=7.724(4) c=19.098(5)
alpha=90 beta=125.403(5) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	3754(2)	3754(3)
Space group	C 2/c	C 2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	2(C22 H19 N6), H2 O	C22 H19 N6, H1 O0.5
Sum formula	C44 H40 N12 O	C22 H20 N6 O0.5
Mr	752.88	376.44
Dx,g cm-3	1.332	1.332
Z	4	8
Mu (mm-1)	0.085	0.085
F000	1584.0	1584.0
F000'	1584.51	
h,k,lmax	38,9,23	38,9,23
Nref	3708	3700
Tmin,Tmax	0.962,0.992	0.963,0.992
Tmin'	0.962	

Correction method= MULTI-SCAN

Data completeness= 0.998 Theta(max)= 26.030

R(reflections)= 0.0549(2461) wR2(reflections)= 0.1624(3700)

S = 0.968 Npar= 281

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.

Alert level C

DIFMX01_ALERT_2_C The maximum difference density is > 0.1*ZMAX*0.75
_refine_diff_density_max given = 0.600
Test value = 0.600

DIFMX02_ALERT_1_C The maximum difference density is > 0.1*ZMAX*0.75
The relevant atom site should be identified.

PLAT041_ALERT_1_C Calc. and Reported SumFormulaStrings Differ ?

PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 4.6 Ratio

PLAT230_ALERT_2_CHirshfeld Test Diff for C021 -- C030 .. 5.7 su

PLAT230_ALERT_2_CHirshfeld Test Diff for C023 -- C026 .. 5.7 su

PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0041 Ang

PLAT906_ALERT_3_C Large K value in the Analysis of Variance 7.078

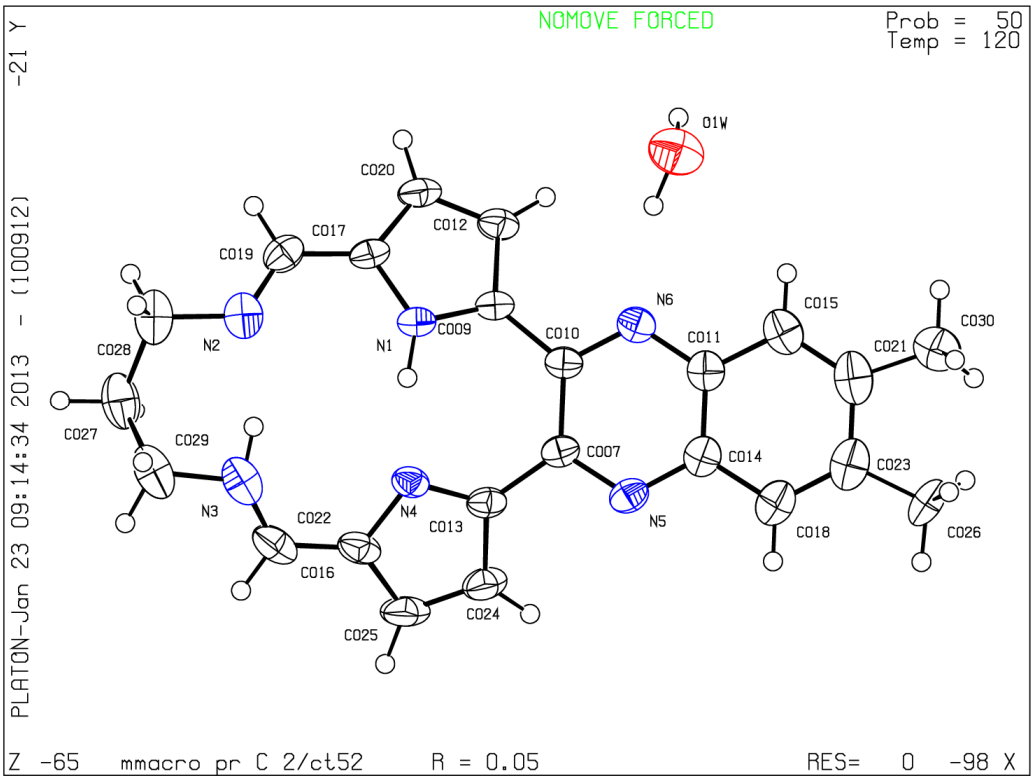
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 6

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 6
PLAT042_ALERT_1_G Calc. and Reported MoietyFormulaStrings Differ ?
PLAT045_ALERT_1_G Calculated and Reported Z Differ by ..... 0.50 Ratio
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.11
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 4 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 40
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 3
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 4

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock H_2L6- ellipsoid plot



A.4: Crystallographic Data Tables for H_2L7

Table A.4.1 Crystal data and structure refinement details for H_2L7

Identification code	H_2L7	
Empirical formula	$C_{21}H_{16}FN_6$	
Formula weight	371.40	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P\,2_1/c$	
Unit cell dimensions	a = 9.396(5) Å	α= 90°.
	b = 10.667(5) Å	β= 90.254(5)°.
	c = 17.165(5) Å	γ= 90°.
Volume	1720.4(13) $Å^3$	
Z	4	
Density (calculated)	1.434 Mg/m^3	
Absorption coefficient	0.098 mm^{-1}	
F(000)	772	
Crystal size	0.30 x 0.30 x 0.15 mm^3	
Theta range for data collection	2.89 to 32.00°.	
Index ranges	-13<=h<=9, -11<=k<=15, -24<=l<=25	
Reflections collected	10797	
Independent reflections	5271 [R(int) = 0.0847]	
Completeness to theta = 25.00°	99.2 %	
Max. and min. transmission	0.9855 and 0.9713	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5271 / 2 / 270	
Goodness-of-fit on F^2	0.821	
Final R indices [I>2sigma(I)]	R1 = 0.0608, wR2 = 0.1269	
R indices (all data)	R1 = 0.1374, wR2 = 0.1442	
Largest diff. peak and hole	0.288 and -0.338 $e.Å^{-3}$	

Table A.4.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for H_2L7. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
N(4)	7025(2)	1236(2)	6637(1)	27(1)
F(2)	572(2)	1781(2)	3014(1)	39(1)
N(1)	4631(2)	384(2)	7224(1)	27(1)
N(2)	5983(2)	18(2)	8661(1)	34(1)
N(5)	5346(2)	1873(2)	4788(1)	27(1)
N(6)	2768(2)	1079(2)	5439(1)	28(1)
N(3)	8488(2)	771(2)	8055(1)	37(1)
C(008)	6736(2)	1490(2)	5882(1)	26(1)
C(009)	5306(2)	1452(2)	5520(1)	25(1)
C(010)	2703(2)	-719(2)	7572(1)	31(1)
C(011)	3965(2)	1007(2)	5851(1)	25(1)
C(012)	4036(2)	-289(2)	7812(1)	29(1)
C(013)	2973(2)	2191(2)	3122(1)	35(1)
C(014)	3713(2)	403(2)	6608(1)	26(1)
C(015)	1700(2)	1819(2)	3478(1)	35(1)
C(016)	2833(2)	1483(2)	4688(1)	26(1)
C(017)	4133(2)	1858(2)	4354(1)	26(1)
C(018)	1574(2)	1481(2)	4233(1)	30(1)
C(019)	4193(2)	2225(2)	3560(1)	33(1)
C(020)	2503(2)	-277(2)	6818(1)	31(1)
C(021)	8288(2)	-571(2)	9214(1)	44(1)
C(022)	4767(2)	-486(2)	8534(1)	32(1)
C(023)	8482(2)	1319(2)	6710(1)	30(1)
C(024)	9157(2)	1049(2)	7418(1)	34(1)
C(025)	9104(2)	1652(2)	5991(1)	35(1)
C(026)	8011(2)	1767(2)	5470(1)	33(1)
C(027)	6755(2)	-205(2)	9393(1)	41(1)
C(028)	9144(2)	442(2)	8807(1)	42(1)
F(1)	2810(6)	2339(6)	2376(3)	33(1)

Table A.4.3: IUCR CIF Check Report

Datablock: H_2L7

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=9.396(5) b=10.667(5) c=17.165(6)
alpha=90 beta=90.254(5) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	1720.4(14)	1720.4(13)
Space group	P 21/c	P 21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C21 H16 F N6	C21 H16 F N6
Sum formula	C21 H16 F N6	C21 H16 F N6
Mr	371.40	371.40
Dx,g cm-3	1.434	1.434
Z	4	4
Mu (mm-1)	0.098	0.098
F000	772.0	772.0
F000'	772.29	
h,k,lmax	14,15,25	13,15,25
Nref	5963	5271
Tmin,Tmax	0.971,0.985	0.971,0.985
Tmin'	0.971	

Correction method= MULTI-SCAN

Data completeness= 0.884 Theta(max)= 32.000

R(reflections)= 0.0608(2331) wR2(reflections)= 0.1438(5271)

S = 0.824 Npar= 270

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level C

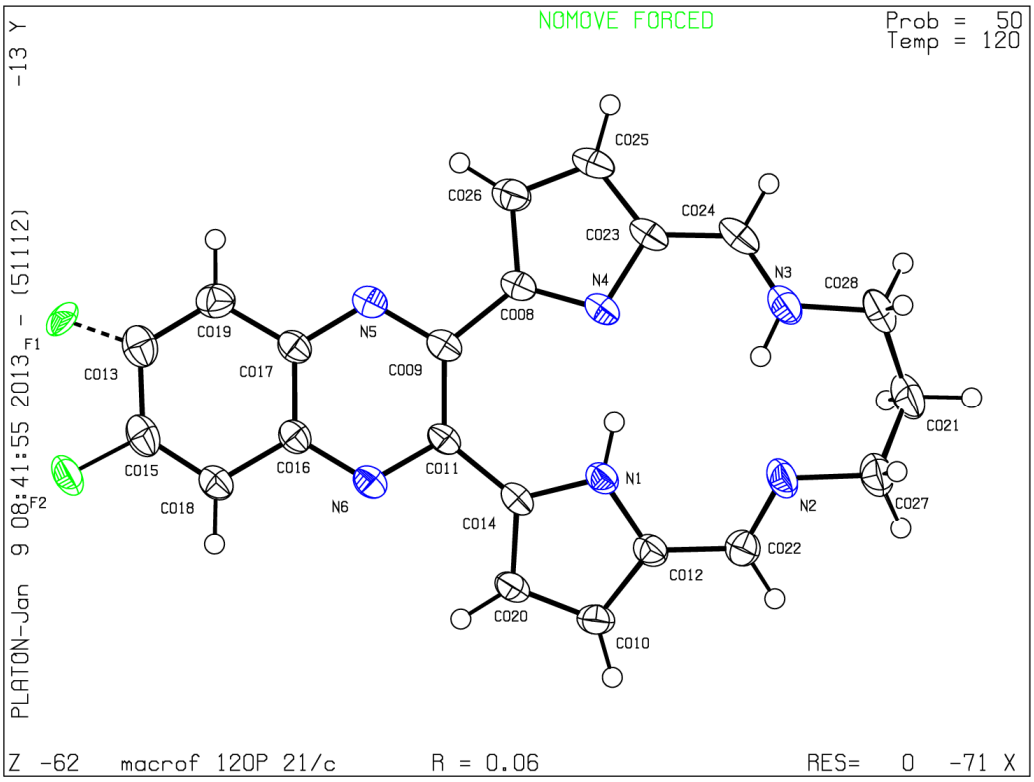
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low .... 44 Perc.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C013 - C019 ... 1.37 Ang.
PLAT366_ALERT_2_C Short? C(sp?)-C(sp?) Bond C015 - C018 ... 1.35 Ang.
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 15.895
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.873
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 3
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 25

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4
PLAT301_ALERT_3_G Note: Main Residue Disorder ..... 4 Perc.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 35

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock H_2L7 - ellipsoid plot



A.5: Crystallographic Data Tables for H_2L8a

Table A.5.1 Crystal data and structure refinement details for H_2L8a

Identification code	H_2L8a	
Empirical formula	$C_{19}H_{14}N_8$	
Formula weight	354.38	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_12_12_1$	
Unit cell dimensions	a = 6.9450(3) Å	α= 90°.
	b = 19.3867(11) Å	β= 90°.
	c = 24.0176(15) Å	γ = 90°.
Volume	3233.7(3) $Å^3$	
Z	4	
Density (calculated)	1.456 Mg/m^3	
Absorption coefficient	0.095 mm^{-1}	
F(000)	1472	
Crystal size	0.25 x 0.07 x 0.03 mm^3	
Theta range for data collection	1.35 to 28.74°.	
Index ranges	-9<=h<=9, -26<=k<=26, -29<=l<=32	
Reflections collected	18286	
Independent reflections	4670 [R(int) = 0.0565]	
Completeness to theta = 25.00°	98.6 %	
Max. and min. transmission	0.9972 and 0.9766	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4670 / 4 / 503	
Goodness-of-fit on F^2	1.043	
Final R indices [I>2sigma(I)]	R1 = 0.0588, wR2 = 0.1277	
R indices (all data)	R1 = 0.1015, wR2 = 0.1477	
Absolute structure parameter	-2(3)	
Largest diff. peak and hole	0.397 and -0.312 e.$Å^{-3}$	

Table A.5.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for H_2L8a. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
N(1)	5845(6)	8319(2)	5931(1)	36(1)
N(2)	6621(5)	8984(2)	6948(1)	24(1)
N(3)	5915(5)	7836(2)	7492(1)	24(1)
N(4)	5100(6)	7151(2)	6489(2)	32(1)
N(5)	7703(5)	9874(2)	8230(1)	27(1)
N(6)	6880(5)	8670(2)	8808(1)	27(1)
N(7)	12124(5)	8307(2)	8892(1)	27(1)
N(8)	12070(5)	9051(2)	7883(1)	23(1)
N(9)	11269(5)	8926(2)	6016(1)	26(1)
N(10)	12463(5)	10060(2)	6630(1)	24(1)
N(15)	11047(5)	7961(2)	7301(1)	23(1)
N(16)	11067(5)	7203(2)	8290(1)	28(1)
C(1)	6399(6)	8956(2)	5942(2)	28(1)
C(2)	6762(6)	9307(2)	6446(2)	26(1)
C(3)	7080(6)	9447(2)	7350(2)	24(1)
C(4)	7160(5)	9312(2)	7949(2)	23(1)
C(5)	6784(5)	8671(2)	8245(2)	23(1)
C(6)	6250(6)	7992(2)	8034(2)	23(1)
C(7)	5457(6)	7149(2)	7469(2)	26(1)
C(8)	5026(6)	6825(2)	6954(2)	28(1)
C(9)	4639(8)	6844(2)	5949(2)	44(1)
C(10)	5673(9)	7198(2)	5492(2)	52(2)
C(11)	7486(6)	10092(2)	7096(2)	27(1)
C(12)	7289(6)	9998(2)	6528(2)	28(1)
C(13)	7854(6)	9842(2)	8783(2)	26(1)
C(14)	8577(7)	10440(2)	9074(2)	30(1)
C(15)	7384(6)	9243(2)	9070(2)	26(1)
C(16)	5509(6)	6871(2)	8006(2)	26(1)
C(17)	6005(6)	7392(2)	8363(2)	30(1)
C(18)	7385(7)	9237(2)	9674(2)	33(1)
N(14)	7348(7)	9263(2)	10147(2)	51(1)
C(20)	12076(7)	7862(2)	9384(2)	33(1)
C(21)	12345(6)	8970(2)	8886(2)	27(1)
C(22)	12354(6)	9361(2)	8390(2)	24(1)

Table A.5.2 continued…

	x	y	z	U(eq)
C(23)	12182(6)	9553(2)	7501(2)	22(1)
C(24)	12002(5)	9471(2)	6900(2)	23(1)
C(25)	11432(6)	8870(2)	6573(2)	23(1)
C(26)	11700(6)	9519(2)	5776(2)	27(1)
C(27)	11438(7)	9570(2)	5174(2)	31(1)
N(12)	11221(7)	9627(2)	4706(2)	46(1)
N(11)	13437(6)	11215(2)	5592(2)	41(1)
C(30)	12943(7)	10716(2)	5805(2)	31(1)
C(31)	12340(6)	10086(2)	6078(2)	25(1)
C(32)	10940(5)	8185(2)	6763(2)	23(1)
C(33)	10463(6)	7290(2)	7325(2)	25(1)
C(34)	10424(6)	6927(2)	7845(2)	26(1)
C(35)	11058(7)	6821(2)	8818(2)	32(1)
C(36)	12533(6)	10206(2)	7765(2)	25(1)
C(37)	12627(6)	10079(2)	8324(2)	24(1)
C(38)	9989(6)	7078(2)	6791(2)	29(1)
C(39)	10269(6)	7635(2)	6440(2)	29(1)
C(1')	10589(7)	7295(2)	9302(2)	33(1)
C(2')	5375(10)	7946(2)	5423(2)	50(1)
N(13)	9203(6)	10890(2)	9321(2)	44(1)

Table A.5.3: IUCR CIF Check Report

Datablock: H_2L8a

Bond precision: C-C = 0.0053 A Wavelength=0.71073

Cell: a=6.9450(3) b=19.3867(11) c=24.0176(15)
alpha=90 beta=90 gamma=90

Temperature: 296 K

	Calculated	Reported
Volume	3233.7(3)	3233.7(3)
Space group	P 21 21 21	P212121
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C19 H14 N8	C19 H14 N8
Sum formula	C19 H14 N8	C19 H14 N8
Mr	354.38	354.38
Dx,g cm-3	1.456	1.456
Z	8	8
Mu (mm-1)	0.095	0.095
F000	1472.0	1472.0
F000'	1472.42	
h,k,lmax	9,26,32	9,26,32
Nref	4740[8408]	4670
Tmin,Tmax	0.992,0.997	0.977,0.997
Tmin'	0.977	

Correction method= MULTI-SCAN

Data completeness= 0.99/0.56 Theta(max)= 28.740

R(reflections)= 0.0570(3195) wR2(reflections)= 0.1383(4670)

S = 1.043 Npar= 503

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.

Alert level C

PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) .. 4.8 Ratio
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0053 Ang
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin&STh/L= 0.600 45

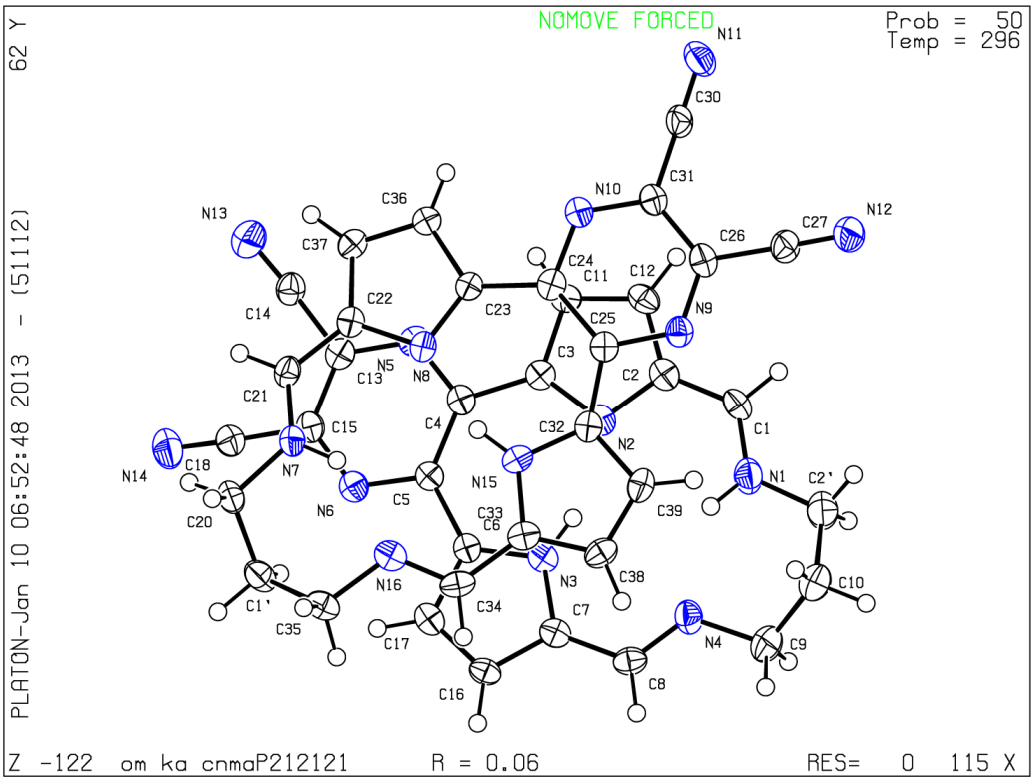
Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 8
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C13 - C14 ... 1.44 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C15 - C18 ... 1.45 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C26 - C27 ... 1.46 Ang.
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C30 - C31 ... 1.45 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 4
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 4

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 23

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablockom_H_2L8a - ellipsoid plot



A.6: Crystallographic Data Tables for H_2L8b

Table A.6.1 Crystal data and structure refinement details for H_2L8b

Identification code	H_2L8b	
Empirical formula	C_{19} H_{17} N_7 O	
Formula weight	359.40	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P n a 21	
Unit cell dimensions	a = 9.792(3) Å	α= 90°.
	b = 17.151(6) Å	β= 90°.
	c = 10.407(4) Å	γ = 90°.
Volume	1747.7(10) $Å^3$	
Z	4	
Density (calculated)	1.366 Mg/m^3	
Absorption coefficient	0.091 mm^{-1}	
F(000)	752	
Crystal size	0.35 x 0.30 x 0.15 mm^3	
Theta range for data collection	2.29 to 25.33°.	
Index ranges	-11<=h<=9, -10<=k<=20, -11<=l<=12	
Reflections collected	7081	
Independent reflections	1671 [R(int) = 0.0420]	
Completeness to theta = 25.3°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9864 and 0.9688	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1671 / 3 / 253	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0588, wR2 = 0.1600	
R indices (all data)	R1 = 0.0819, wR2 = 0.1755	
Largest diff. peak and hole	0.402 and -0.209 $e.Å^{-3}$	

Table A.6.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for H_2L8b. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
O(1)	13359(4)	2008(2)	1761(4)	55(1)
C(16)	12459(5)	2355(3)	2547(6)	41(1)
N(5)	11551(4)	3530(3)	3320(5)	44(1)
N(4)	8896(4)	3421(2)	5724(4)	42(1)
N(1)	8910(4)	1899(2)	5630(5)	44(1)
C(1)	9925(5)	1729(3)	4770(6)	43(1)
C(15)	10726(5)	2291(3)	4059(6)	41(1)
N(6)	11624(5)	1924(2)	3260(5)	42(1)
C(19)	13314(7)	1182(3)	1638(8)	69(2)
C(17)	12425(5)	3161(3)	2575(6)	45(1)
C(14)	10698(5)	3124(3)	4088(5)	39(1)
C(13)	9844(5)	3650(3)	4868(5)	42(1)
C(10)	8372(6)	4099(3)	6268(6)	51(1)
C(9)	7376(6)	4075(4)	7230(6)	57(2)
N(3)	6878(5)	3424(3)	7667(5)	62(1)
C(8)	5840(7)	3352(5)	8673(7)	69(2)
C(7)	5969(9)	2580(5)	9346(8)	88(3)
C(6)	5842(8)	1862(4)	8551(7)	74(2)
N(2)	6891(5)	1863(3)	7540(6)	63(1)
C(5)	7369(6)	1222(4)	7085(7)	59(2)
C(4)	8404(6)	1226(3)	6120(6)	53(2)
C(11)	9022(7)	4746(4)	5716(8)	76(2)
C(12)	9941(6)	4472(3)	4832(7)	64(2)
C(18)	13315(6)	3612(3)	1765(7)	55(1)
N(7)	14006(7)	3957(3)	1123(7)	84(2)
C(2)	10051(6)	917(3)	4707(7)	60(2)
C(3)	9098(6)	609(3)	5562(8)	70(2)

Table A.6.3: IUCR CIF Check Report

Datablock: H_2L8b

Bond precision: C-C = 0.0085 A Wavelength=0.71073

Cell: a=9.792(3) b=17.151(6) c=10.407(4)
alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1747.8(11)	1747.7(10)
Space group	P n a 21	P n a 21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C19 H17 N7 O	C19 H17 N7 O
Sum formula	C19 H17 N7 O	C19 H17 N7 O
Mr	359.40	359.40
Dx,g cm-3	1.366	1.366
Z	4	4
Mu (mm-1)	0.091	0.091
F000	752.0	752.0
F000'	752.25	
h,k,lmax	11,20,12	11,20,12
Nref	1688[3187]	1671
Tmin,Tmax	0.969,0.986	0.969,0.986
Tmin'	0.969	

Correction method= MULTI-SCAN

Data completeness= 0.99/0.52 Theta(max)= 25.330

R(reflections)= 0.0588(1241) wR2(reflections)= 0.1755(1671)

S = 1.071 Npar= 253

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level C

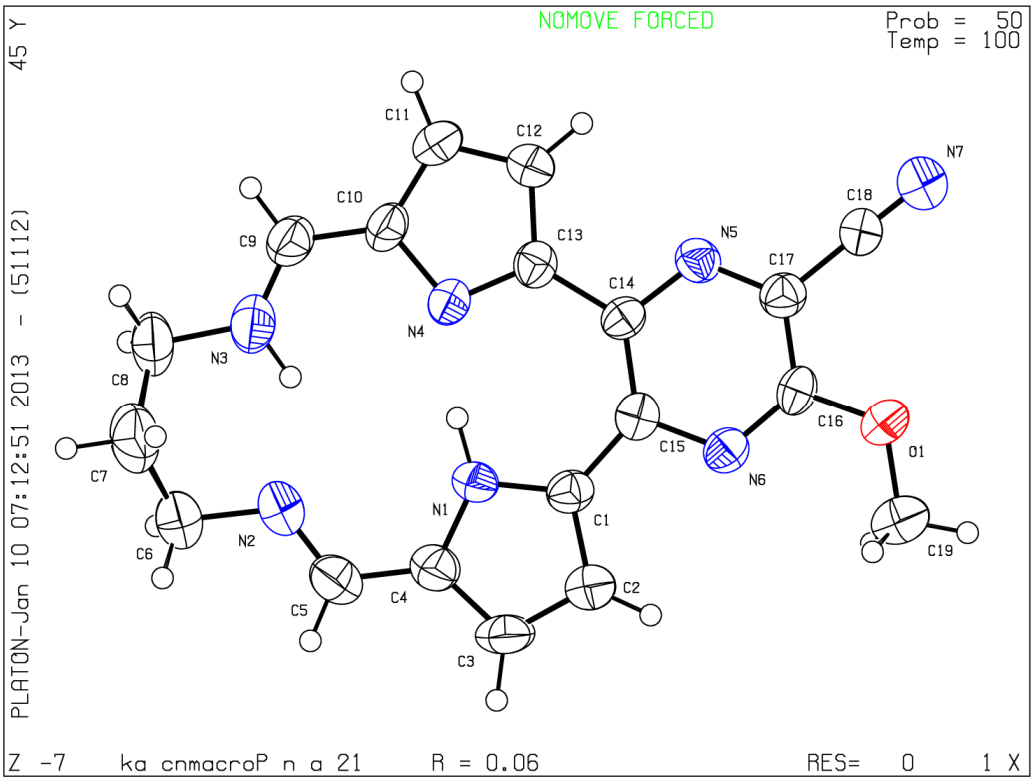
PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax .LT. 18) 6.60
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C7
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C11
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0085 Ang
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 16

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 4
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C17 - C18 ... 1.44 Ang.
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 3
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 36 Perc.

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock H_2L8b- ellipsoid plot



A.7: Crystallographic Data Tables for H_2L8c

Table A.7.1 Crystal data and structure refinement details for H_2L8c.

Identification code	H_2L8c	
Empirical formula	$C_{20}\ H_{18}\ N_8\ O$	
Formula weight	386.42	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 8.8718(2) Å	α= 90°.
	b = 20.4106(3) Å	β= 98.3440(10)°.
	c = 10.0909(2) Å	γ = 90°.
Volume	1807.91(6) $Å^3$	
Z	4	
Density (calculated)	1.420 Mg/m^3	
Absorption coefficient	0.774 mm^{-1}	
F(000)	808	
Crystal size	0.15 x 0.15 x 0.05 mm^3	
Theta range for data collection	4.33 to 68.31°.	
Index ranges	-10<=h<=10, -23<=k<=24, -12<=l<=11	
Reflections collected	11955	
Independent reflections	3279 [R(int) = 0.0189]	
Completeness to theta = 25.00°	96.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9623 and 0.8927	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3279 / 0 / 267	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0557, wR2 = 0.1499	
R indices (all data)	R1 = 0.0597, wR2 = 0.1534	
Largest diff. peak and hole	0.531 and -0.322 e.$Å^{-3}$	

Table A.7.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for H_2L8c. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
O(1)	4391(2)	3904(1)	9394(2)	40(1)
N(1)	-420(2)	6152(1)	908(2)	34(1)
N(2)	844(2)	5292(1)	2990(2)	27(1)
N(3)	4223(2)	5009(1)	6758(2)	31(1)
N(5)	2122(2)	4115(1)	5579(2)	30(1)
N(6)	1613(2)	7030(1)	2084(2)	35(1)
N(7)	2849(2)	6143(1)	4087(2)	28(1)
C(1)	-941(3)	6649(1)	-108(2)	38(1)
C(2)	-877(3)	5552(1)	953(2)	31(1)
C(3)	-299(2)	5118(1)	1979(2)	29(1)
C(4)	1076(2)	4765(1)	3795(2)	27(1)
C(5)	2190(2)	4709(1)	5017(2)	28(1)
C(6)	3309(2)	5177(1)	5623(2)	29(1)
C(7)	4085(3)	4423(1)	7314(2)	32(1)
C(8)	5101(3)	4307(1)	8605(2)	34(1)
C(9)	5261(3)	3730(1)	10653(3)	44(1)
C(10)	3041(3)	3971(1)	6698(2)	31(1)
C(11)	2925(3)	3298(1)	7169(2)	35(1)
N(8)	2816(3)	2764(1)	7470(2)	45(1)
C(13)	341(3)	7116(1)	-250(3)	42(1)
C(14)	951(3)	7482(1)	1030(3)	41(1)
C(15)	2837(3)	7173(1)	2847(2)	34(1)
C(16)	3464(3)	6745(1)	3927(2)	32(1)
C(17)	3617(2)	5837(1)	5178(2)	29(1)
C(18)	4763(3)	6265(1)	5754(2)	34(1)
C(19)	4669(3)	6825(1)	4980(2)	36(1)
C(20)	-793(3)	4474(1)	2162(2)	34(1)
C(21)	63(3)	4249(1)	3306(2)	35(1)
N(9)	6394(3)	4543(1)	8984(2)	44(1)

Table A.7.3: IUCR CIF Check Report

Datablock: H_2L8c

Bond precision: C-C = 0.0031 A Wavelength=1.54178

Cell: a=8.8718(2) b=20.4106(3) c=10.0909(2)
alpha=90 beta=98.344(1) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	1807.91(6)	1807.91(6)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H18 N8 O	C20 H18 N8 O
Sum formula	C20 H18 N8 O	C20 H18 N8 O
Mr	386.42	386.42
Dx,g cm-3	1.420	1.420
Z	4	4
Mu (mm-1)	0.774	0.774
F000	808.0	808.0
F000'	810.40	
h,k,lmax	10,24,12	10,24,12
Nref	3311	3279
Tmin,Tmax	0.890,0.962	0.893,0.962
Tmin'	0.890	

Correction method= MULTI-SCAN

Data completeness= 0.990 Theta(max)= 68.310

R(reflections)= 0.0557(3019) wR2(reflections)= 0.1534(3279)

S = 1.061 Npar= 267

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level B

PLAT019_ALERT_1_B Check _diffrn_measured_fraction_theta_full/_max 0.978

Alert level C

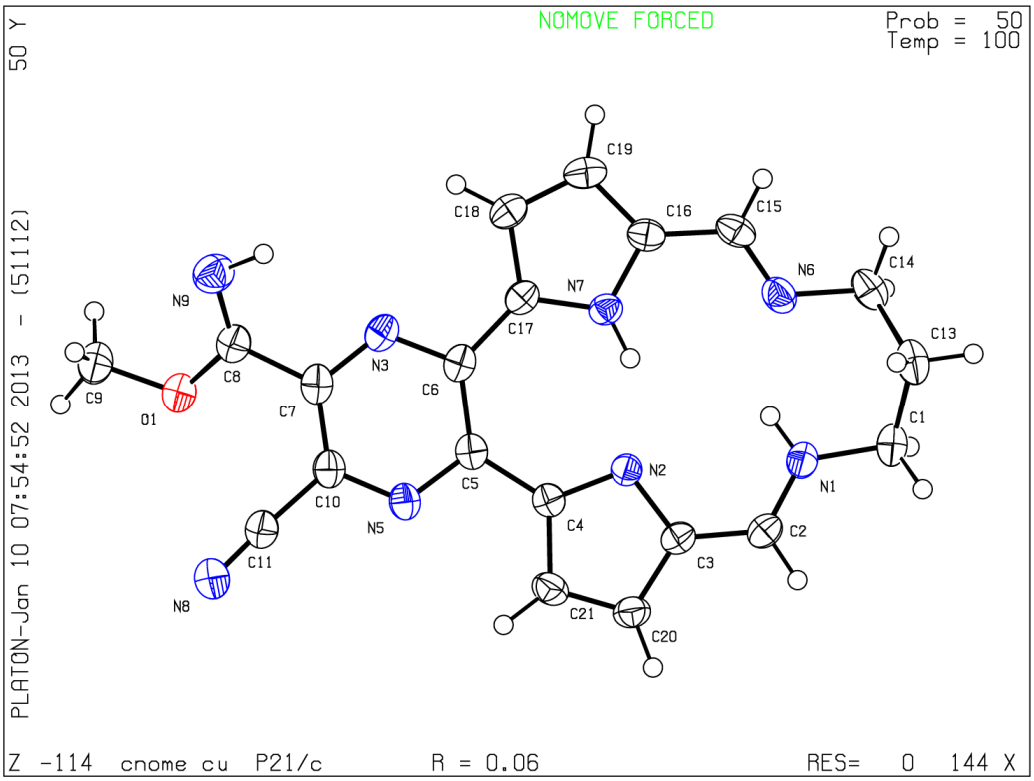
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.173
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 25

Alert level G

PLAT007_ALERT_5_G Note: Number of Unrefined D-H Atoms 2
PLAT371_ALERT_2_G Long C(sp2)-C(sp1) Bond C10 - C11 ... 1.46 Ang.
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 7

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock H_2L8c - ellipsoid plot



A.8: Crystallographic Data Tables for H_2L9

Table A.8.1 Crystal data and structure refinement details for H_2L9

Identification code	H_2L9	
Empirical formula	$C_{20}\ H_{18}\ N_6$	
Formula weight	342.40	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.174(4) Å	α= 90°.
	b = 17.089(5) Å	β= 108.624(5)°.
	c = 11.072(5) Å	γ = 90°.
Volume	1644.9(11) $Å^3$	
Z	4	
Density (calculated)	1.383 Mg/m^3	
Absorption coefficient	0.087 mm^{-1}	
F(000)	720	
Crystal size	0.40 x 0.30 x 0.10 mm^3	
Theta range for data collection	3.07 to 26.05°.	
Index ranges	-11<=h<=11, -21<=k<=21, -10<=l<=13	
Reflections collected	12114	
Independent reflections	3248 [R(int) = 0.0414]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9913 and 0.9659	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3248 / 0 / 245	
Goodness-of-fit on F^2	0.911	
Final R indices [I>2sigma(I)]	R1 = 0.0391, wR2 = 0.0913	
R indices (all data)	R1 = 0.0535, wR2 = 0.0947	
Largest diff. peak and hole	0.159 and -0.295 $e.Å^{-3}$	

Table A.8.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for H_2L9. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(1)	8310(2)	451(1)	67(1)	31(1)
C(2)	6177(2)	1228(1)	-99(1)	24(1)
C(3)	4848(2)	1530(1)	166(1)	22(1)
C(4)	3886(2)	2139(1)	-441(1)	26(1)
C(5)	2745(2)	2216(1)	134(1)	25(1)
C(6)	3033(2)	1649(1)	1092(1)	21(1)
C(7)	2083(2)	1490(1)	1906(1)	21(1)
C(8)	-99(2)	1921(1)	2343(1)	22(1)
C(9)	-1367(2)	2441(1)	2105(1)	26(1)
C(10)	-2434(2)	2334(1)	2706(1)	29(1)
C(11)	-2294(2)	1711(1)	3577(1)	30(1)
C(12)	-1077(2)	1208(1)	3833(1)	28(1)
C(13)	41(2)	1303(1)	3213(1)	22(1)
C(14)	2233(2)	847(1)	2808(1)	20(1)
C(15)	3362(2)	203(1)	3131(1)	21(1)
C(16)	3255(2)	-440(1)	3918(1)	24(1)
C(17)	4491(2)	-911(1)	4019(1)	25(1)
C(18)	5325(2)	-552(1)	3295(1)	22(1)
C(19)	6691(2)	-835(1)	3166(1)	24(1)
C(20)	8919(2)	-890(1)	2456(2)	32(1)
N(1)	7019(1)	666(1)	501(1)	24(1)
N(2)	4313(1)	1243(1)	1092(1)	22(1)
N(3)	944(1)	2008(1)	1719(1)	23(1)
N(4)	1218(1)	783(1)	3437(1)	23(1)
N(5)	4613(1)	133(1)	2752(1)	21(1)
N(6)	7491(1)	-535(1)	2496(1)	25(1)

Table A.8.3: IUCR CIF Check Report

Datablock: H_2L9

Bond precision: C-C = 0.0020 A Wavelength=0.71073

Cell: a=9.174(4) b=17.089(5) c=11.072(5)
alpha=90 beta=108.624(5) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	1644.9(11)	1644.9(11)
Space group	P 21/c	P21/c
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C20 H18 N6	C20 H18 N6
Sum formula	C20 H18 N6	C20 H18 N6
Mr	342.40	342.40
Dx,g cm-3	1.383	1.383
Z	4	4
Mu (mm-1)	0.087	0.087
F000	720.0	720.0
F000'	720.21	
h,k,lmax	11,21,13	11,21,13
Nref	3250	3248
Tmin,Tmax	0.969,0.991	0.966,0.991
Tmin'	0.966	

Correction method= MULTI-SCAN

Data completeness= 0.999 Theta(max)= 26.050

R(reflections)= 0.0391(2421) wR2(reflections)= 0.0947(3248)

S = 0.911 Npar= 245

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.

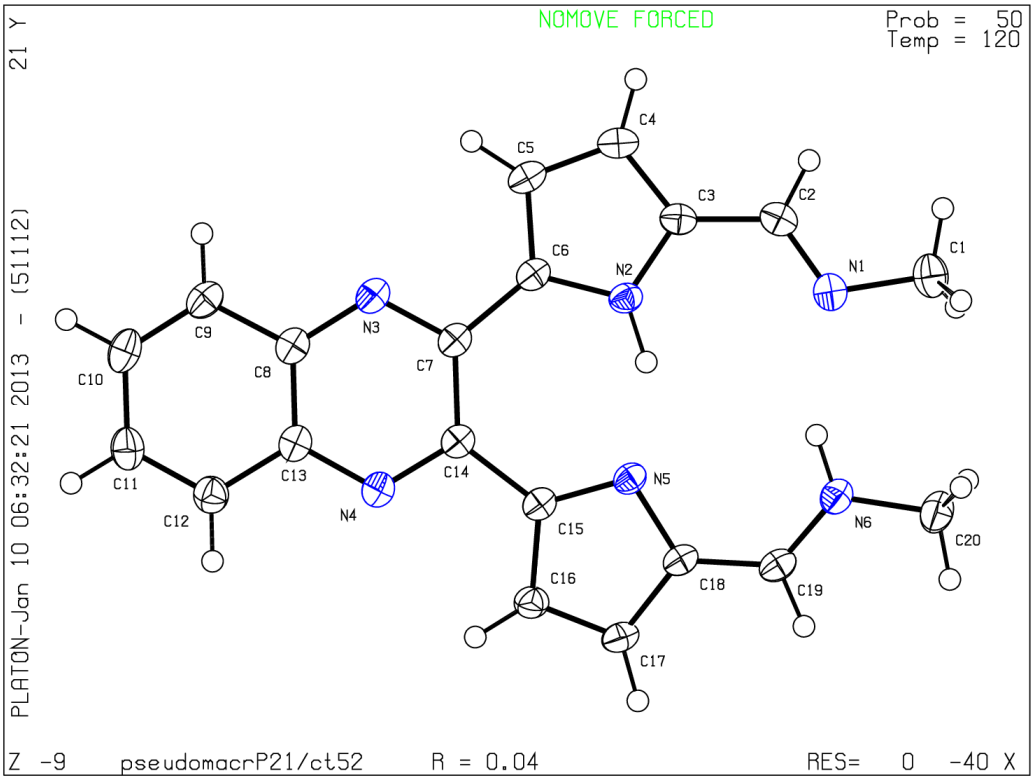
Alert level C

PLAT906_ALERT_3_C Large K value in the Analysis of Variance 3.022

PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 5

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock H_2L9 - ellipsoid plot



A.9: Crystallographic Data Tables for H_2L12

Table A.9.1 Crystal data and structure refinement details for H_2L12

Identification code	H_2L12	
Empirical formula	$C_{14}H_{18}N_4$	
Formula weight	242.32	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/*c*	
Unit cell dimensions	a = 18.140(5) Å	α= 90°.
	b = 5.129(4) Å	β= 102.177(5)°.
	c = 14.310(5) Å	γ = 90°.
Volume	1301.5(12) $Å^3$	
Z	4	
Density (calculated)	1.237 Mg/m^3	
Absorption coefficient	0.077 mm^{-1}	
F(000)	520	
Crystal size	0.50 x 0.29 x 0.22 mm^3	
Theta range for data collection	4.07 to 32.10°.	
Index ranges	-26<=h<=26, -7<=k<=5, -20<=l<=21	
Reflections collected	6311	
Independent reflections	2095 [R(int) = 0.0260]	
Completeness to theta = 25.00°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9833 and 0.9625	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2095 / 0 / 86	
Goodness-of-fit on F^2	0.977	
Final R indices [I>2sigma(I)]	R1 = 0.0425, wR2 = 0.1194	
R indices (all data)	R1 = 0.0522, wR2 = 0.1232	
Largest diff. peak and hole	0.217 and -0.353 $e.Å^{-3}$	

Table A.9.2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for H_2L12. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(1)	3972(1)	-1719(2)	6860(1)	25(1)
C(2)	4040(1)	225(2)	7535(1)	25(1)
C(3)	3374(1)	1729(2)	7306(1)	24(1)
C(4)	2920(1)	649(2)	6500(1)	20(1)
C(5)	2176(1)	1495(2)	6026(1)	21(1)
C(6)	1000(1)	1407(2)	4987(1)	20(1)
C(7)	401(1)	-436(2)	5221(1)	21(1)
N(1)	3294(1)	-1467(2)	6237(1)	22(1)
N(2)	1757(1)	315(2)	5324(1)	21(1)

Table A.9.3: IUCR CIF Check Report

Datablock: H_2L12

Bond precision: C-C = 0.0017 A Wavelength=0.71073

Cell: a=18.140(5) b=5.129(4) c=14.310(5)
alpha=90 beta=102.177(5) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	1301.5(12)	1301.5(12)
Space group	C 2/c	C2/c
Hall group	-C 2yc	-C2yc
Moiety formula	C14 H18 N4	C14 H18 N4
Sum formula	C14 H18 N4	C14 H18 N4
Mr	242.32	242.32
Dx,g cm-3	1.237	1.237
Z	4	4
Mu (mm-1)	0.077	0.077
F000	520.0	520.0
F000'	520.15	
h,k,lmax	26,7,21	26,7,21
Nref	2278	2095
Tmin,Tmax	0.974,0.983	0.962,0.983
Tmin'	0.962	

Correction method= MULTI-SCAN

Data completeness= 0.920 Theta(max)= 32.100

R(reflections)= 0.0425(1666) wR2(reflections)= 0.1232(2095)

S = 0.977 Npar= 86

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level C

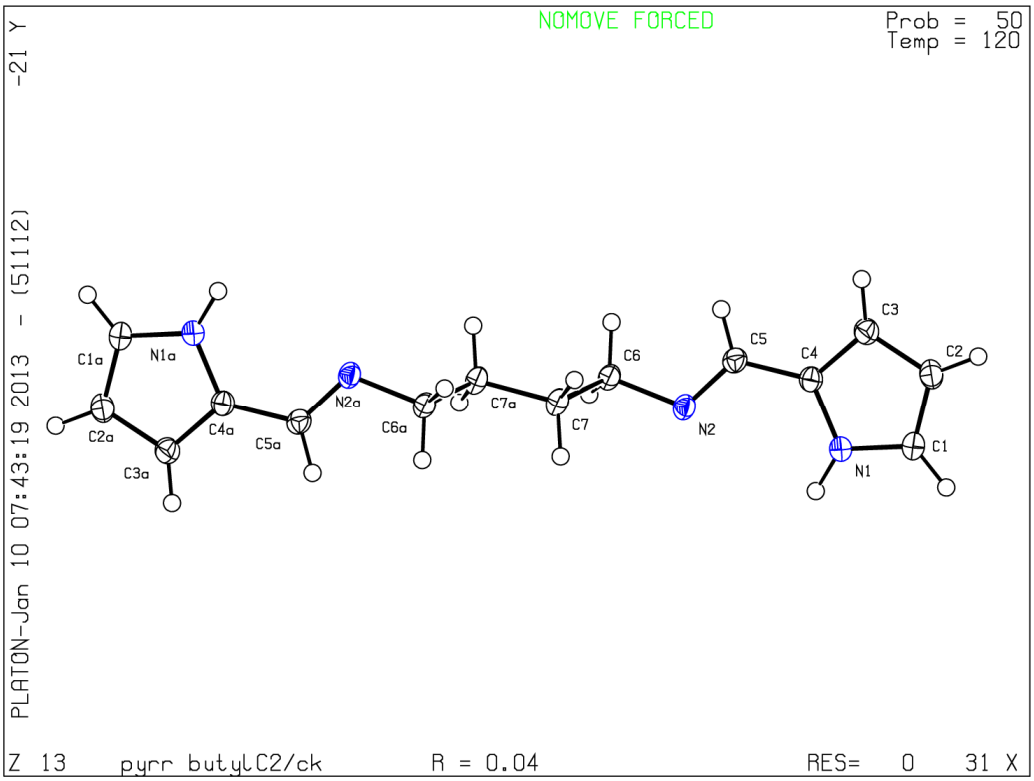
PLAT906_ALERT_3_C Large K value in the Analysis of Variance 2.154
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 3

Alert level G

PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 177

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock H_2L12 - ellipsoid plot



APPENDIX B: *CRYSTOLLOGRAPHIC DATA TABLES OF GOLD(III) COMPLEXES*

B.1: Crystallographic Data Tables for [Au(L1)](PF_6)

Table B.1.1: Crystal data and structure refinement details for [Au(L1)](PF_6).

Identification code	[Au(L1)](PF_6)	
Empirical formula	C_{21} H_{16} Au F_6 N_6 P	
Formula weight	694.33	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2/c	
Unit cell dimensions	a = 16.473(5) Å	□= 90.000°.
	b = 6.980(5) Å	□= 105.675(5)°.
	c = 18.804(5) Å	□ = 90.000°.
Volume	2081.7(17) $Å^3$	
Z	4	
Density (calculated)	2.215 Mg/m^3	
Absorption coefficient	7.223 mm^{-1}	
F(000)	1328	
Crystal size	0.50 x 0.02 x 0.01 mm^3	
Theta range for data collection	2.92 to 25.97°.	
Index ranges	-19<=h<=20, -6<=k<=8, -22<=l<=22	
Reflections collected	14581	
Independent reflections	4010 [R(int) = 0.0603]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.49688	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4010 / 0 / 316	
Goodness-of-fit on F^2	0.940	
Final R indices [I>2sigma(I)]	R1 = 0.0320, wR2 = 0.0703	
R indices (all data)	R1 = 0.0452, wR2 = 0.0733	
Largest diff. peak and hole	2.282 and -1.453 $e.Å^{-3}$	

Table B.1.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Au(L1)](PF_6). U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
Au(1)	7252(1)	3853(1)	613(1)	21(1)
P	9026(1)	842(2)	-1505(1)	26(1)
N(1)	6499(3)	3010(7)	1223(2)	21(1)
N(4)	6441(3)	3727(6)	-375(3)	21(1)
N(6)	4229(3)	2414(6)	-862(2)	18(1)
C(14)	4957(3)	2643(7)	-338(3)	15(1)
F(5)	10026(2)	800(6)	-1272(2)	50(1)
F(6)	8982(3)	-1321(5)	-1206(2)	46(1)
N(2)	8102(3)	3892(7)	1603(3)	31(1)
C(15)	4990(3)	2274(7)	440(3)	17(1)
N(5)	4292(3)	1682(6)	620(3)	20(1)
C(10)	6834(4)	4090(8)	-938(4)	25(1)
F(2)	9037(3)	1658(6)	-705(2)	50(1)
C(1)	5695(4)	2373(8)	1123(3)	22(1)
C(2)	5610(4)	1768(9)	1827(3)	28(1)
C(13)	5629(4)	3190(8)	-691(3)	19(1)
F(4)	9017(3)	26(8)	-2303(2)	73(2)
F(3)	9044(3)	3017(6)	-1797(3)	60(1)
C(19)	2056(4)	912(8)	-1030(4)	29(2)
N(3)	8044(3)	4613(7)	6(3)	23(1)
C(21)	3532(3)	1817(7)	-675(3)	17(1)
C(12)	5503(4)	3223(9)	-1468(3)	25(1)
C(17)	2820(4)	774(8)	272(4)	24(1)
C(16)	3572(4)	1424(7)	88(3)	22(1)
C(3)	6373(4)	2054(10)	2345(3)	34(2)
C(9)	7692(4)	4574(9)	-705(3)	27(1)
C(7)	9317(4)	3940(9)	1046(4)	44(2)
C(5)	7784(4)	3316(9)	2137(4)	33(2)
C(8)	8941(4)	5104(10)	341(4)	35(2)
F(1)	8013(2)	903(6)	-1738(3)	54(1)
C(6)	8985(4)	4448(10)	1706(4)	40(2)
C(18)	2096(4)	531(8)	-274(4)	28(2)
C(11)	6253(4)	3791(8)	-1628(3)	26(1)
C(4)	6924(4)	2814(8)	1964(3)	26(1)
C(20)	2768(4)	1539(8)	-1227(3)	26(1)

Table B.1.3: IUCR CIF Check Report.

Datablock: [Au(L1)](PF_6)

Bond precision: C-C = 0.0090 A Wavelength=0.71073

Cell: a=16.473(5) b=6.980(5) c=18.804(5)
alpha=90 beta=105.675(5) gamma=90

Temperature: 173 K

	Calculated	Reported
Volume	2081.7(17)	2081.7(17)
Space group	P 2/c	P2/c
Hall group	-P 2yc	-P 2yc
Moiety formula	C21 H16 Au N6, F6 P	C21 H16 Au N6, F6 P
Sum formula	C21 H16 Au F6 N6 P	C21 H16 Au F6 N6 P
Mr	694.34	694.33
Dx,g cm-3	2.216	2.215
Z	4	4
Mu (mm-1)	7.223	7.223
F000	1328.0	1328.0
F000'	1321.29	
h,k,lmax	20,8,23	20,8,22
Nref	4088	4010
Tmin,Tmax	0.841,0.930	0.497,1.000
Tmin'	0.027	

Correction method= MULTI-SCAN

Data completeness= 0.981 Theta(max)= 25.970

R(reflections)= 0.0320(3153) wR2(reflections)= 0.0733(4010)

S = 0.940 Npar= 316

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level C

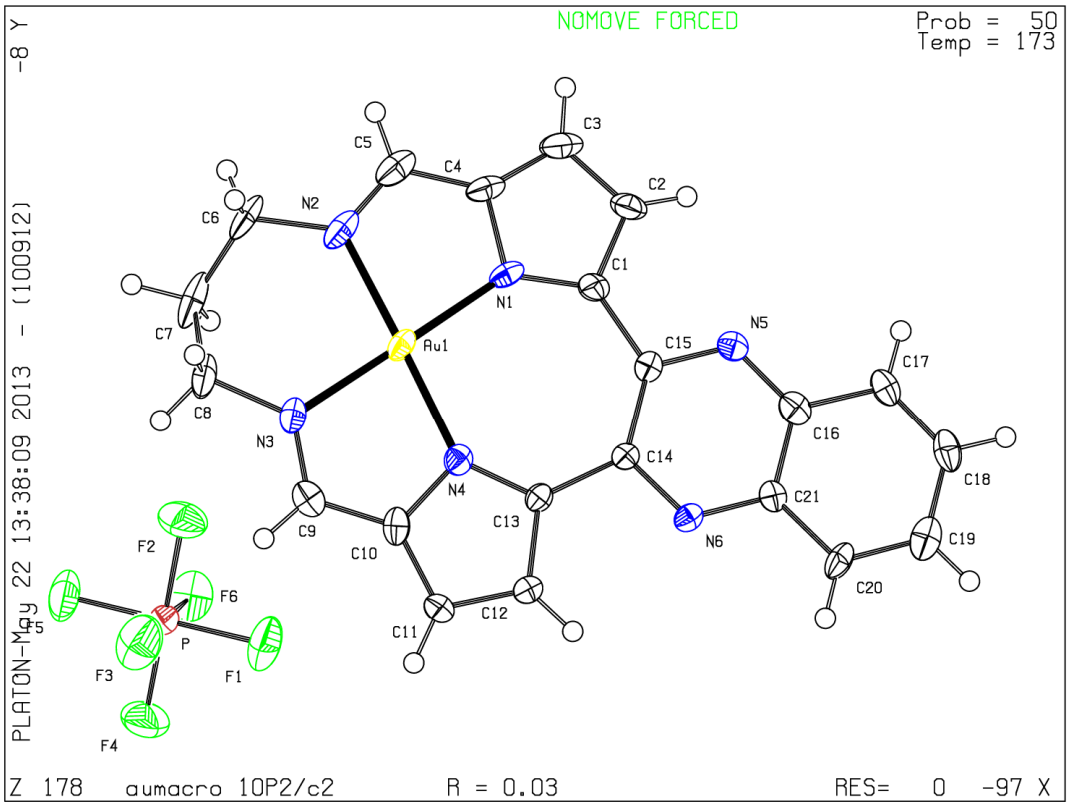
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of P
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0090 Ang
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 5
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3

Alert level G

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
PLAT153_ALERT_1_G The su's on the Cell Axes are Equal ..... 0.00500 Ang.
PLAT790_ALERT_4_G Centre of Gravity not Within Unit Cell: Resd. # 2
F6 P
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 70

PLATON version of 24/04/2013; check.def file version of 23/04/2013

Datablock [Au(L1)](PF$_6$)- ellipsoid plot



B.2: Crystallographic Data Tables for [Au(L2)](CF_3SO_3)

Table B.2.1: Crystal data and structure refinement details for [Au(L2)](CF_3SO_3).

Identification code	[Au(L2)](CF_3SO_3)	
Empirical formula	C_{24} H_{20} Au F_3 N_6 O_3 S	
Formula weight	726.50	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 17.092(5) Å	α= 90.000(5)°.
	b = 25.520(5) Å	β= 119.057(5)°.
	c = 13.625(5) Å	= 90.000(5)°.
Volume	5195(3) $Å^3$	
Z	2	
Density (calculated)	1.860 Mg/m^3	
Absorption coefficient	5.805 mm^{-1}	
F(000)	2820	
Crystal size	0.30 x 0.10 x 0.07 mm^3	
Theta range for data collection	2.77 to 26.05°.	
Index ranges	-21<=h<=20, -30<=k<=31, -13<=l<=16	
Reflections collected	19009	
Independent reflections	7804 [R(int) = 0.0737]	
Completeness to theta = 25.00°	99.9 %	
Max. and min. transmission	0.6867 and 0.2748	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7804 / 8 / 689	
Goodness-of-fit on F^2	1.003	
Final R indices [I>2sigma(I)]	R1 = 0.0646, wR2 = 0.1599	
R indices (all data)	R1 = 0.0897, wR2 = 0.1697	
Absolute structure parameter	0.659(18)	
Largest diff. peak and hole	2.382 and -1.468 $e.Å^{-3}$	

Table B.2.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Au(L2)](CF_3SO_3). U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(1A)	10870(17)	400(11)	2603(19)	41(7)
C(1B)	-316(18)	9363(11)	4170(20)	39(6)
C(2A)	11752(13)	601(8)	3298(16)	33(5)
C(2B)	-518(17)	8858(11)	3990(20)	55(7)
C(3A)	11760(12)	1129(8)	3285(15)	31(5)
C(3B)	257(15)	8553(10)	4575(19)	48(5)
C(4A)	10889(13)	1310(7)	2561(17)	30(4)
C(4B)	935(15)	8914(10)	5128(18)	49(6)
C(5A)	10455(15)	1763(8)	2157(17)	32(5)
C(5B)	1857(17)	8862(11)	5880(20)	51(7)
C(6A)	9038(18)	2192(8)	880(20)	47(6)
C(6B)	3180(20)	9355(18)	7010(30)	106(16)
C(7A)	8013(13)	2160(9)	566(19)	51(6)
C(7B)	3687(15)	9830(11)	6950(20)	57(7)
C(8A)	7489(17)	1708(11)	-390(20)	49(7)
C(8B)	3414(17)	10319(13)	7200(20)	76(9)
C(9A)	7310(14)	775(10)	-327(18)	39(5)
C(9B)	2170(14)	10961(11)	6188(19)	50(6)
C(10A)	7420(18)	-215(9)	-178(19)	47(7)
C(10B)	1213(16)	11066(9)	5438(19)	44(6)
C(11A)	7690(20)	313(10)	40(20)	55(8)
C(11B)	662(17)	11462(10)	5000(20)	50(6)
C(12A)	8136(15)	-538(11)	420(20)	49(7)
C(13A)	8905(16)	-206(9)	1011(19)	42(6)
C(13B)	-208(16)	11263(11)	4300(17)	48(6)
C(14A)	9796(16)	-424(8)	1761(19)	29(5)
C(14B)	-911(15)	10300(30)	3640(20)	84(15)
C(15A)	10522(16)	-1210(8)	2371(19)	39(5)
C(15B)	-2452(14)	10409(9)	2378(18)	39(5)
C(16A)	10570(20)	-1734(10)	2370(30)	64(8)
C(16B)	-3220(17)	10744(14)	1720(20)	73(8)
C(17A)	11222(18)	-2024(9)	2890(20)	62(7)
C(17B)	-4001(14)	10494(12)	1170(20)	57(8)
C(18B)	-4068(16)	9940(8)	1190(20)	47(6)

Table B.2.2. continued…

	x	y	z	U(eq)
C(19A)	12070(20)	-1783(9)	3550(30)	68(8)
C(19B)	-3395(12)	9694(7)	1766(14)	27(4)
C(20A)	12097(14)	-1251(9)	3576(17)	38(5)
C(20B)	-2523(14)	9879(9)	2410(17)	43(5)
C(21A)	11352(17)	-934(12)	3005(19)	54(7)
C(21B)	-997(15)	9729(16)	3624(17)	50(8)
C(22A)	7925(13)	2058(8)	1608(18)	44(5)
C(22B)	4687(14)	9813(11)	7930(20)	65(7)
C(23A)	7575(14)	2679(9)	40(20)	59(7)
C(23B)	3645(16)	9872(10)	5850(20)	61(7)
C(24A)	9750(20)	3135(14)	4730(50)	130(20)
C(24B)	7510(40)	1900(40)	6120(40)	220(50)
C(047)	10689(14)	-161(10)	2451(16)	31(6)
N(1A)	10355(11)	868(7)	2159(14)	35(4)
N(1B)	2298(14)	9334(10)	6233(16)	54(6)
N(2A)	9538(11)	1748(7)	1446(14)	41(4)
N(2B)	593(13)	9416(8)	4869(16)	40(5)
N(3A)	7814(15)	1198(9)	63(17)	51(5)
N(3B)	712(11)	10604(9)	5005(14)	42(5)
N(4A)	8592(12)	293(7)	767(14)	36(4)
N(4B)	2474(15)	10520(10)	6360(20)	63(7)
N(5A)	11371(12)	-424(7)	3023(16)	37(4)
N(5B)	-1612(14)	10643(8)	3009(16)	44(5)
N(6A)	9767(10)	-926(6)	1747(12)	33(4)
N(6B)	-1764(12)	9559(9)	3079(16)	48(5)
N(027)	-150(20)	10707(17)	4300(20)	97(12)
O(1A)	8892(12)	3313(8)	2685(18)	77(6)
O(1B)	8310(30)	2974(11)	6770(40)	200(20)
O(2A)	10286(12)	2809(10)	3420(20)	121(10)
O(2B)	6990(40)	2560(20)	7050(40)	330(40)
O(3A)	10313(12)	3759(8)	3820(19)	90(6)
O(3B)	8560(30)	2284(11)	8140(20)	157(15)
F(1A)	9308(13)	2654(7)	4680(20)	115(7)
F(1B)	6943(19)	2254(14)	5120(30)	215(19)
F(2A)	9316(14)	3475(8)	4930(20)	123(9)
F(2B)	7400(30)	1614(16)	6340(50)	290(40)

Table B.2.2. continued…

	x	y	z	U(eq)
F(3A)	10601(11)	3050(9)	5642(18)	112(7)
F(3B)	8290(20)	1915(12)	5970(30)	184(14)
S(1A)	9803(5)	3268(3)	3522(8)	85(2)
S(1B)	7889(10)	2540(5)	7128(10)	131(5)
Au(1A)	9092(1)	1017(1)	1045(1)	29(1)
Au(1B)	1492(1)	9962(1)	5547(1)	41(1)

Table B.1.3: IUCR CIF Check Report.

Datablock: [Au(L2)](CF_3SO_3)

Bond precision: C-C = 0.0220 A Wavelength=0.71073

Cell: a=17.092(5) b=25.520(5) c=13.625(5)
alpha=90 beta=119.057(5) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	5195(3)	5195(3)
Space group	C c	C c
Hall group	C -2yc	C -2yc
Moiety formula	C23 H20 Au N6, C F3 O3 S	C23 H20 Au N6, C F3 O3 S
Sum formula	C24 H20 Au F3 N6 O3 S	C24 H20 Au F3 N6 O3 S
Mr	726.50	726.49
Dx,g cm-3	1.858	1.858
Z	8	8
Mu (mm-1)	5.804	5.804
F000	2816.0	2816.0
F000'	2802.62	
h,k,lmax	21,31,16	21,31,16
Nref	10271[5143]	7796
Tmin,Tmax	0.503,0.666	0.404,1.000
Tmin'	0.174	

Correction method= MULTI-SCAN

Data completeness= 1.52/0.76 Theta(max)= 26.050

R(reflections)= 0.0544(5727) wR2(reflections)= 0.1246(7796)

S = 0.980 Npar= 665

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0220 Ang
PLAT601_ALERT_2_B Structure Contains Solvent Accessible VOIDS of . 175 Ang3
PLAT973_ALERT_2_B Large Calcd. Positive Residual Density on Au2 1.51 eA-3

Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 7.72
PLAT234_ALERT_4_C Large Hirshfeld Difference Au2 -- N2B .. 0.16 Ang.
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of C1C
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 3.7
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 6
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 3
PLAT915_ALERT_3_C Low Friedel Pair Coverage ..... 52 %
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density 2.24 eA-3

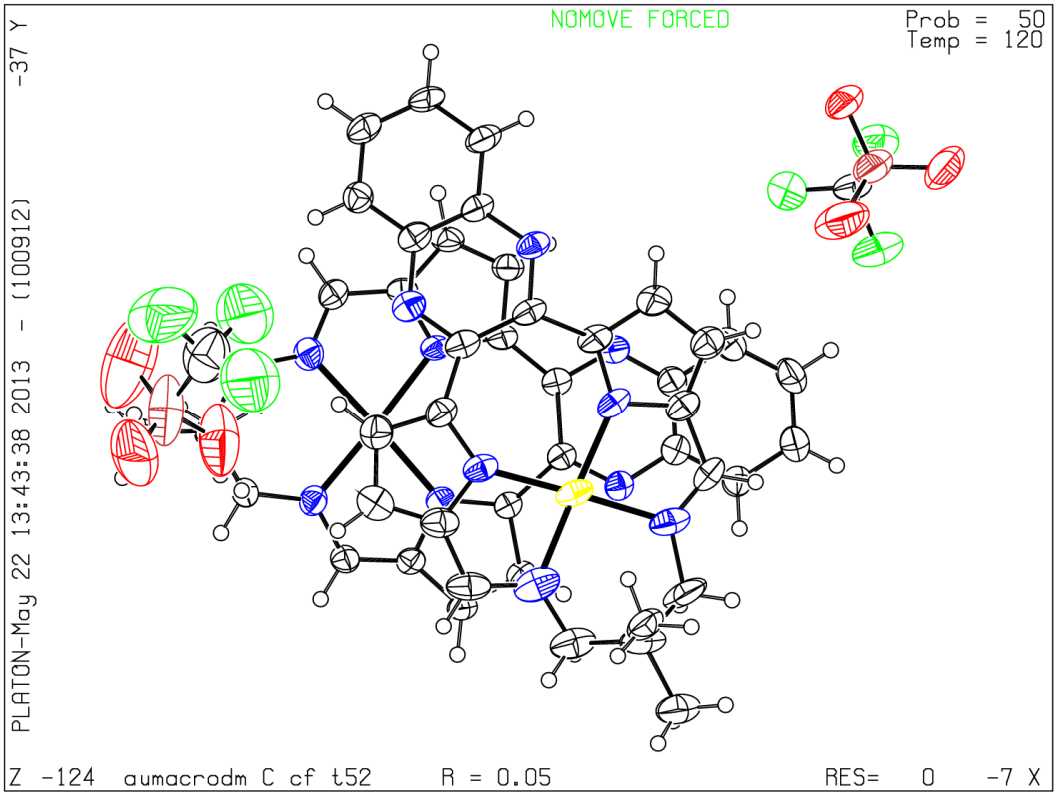
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density 2.02 eA-3
PLAT973_ALERT_2_C Large Calcd. Positive Residual Density on Au1 1.44 eA-3

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 10
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 74
PLAT153_ALERT_1_G The su's on the Cell Axes are Equal ..... 0.00500 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 8
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su .. 0.01
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 455

PLATON version of 24/04/2013; check.def file version of 23/04/2013

Datablock [Au(L2)](CF$_3$SO$_3$)- ellipsoid plot



B.3: Crystallographic Data Tables for [Au(L3)](PF_6)

Table B.3.1: Crystal data and structure refinement details for [Au(L3)](PF_6).

Identification code	[Au(L3)](PF_6)	
Empirical formula	C_{24} H_{21} Au F_6 N_7 P	
Formula weight	749.41	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pna21	
Unit cell dimensions	a = 43.9022(11) Å	α= 90°.
	b = 6.7597(2) Å	β= 90°.
	c = 48.8964(12) Å	γ = 90°.
Volume	14510.8(7) $Å^3$	
Z	24	
Density (calculated)	2.058 Mg/m^3	
Absorption coefficient	12.760 mm^{-1}	
F(000)	8688	
Crystal size	0.12 x 0.02 x 0.02 mm^3	
Theta range for data collection	1.81 to 66.59°.	
Index ranges	-45<=h<=52, -8<=k<=8, -57<=l<=56	
Reflections collected	101016	
Independent reflections	24413 [R(int) = 0.0978]	
Completeness to theta = 67.0°	99.4 %	
Absorption correction	Numerical	
Max. and min. transmission	0.8123 and 0.3097	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	24413 / 2247 / 2114	
Goodness-of-fit on F^2	1.055	
Final R indices [I>2sigma(I)]	R1 = 0.0520, wR2 = 0.1067	
R indices (all data)	R1 = 0.0680, wR2 = 0.1131	
Absolute structure parameter	0.00(6)	
Largest diff. peak and hole	2.016 and -2.003 e.$Å^{-3}$	

Table B.3.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Au(L3)](PF_6). U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
Au(1)	5526(1)	1621(1)	7879(1)	19(1)
Au(2)	6955(1)	7984(1)	6761(1)	19(1)
Au(3)	9705(1)	2191(1)	5259(1)	21(1)
Au(4)	9568(1)	8286(1)	6177(1)	18(1)
Au(5)	7917(1)	3127(1)	8461(1)	17(1)
Au(6)	7783(1)	7056(1)	9389(1)	24(1)
P(1)	5498(1)	6927(5)	8898(1)	29(1)
P(2)	8096(1)	3846(5)	7119(1)	27(1)
P(3)	6992(1)	2566(5)	5746(1)	26(1)
P(4)	5882(1)	7507(5)	5501(1)	26(1)
P(5)	9386(1)	9088(5)	7520(1)	26(1)
P(6)	6609(1)	2167(6)	9140(1)	26(1)
F(1)	5750(2)	6887(15)	9132(2)	44(2)
F(2)	5694(2)	5371(13)	8728(3)	51(3)
F(3)	5250(3)	6953(14)	8660(2)	42(3)
F(4)	5302(3)	8476(15)	9063(3)	56(3)
F(5)	5670(2)	8715(12)	8757(2)	42(2)
F(6)	5324(2)	5117(14)	9043(2)	46(2)
F(7)	7951(2)	5645(13)	7287(2)	43(2)
F(8)	8380(2)	3829(14)	7328(2)	37(2)
F(9)	8234(3)	2052(17)	6955(3)	57(3)
F(10)	7813(2)	3850(15)	6911(2)	44(2)
F(11)	7908(3)	2317(16)	7320(3)	62(4)
F(12)	8270(2)	5340(17)	6926(2)	54(3)
F(13)	6752(3)	2515(15)	5500(3)	51(3)
F(14)	7191(2)	899(15)	5599(2)	53(3)
F(15)	7225(2)	2607(13)	5993(2)	38(2)
F(16)	6790(2)	4214(13)	5896(2)	41(2)
F(17)	6796(2)	890(12)	5899(2)	36(2)
F(18)	7182(3)	4224(16)	5594(3)	65(4)
F(19)	6023(2)	9227(12)	5314(2)	39(2)
F(20)	6019(2)	5878(13)	5300(2)	43(2)
F(21)	5730(2)	5807(13)	5689(2)	40(2)
F(22)	5734(2)	9141(13)	5700(2)	43(3)

Table B.3.2. continued…

	x	y	z	U(eq)
F(23)	6178(3)	7450(13)	5688(3)	40(3)
F(24)	5571(3)	7554(12)	5323(2)	39(3)
F(25)	9669(2)	9142(14)	7724(2)	38(2)
F(26)	9556(3)	7552(14)	7331(2)	39(3)
F(27)	9104(2)	9046(13)	7311(2)	36(2)
F(28)	9209(2)	10599(15)	7709(2)	50(3)
F(29)	9237(3)	7260(15)	7683(3)	50(3)
F(30)	9532(2)	10864(12)	7352(2)	41(2)
F(31)	6467(2)	3758(13)	9336(2)	44(2)
F(32)	6916(2)	2165(12)	9316(2)	33(2)
F(33)	6759(2)	580(13)	8936(2)	40(2)
F(34)	6307(3)	2191(14)	8958(3)	40(3)
F(35)	6477(2)	410(14)	9318(2)	47(3)
F(36)	6750(2)	3918(12)	8955(2)	36(2)
N(1A)	5534(2)	1641(13)	7472(2)	17(2)
N(1B)	6517(3)	7498(13)	6705(3)	18(2)
N(1C)	9631(3)	2612(14)	5653(3)	20(2)
N(1D)	9522(3)	7730(16)	5778(3)	22(2)
N(1E)	8359(3)	3291(16)	8364(2)	24(2)
N(1F)	8217(3)	7316(17)	9503(3)	25(2)
N(1S)	5272(3)	1660(20)	9688(3)	40(3)
N(2A)	5080(3)	1002(15)	7813(3)	26(2)
N(2B)	6962(3)	7809(15)	6346(3)	20(2)
N(2C)	10154(3)	2273(16)	5385(3)	26(2)
N(2D)	10012(3)	7959(16)	6087(3)	23(2)
N(2E)	7871(2)	3813(14)	8063(2)	16(2)
N(2F)	7716(3)	6612(19)	9782(3)	32(2)
N(2S)	6873(4)	7413(19)	8386(4)	37(3)
N(3A)	5523(3)	1738(16)	8292(3)	26(2)
N(3B)	7399(3)	8664(14)	6825(2)	23(2)
N(3C)	9766(3)	1698(17)	4854(3)	26(2)
N(3D)	9605(2)	9040(15)	6574(2)	21(2)
N(3E)	7469(3)	2734(15)	8562(3)	21(2)
N(3F)	7347(3)	7024(17)	9267(3)	28(2)
N(3S)	7954(3)	8869(16)	7858(3)	31(3)
N(4A)	5967(3)	2091(15)	7932(3)	19(2)

Table B.3.2. continued…

	x	y	z	U(eq)
N(4B)	6948(2)	8028(14)	7166(3)	18(2)
N(4C)	9275(3)	2228(16)	5134(3)	24(2)
N(4D)	9129(3)	8378(15)	6266(2)	22(2)
N(4E)	7972(3)	2587(15)	8855(3)	20(2)
N(4F)	7856(3)	7433(16)	8992(3)	24(2)
N(4S)	9529(3)	4066(16)	6784(3)	33(3)
N(5A)	6573(3)	2703(15)	7433(3)	22(2)
N(5B)	6315(3)	7472(14)	7631(3)	19(2)
N(5C)	8590(3)	2475(17)	5545(4)	29(2)
N(5E)	8658(4)	2584(16)	9259(3)	31(2)
N(5F)	8566(3)	7915(16)	8625(3)	26(2)
N(5S)	5612(4)	2280(20)	6254(4)	42(4)
N(6A)	6167(3)	2174(15)	7006(3)	20(2)
N(6B)	5912(3)	6934(15)	7205(3)	22(2)
N(6C)	8912(3)	2898(16)	6026(3)	24(2)
N(6E)	9017(3)	2827(17)	8796(4)	32(2)
N(6F)	8898(3)	7584(15)	9097(3)	24(2)
N(6S)	7214(3)	6520(20)	4949(3)	43(3)
N(41)	8473(3)	7574(16)	5838(4)	33(2)
N(42)	8835(4)	7645(15)	5370(3)	29(2)
C(1A)	5730(3)	1904(17)	7265(3)	18(2)
C(1B)	6251(3)	7242(18)	6851(3)	19(2)
C(1C)	9387(3)	2816(17)	5829(3)	21(2)
C(1D)	9303(4)	7660(20)	5583(4)	27(2)
C(1E)	8628(3)	3026(18)	8481(3)	24(2)
C(1F)	8495(4)	7478(19)	9402(4)	27(2)
C(1S)	5485(4)	1730(20)	9569(4)	31(3)
C(2A)	5561(3)	1904(18)	7018(3)	24(2)
C(2B)	6013(3)	7008(19)	6670(3)	24(2)
C(2C)	9520(3)	3037(16)	6100(3)	21(2)
C(2D)	9459(4)	7411(18)	5332(4)	27(2)
C(2E)	8854(3)	3190(20)	8271(3)	29(2)
C(2F)	8709(5)	7570(20)	9621(5)	33(2)
C(2S)	5760(4)	1790(20)	9396(4)	42(4)
C(3A)	5256(3)	1574(17)	7081(3)	23(2)
C(3B)	6131(4)	7139(18)	6406(4)	22(2)

Table B.3.2. continued…

	x	y	z	U(eq)
C(3C)	9831(3)	2979(16)	6070(3)	19(2)
C(3D)	9757(4)	7334(18)	5368(4)	25(2)
C(3E)	8712(3)	3560(20)	8035(3)	29(2)
C(3F)	8548(4)	7340(20)	9870(4)	34(2)
C(3S)	6646(4)	7401(19)	8505(4)	30(3)
C(4A)	5241(3)	1411(17)	7367(3)	22(2)
C(4B)	6439(3)	7468(17)	6424(3)	19(2)
C(4C)	9897(3)	2684(17)	5799(3)	19(2)
C(4D)	9794(4)	7516(17)	5655(4)	21(2)
C(4E)	8398(3)	3580(20)	8087(3)	24(2)
C(4F)	8241(4)	7070(20)	9788(4)	29(2)
C(4S)	6368(4)	7340(20)	8656(4)	30(3)
C(5A)	5012(3)	1045(17)	7554(3)	23(2)
C(5B)	6677(3)	7565(16)	6249(3)	19(2)
C(5C)	10165(4)	2483(19)	5646(4)	27(3)
C(5D)	10061(4)	7650(20)	5823(4)	29(3)
C(5E)	8126(3)	3954(16)	7936(3)	20(2)
C(5F)	7970(4)	6790(20)	9936(3)	30(3)
C(5S)	8169(3)	8904(19)	7736(3)	27(3)
C(6A)	4860(3)	309(19)	8025(3)	30(2)
C(6B)	7225(3)	7740(19)	6169(3)	26(2)
C(6C)	10419(4)	2240(20)	5207(4)	31(3)
C(6D)	10270(3)	7900(20)	6273(4)	22(2)
C(6E)	7590(3)	4488(18)	7931(3)	22(2)
C(6F)	7437(4)	5850(20)	9921(4)	38(3)
C(6S)	8454(4)	8960(20)	7572(4)	43(4)
C(7A)	4758(4)	1970(20)	8210(4)	28(2)
C(7B)	7483(3)	6511(19)	6283(3)	28(2)
C(7C)	10393(3)	3610(19)	4967(3)	27(2)
C(7D)	10192(3)	6759(19)	6541(3)	23(2)
C(7E)	7376(3)	2782(18)	7863(3)	25(2)
C(7F)	7189(4)	7320(20)	9949(5)	37(3)
C(7S)	9311(3)	4098(19)	6905(3)	26(3)
C(8A)	5001(3)	3078(19)	8354(3)	27(2)
C(8B)	7741(3)	7718(19)	6426(4)	26(2)
C(8C)	10297(4)	2494(18)	4700(4)	26(3)

Table B.3.2. continued…

	x	y	z	U(eq)
C(8D)	10109(3)	8060(20)	6776(3)	26(2)
C(8E)	7300(3)	1499(19)	8110(3)	23(2)
C(8F)	7092(4)	8320(20)	9678(4)	41(3)
C(8S)	9029(4)	4170(30)	7074(4)	43(4)
C(9A)	5251(3)	1785(19)	8473(3)	26(2)
C(9B)	7615(3)	9345(18)	6616(3)	23(2)
C(9C)	10058(3)	940(20)	4737(3)	32(3)
C(9D)	9891(3)	9723(18)	6710(3)	24(2)
C(9E)	7211(4)	2573(19)	8365(4)	24(2)
C(9F)	7068(4)	6960(20)	9437(4)	36(3)
C(9S)	5828(4)	2330(20)	6139(5)	34(4)
C(10A)	5794(3)	1990(20)	8394(3)	25(2)
C(10B)	7475(3)	8663(18)	7080(3)	23(2)
C(10C)	9518(3)	1750(20)	4723(3)	29(3)
C(10D)	9347(3)	9102(19)	6698(3)	27(2)
C(10E)	7438(4)	2399(17)	8817(4)	20(2)
C(10F)	7314(4)	7215(17)	8999(4)	22(2)
C(10S)	6119(4)	2380(20)	5983(5)	42(4)
C(11A)	6044(3)	2146(19)	8208(3)	22(2)
C(11B)	7243(3)	8254(17)	7272(3)	21(2)
C(11C)	9252(4)	2200(20)	4854(3)	24(2)
C(11D)	9085(3)	8646(19)	6549(3)	24(2)
C(11E)	7693(4)	2386(18)	8989(4)	23(2)
C(11F)	7583(4)	7420(17)	8842(4)	24(2)
C(11S)	7002(5)	6920(30)	5079(4)	41(4)
C(12A)	6355(4)	2549(19)	8237(4)	26(2)
C(12B)	7224(3)	8135(17)	7555(3)	21(2)
C(12C)	8950(4)	2280(20)	4787(4)	27(2)
C(12D)	8772(3)	8440(20)	6607(3)	30(2)
C(12E)	7747(4)	2190(19)	9263(4)	25(2)
C(12F)	7646(4)	7750(19)	8574(4)	28(2)
C(12S)	6727(4)	7210(30)	5238(5)	46(4)
C(13A)	6471(3)	2584(18)	7980(3)	24(2)
C(13B)	6921(3)	7822(18)	7621(3)	22(2)
C(13C)	8791(4)	2560(20)	5027(4)	28(2)
C(13D)	8637(4)	8010(20)	6360(3)	30(2)

Table B.3.2. continued…

	x	y	z	U(eq)
C(13E)	8068(4)	2310(19)	9309(4)	28(2)
C(13F)	7958(3)	7887(17)	8543(3)	24(2)
C(14A)	6227(3)	2399(17)	7789(3)	19(2)
C(14B)	6753(3)	7784(18)	7377(3)	19(2)
C(14C)	8992(4)	2516(18)	5243(4)	23(2)
C(14D)	8848(3)	7950(20)	6148(3)	26(2)
C(14E)	8201(4)	2578(18)	9048(4)	23(2)
C(14F)	8081(4)	7711(18)	8809(3)	24(2)
C(15A)	6275(3)	2398(15)	7495(3)	15(2)
C(15B)	6411(3)	7485(16)	7370(3)	17(2)
C(15C)	8893(4)	2605(17)	5533(4)	21(2)
C(15D)	8776(4)	7730(20)	5854(4)	28(2)
C(15E)	8529(4)	2643(18)	9014(4)	26(2)
C(15F)	8418(4)	7736(18)	8861(4)	23(2)
C(16A)	6065(3)	2162(18)	7261(3)	20(2)
C(16B)	6205(3)	7214(18)	7151(3)	19(2)
C(16C)	9059(4)	2771(18)	5787(4)	23(2)
C(16D)	8967(4)	7661(18)	5620(4)	25(2)
C(16E)	8717(4)	2843(19)	8762(3)	24(2)
C(16F)	8590(4)	7581(19)	9109(4)	25(2)
C(17A)	6673(3)	2747(18)	7169(3)	21(2)
C(17B)	6019(3)	7157(17)	7680(3)	18(2)
C(17C)	8440(4)	2501(18)	5786(4)	26(2)
C(17D)	8356(5)	7400(20)	5576(5)	40(2)
C(17E)	8960(5)	2580(20)	9286(5)	36(2)
C(17F)	8870(4)	7936(19)	8611(4)	27(2)
C(18A)	6977(3)	3073(17)	7113(3)	21(2)
C(18B)	5919(4)	7126(19)	7958(3)	24(2)
C(18C)	8117(4)	2356(19)	5793(4)	29(2)
C(18D)	8028(5)	7260(20)	5554(5)	47(3)
C(18E)	9111(5)	2560(20)	9535(5)	40(2)
C(18F)	9027(4)	8145(19)	8362(3)	29(2)
C(19A)	7088(3)	3133(17)	6850(3)	22(2)
C(19B)	5610(3)	6768(18)	8008(3)	25(2)
C(19C)	7977(4)	2510(20)	6039(4)	32(2)
C(19D)	7913(5)	7170(20)	5282(5)	49(3)

Table B.2.2. continued…

	x	y	z	U(eq)
C(19E)	9442(4)	2580(20)	9537(4)	42(2)
C(19F)	9330(4)	8110(20)	8361(4)	34(2)
C(20A)	6874(3)	2773(17)	6633(3)	23(2)
C(20B)	5405(3)	6507(17)	7786(3)	24(2)
C(20C)	8134(4)	2810(20)	6275(4)	33(2)
C(20D)	8102(5)	7280(30)	5064(5)	50(3)
C(20E)	9614(4)	2670(20)	9302(4)	40(3)
C(20F)	9507(4)	7870(20)	8607(4)	33(2)
C(21A)	6579(4)	2471(18)	6684(4)	24(2)
C(21B)	5496(3)	6552(16)	7522(3)	20(2)
C(21C)	8455(4)	2980(20)	6276(3)	31(2)
C(21D)	8393(6)	7490(20)	5079(5)	47(3)
C(21E)	9473(5)	2760(20)	9068(5)	39(2)
C(21F)	9355(4)	7715(19)	8852(4)	29(2)
C(22A)	6467(3)	2458(17)	6954(4)	23(2)
C(22B)	5811(3)	6895(17)	7462(3)	17(2)
C(22C)	8608(4)	2820(20)	6019(3)	28(2)
C(22D)	8527(5)	7560(20)	5360(5)	41(2)
C(22E)	9152(4)	2720(20)	9043(4)	33(2)
C(22F)	9038(4)	7751(18)	8859(4)	26(2)

Table B.3.3: IUCR CIF Check Report.

Datablock: [Au(L3)](PF_6)

Bond precision: C-C = 0.0230 A Wavelength=1.54178

Cell: a=43.9022(11) b=6.7597(2) c=48.8964(12)
alpha=90 beta=90 gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	14510.8(7)	14510.8(7)
Space group	P n a 21	Pna21
Hall group	P 2c -2n	P 2c -2n
Moiety formula	C22 H18 Au N6, F6 P, C2 H3 N	C22 H18 Au N6, F6 P, C2 H3 N
Sum formula	C24 H21 Au F6 N7 P	C24 H21 Au F6 N7 P
Mr	749.42	749.41
Dx,g cm-3	2.058	2.058
Z	24	24
Mu (mm-1)	12.760	12.760
F000	8688.0	8688.0
F000'	8614.96	
h,k,lmax	52,8,58	52,8,57
Nref	25548[12938]	24413
Tmin,Tmax	0.773,0.775	0.310,0.812
Tmin'	0.206	

Correction method= NUMERICAL

Data completeness= 1.89/0.96 Theta(max)= 66.590

R(reflections)= 0.0520(20623) wR2(reflections)= 0.1131(24413)

S = 1.055 Npar= 2114

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level B

PLAT342_ALERT_3_B Low Bond Precision on C-C Bonds ..... 0.0230 Ang

Alert level C

PLAT089_ALERT_3_C Poor Data / Parameter Ratio (Zmax < 18) 6.08
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of P1
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.595 95
PLAT926_ALERT_1_C Reported and Calculated R1 Differ by ..... -0.0021
PLAT927_ALERT_1_C Reported and Calculated wR2 Differ by ..... -0.0045
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density 2.03 eA-3
PLAT972_ALERT_2_C Large Calcd. Non-Metal Negative Residual Density -1.79 eA-3

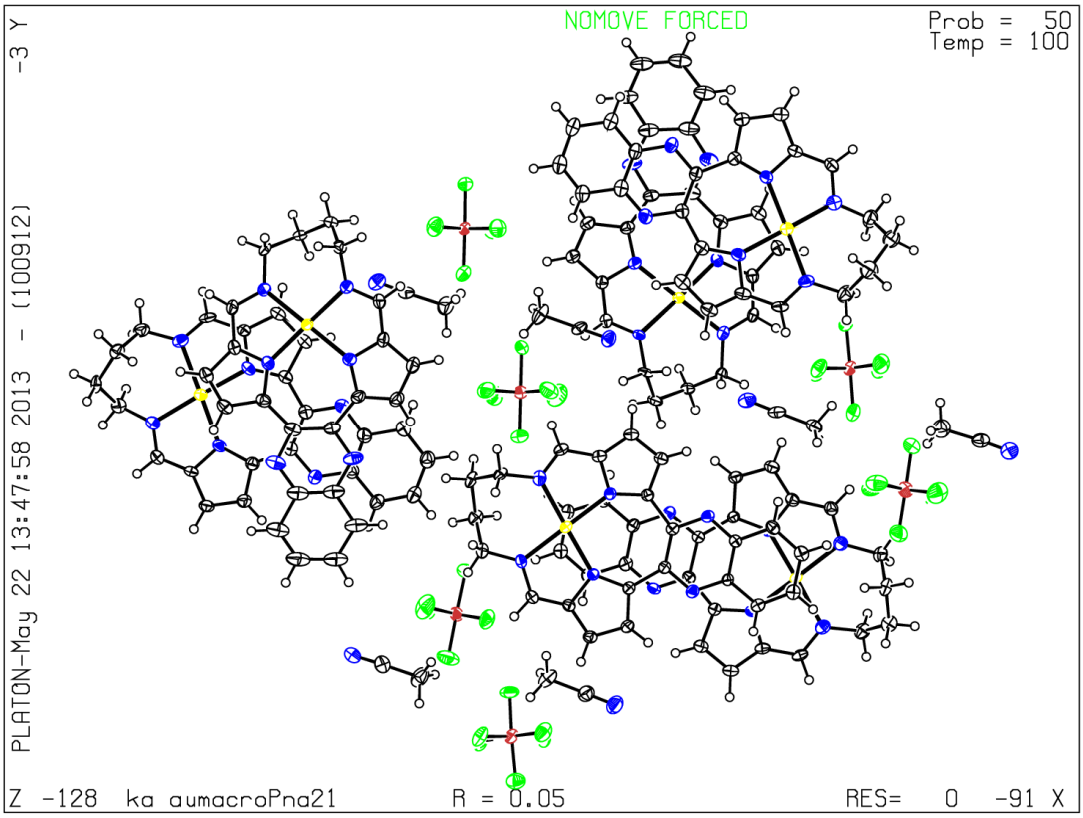
Alert level G

PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 186

PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 102.15
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C17D -C22D 0.21 Ang.
PLAT335_ALERT_2_G Check Large C6 Ring C-C Range C17E -C22E 0.16 Ang.
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 60
PLAT850_ALERT_4_G Check Flack Parameter Exact Value 0.00 and su .. 0.06
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints 2247
PLAT909_ALERT_3_G Percentage of Observed Data at Theta(Max) still 76 %
PLAT916_ALERT_2_G Hooft y and Flack x Parameter values differ by . 0.42

PLATON version of 24/04/2013; check.def file version of 23/04/2013

Datablock [Au(L3)](PF_6)- ellipsoid plot



B.4: Crystallographic Data Tables for [Au(L10)](AuCl$_4$)

Table B.4.1: Crystal data and structure refinement details for [Au(L10)](AuCl$_4$).

Identification code	[Au(L10)](AuCl$_4$)	
Empirical formula	C_{22} H_{18} Au_2 Cl_4 N_6	
Formula weight	902.16	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/*c*	
Unit cell dimensions	a = 9.4669(13) Å	α= 90°.
	b = 31.073(4) Å	β= 103.831(3)°.
	c = 8.3523(12) Å	γ = 90°.
Volume	2385.7(6) Å^3	
Z	4	
Density (calculated)	2.512 Mg/m^3	
Absorption coefficient	12.758 mm^{-1}	
F(000)	1672	
Crystal size	0.10 x 0.05 x 0.01 mm^3	
Theta range for data collection	2.31 to 28.09°.	
Index ranges	-12<=h<=12, -41<=k<=40, -11<=l<=10	
Reflections collected	9729	
Independent reflections	2871 [R(int) = 0.0289]	
Completeness to theta = 25.00°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8830 and 0.3619	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2871 / 0 / 156	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0342, wR2 = 0.1022	
R indices (all data)	R1 = 0.0424, wR2 = 0.1110	
Largest diff. peak and hole	3.719 and -1.556 e.Å^{-3}	

Table B.4.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Au(L10)]($AuCl_4$).. U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
C(10)	1070(9)	6487(3)	1559(10)	20(2)
C(11)	529(8)	6857(2)	2033(10)	18(2)
Au(1)	0	4120(1)	2500	10(1)
N(3)	1059(6)	5713(2)	1604(8)	13(1)
N(2)	1472(7)	3700(2)	1896(8)	14(1)
C	2681(9)	3012(3)	1390(10)	19(2)
C(3)	2470(8)	3906(2)	1381(10)	16(1)
N(1)	1325(6)	4549(2)	1864(8)	14(1)
C(6)	2658(9)	5057(3)	999(11)	20(2)
C(8)	579(7)	5342(2)	2081(9)	13(1)
C(7)	1445(8)	4985(2)	1668(10)	16(1)
C(4)	2430(8)	4356(2)	1327(10)	15(1)
C(2)	1514(8)	3229(2)	2070(10)	15(1)
C(5)	3290(9)	4664(3)	806(11)	21(2)
C(9)	533(8)	6087(2)	2032(9)	15(1)
Au(2)	0	1694(1)	2500	13(1)
Cl(1)	-684(2)	2217(1)	570(3)	26(1)
Cl(2)	-545(2)	1180(1)	485(3)	25(1)

Table B.4.3: IUCR CIF Check Report.

Datablock: [Au(L10)](AuCl$_4$)

Bond precision: C-C = 0.0111 A Wavelength=0.71073

Cell: a=9.4669(13) b=31.073(4) c=8.3523(12)
alpha=90 beta=103.831(3) gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	2385.7(6)	2385.7(6)
Space group	C 2/c	C2/c
Hall group	-C 2yc	-C 2yc
Moiety formula	C22 H18 Au N6, Au Cl4	C22 H18 Au N6, Au Cl4
Sum formula	C22 H18 Au2 Cl4 N6	C22 H18 Au2 Cl4 N6
Mr	902.16	902.16
Dx,g cm-3	2.512	2.512
Z	4	4
Mu (mm-1)	12.758	12.758
F000	1672.0	1672.0
F000'	1659.78	
h,k,lmax	12,41,11	12,41,11
Nref	2915	2871
Tmin,Tmax	0.470,0.880	0.362,0.883
Tmin'	0.276	

Correction method= MULTI-SCAN

Data completeness= 0.985 Theta(max)= 28.090

R(reflections)= 0.0342(2497) wR2(reflections)= 0.1110(2871)

S = 1.048 Npar= 156

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level B

PLAT973_ALERT_2_B Large Calcd. Positive Residual Density on Au1 1.69 eA-3

Alert level C

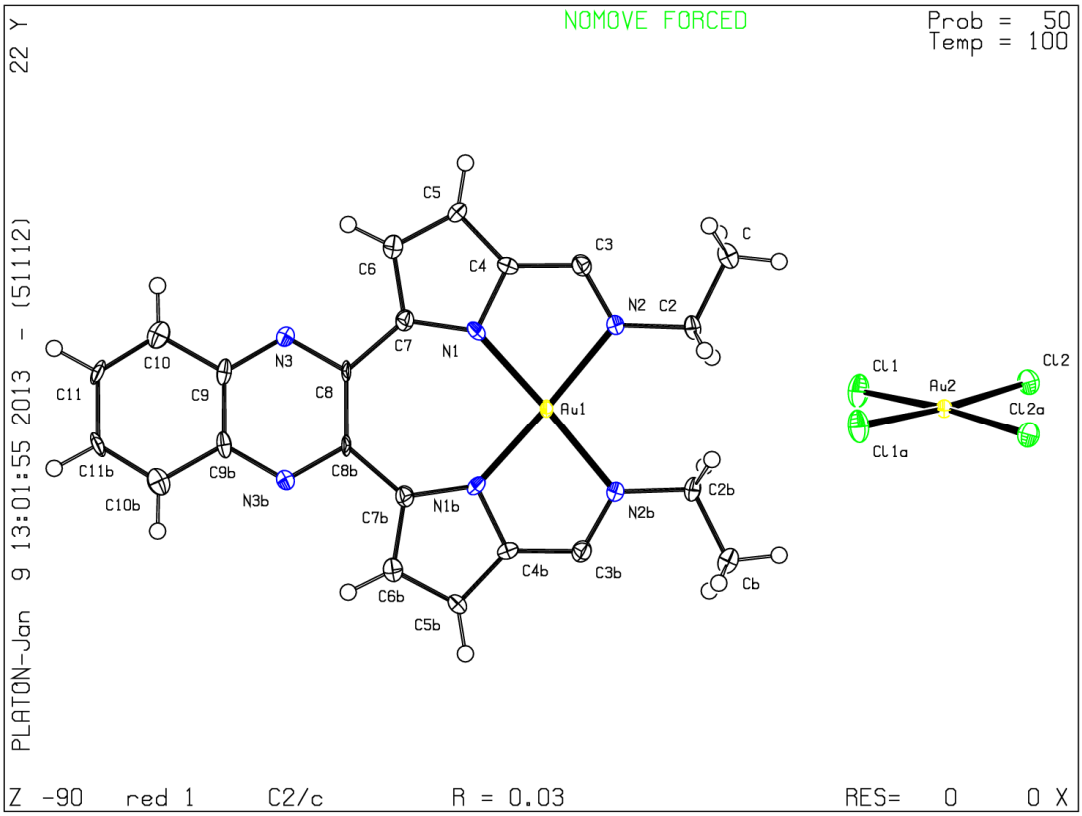
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density 2.39
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0111 Ang
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 1
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 32
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density 2.33 eA-3
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density 2.10 eA-3
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density 1.63 eA-3
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density 1.53 eA-3
PLAT973_ALERT_2_C Large Calcd. Positive Residual Density on Au2 1.20 eA-3

Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 57.93
PLAT343_ALERT_2_G Check sp? Angle Range in Main Residue for .. C3
PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 3
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 12

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock [Au(L10)](AuCl$_4$) - ellipsoid plot



B.5: Crystallographic Data Tables for [Au(L12)](PF_6)

Table B.5.1: Crystal data and structure refinement details for [Au(L12)](PF_6).

Identification code	[Au(L12)](PF_6)	
Empirical formula	C_{14} H_{16} Au F_6 N_4 P	
Formula weight	582.24	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 8.293(5) Å	α= 90°.
	b = 10.903(5) Å	β= 96.808(5)°.
	c = 19.024(6) Å	γ = 90°.
Volume	1708.0(14) $Å^3$	
Z	4	
Density (calculated)	2.264 Mg/m^3	
Absorption coefficient	8.775 mm^{-1}	
F(000)	1104	
Crystal size	0.45 x 0.20 x 0.15 mm^3	
Theta range for data collection	2.85 to 32.08°.	
Index ranges	-11<=h<=11, -14<=k<=15, -27<=l<=28	
Reflections collected	16330	
Independent reflections	5430 [R(int) = 0.0396]	
Completeness to theta = 25.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.3528 and 0.1101	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5430 / 0 / 235	
Goodness-of-fit on F^2	1.054	
Final R indices [I>2sigma(I)]	R1 = 0.0357, wR2 = 0.0848	
R indices (all data)	R1 = 0.0579, wR2 = 0.0985	
Largest diff. peak and hole	3.059 and -2.759 e.$Å^{-3}$	

Table B.5.2: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for [Au(L12)](PF_6). U(eq) is defined as one third of the trace of the orthogonalised Uij tensor.

	x	y	z	U(eq)
Au(01)	8041(1)	4682(1)	4471(1)	19(1)
P	3222(2)	546(1)	3467(1)	25(1)
N(3)	9411(5)	4764(4)	3648(2)	21(1)
N(4)	8473(6)	6467(5)	4469(2)	25(1)
N(1)	6836(6)	4565(4)	5324(2)	21(1)
F(1)	3982(5)	1769(4)	3845(2)	40(1)
F(3)	3816(10)	-203(5)	4145(3)	81(2)
F(4)	2465(6)	-658(5)	3079(3)	61(2)
C(3)	5693(7)	3347(6)	6085(3)	26(1)
C(10)	9900(7)	5894(6)	3528(3)	25(1)
F(5)	4891(5)	288(4)	3157(3)	49(1)
F(2)	1551(6)	855(5)	3757(3)	65(2)
F(6)	2671(8)	1333(6)	2773(3)	72(2)
C(2)	5710(7)	4573(5)	6349(3)	24(1)
C(12)	9585(8)	8120(6)	3971(3)	31(1)
C(14)	8076(7)	7497(6)	4815(4)	28(1)
C(8)	8810(8)	3047(6)	2794(3)	29(1)
C(7)	7369(7)	2547(6)	3142(3)	27(1)
C(9)	10069(7)	3715(6)	3299(3)	27(1)
C(6)	7815(7)	1976(5)	3870(3)	25(1)
N(2)	7544(6)	2845(4)	4443(2)	20(1)
C(1)	6396(7)	5276(6)	5843(3)	23(1)
C(11)	9385(7)	6842(6)	3943(3)	25(1)
C(4)	6408(7)	3369(5)	5460(3)	22(1)
C(13)	8753(8)	8524(6)	4525(3)	32(1)
C(5)	6793(7)	2478(5)	4967(3)	23(1)

Table B.4.3: IUCR CIF Check Report.

Datablock: [Au(L12)](PF_6)

Bond precision: C-C = 0.0085 A Wavelength=0.71073

Cell: a=8.293(5) b=10.903(5) c=19.024(6)
alpha=90 beta=96.808(5) gamma=90

Temperature: 120 K

	Calculated	Reported
Volume	1708.0(14)	1708.0(14)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C14 H16 Au N4, F6 P	C14 H16 Au N4, F6 P
Sum formula	C14 H16 Au F6 N4 P	C14 H16 Au F6 N4 P
Mr	582.25	582.24
Dx,g cm-3	2.264	2.264
Z	4	4
Mu (mm-1)	8.775	8.775
F000	1104.0	1104.0
F000'	1097.31	
h,k,lmax	12,16,28	11,15,28
Nref	5980	5430
Tmin,Tmax	0.140,0.268	0.110,0.353
Tmin'	0.017	

Correction method= MULTI-SCAN

Data completeness= 0.908 Theta(max)= 32.080

R(reflections)= 0.0357(4141) wR2(reflections)= 0.0985(5430)

S = 1.054 Npar= 235

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.

Alert level C

PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors of P
PLAT250_ALERT_2_C Large U3/U1 Ratio for Average U(i,j) Tensor 2.1
PLAT342_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0085 Ang
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.946
PLAT910_ALERT_3_C Missing # of FCF Reflections Below Th(Min) 4
PLAT911_ALERT_3_C Missing # FCF Refl Between THmin & STh/L= 0.600 2
PLAT971_ALERT_2_C Large Calcd. Non-Metal Positive Residual Density 2.06 eA-3
PLAT972_ALERT_2_C Large Calcd. Non-Metal Negative Residual Density -1.53 eA-3

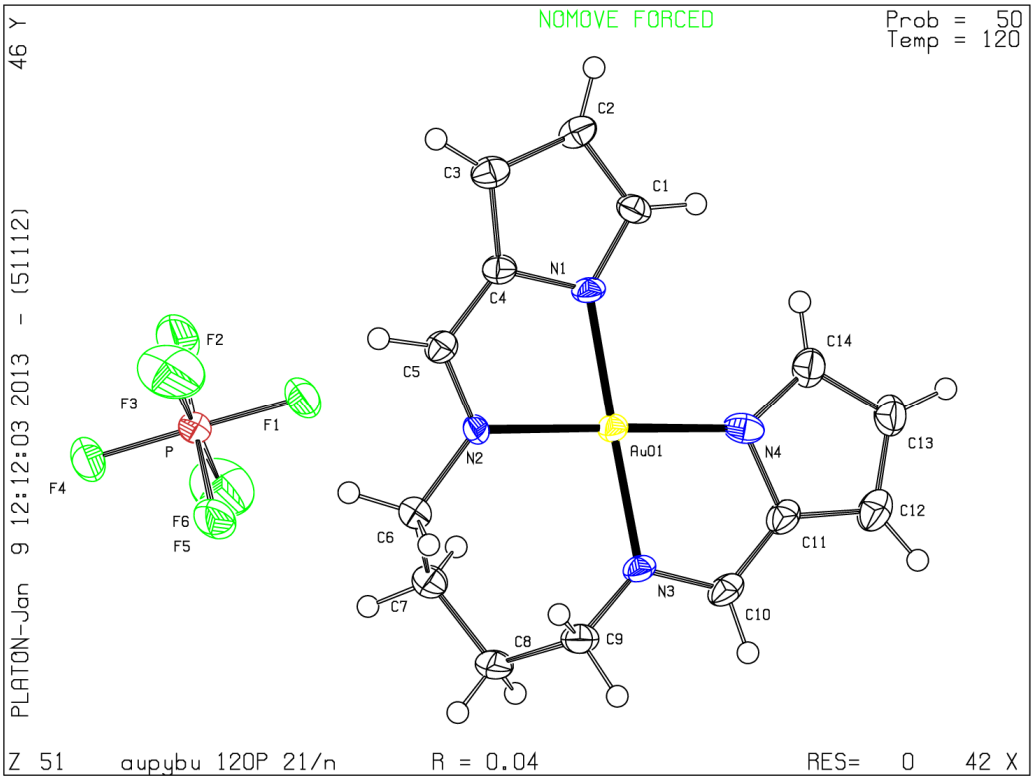
Alert level G

PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 9.06
PLAT128_ALERT_4_G Alternate Setting of Space-group P21/c P21/n
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Au01 -- N4 .. 7.5 su

PLAT720_ALERT_4_G Number of Unusual/Non-Standard Labels 1
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 476

PLATON version of 05/11/2012; check.def file version of 05/11/2012

Datablock [Au(L12)](PF$_6$) - ellipsoid plot



C.1: Full crystallographic Data Tables of H_2L2

Table C.1.1: Bond lengths [Å] and angles [°] for H_2L2

C(1)-N(1)	1.358(3)
C(1)-C(2)	1.403(4)
C(1)-C(21)	1.462(4)
C(2)-C(3)	1.399(4)
C(2)-H(021)	0.9300
C(3)-C(4)	1.400(4)
C(3)-H(026)	0.9300
C(4)-N(1)	1.370(4)
C(4)-C(5)	1.435(4)
C(5)-N(2)	1.291(3)
C(5)-H(019)	0.9300
C(6)-N(2)	1.460(3)
C(6)-C(7)	1.553(4)
C(6)-H(02D)	0.9700
C(6)-H(02E)	0.9700
C(7)-C(23)	1.527(4)
C(7)-C(22)	1.540(4)
C(7)-C(8)	1.546(4)
C(8)-N(3)	1.462(3)
C(8)-H(02F)	0.9700
C(8)-H(02G)	0.9700
C(9)-N(3)	1.302(4)
C(9)-C(10)	1.396(4)
C(9)-H(013)	0.9300
C(10)-N(4)	1.389(3)
C(10)-C(11)	1.409(4)
C(11)-C(12)	1.372(4)
C(11)-H(024)	0.9300
C(12)-C(13)	1.439(4)
C(12)-H(016)	0.9300
C(13)-N(4)	1.339(3)
C(13)-C(14)	1.486(4)
C(14)-N(5)	1.331(3)
C(14)-C(21)	1.475(4)

Table C.1.1. continued…

C(15)-N(5)	1.368(3)
C(15)-C(16)	1.408(4)
C(15)-C(20)	1.420(4)
C(16)-C(17)	1.369(4)
C(16)-H(018)	0.9300
C(17)-C(18)	1.425(4)
C(17)-H(022)	0.9300
C(18)-C(19)	1.359(4)
C(18)-H(027)	0.9300
C(19)-C(20)	1.421(4)
C(19)-H(015)	0.9300
C(20)-N(6)	1.357(3)
C(21)-N(6)	1.338(3)
C(22)-H(02H)	0.9600
C(22)-H(02I)	0.9600
C(22)-H(02J)	0.9600
C(23)-H(02A)	0.9600
C(23)-H(02B)	0.9600
C(23)-H(02C)	0.9600
N(1)-H(101)	0.925(18)
N(3)-H(102)	0.906(17)

N(1)-C(1)-C(2)	108.3(2)
N(1)-C(1)-C(21)	125.2(2)
C(2)-C(1)-C(21)	126.5(2)
C(3)-C(2)-C(1)	107.6(2)
C(3)-C(2)-H(021)	126.2
C(1)-C(2)-H(021)	126.2
C(2)-C(3)-C(4)	106.4(2)
C(2)-C(3)-H(026)	126.8
C(4)-C(3)-H(026)	126.8
N(1)-C(4)-C(3)	108.9(2)
N(1)-C(4)-C(5)	120.8(2)
C(3)-C(4)-C(5)	130.2(3)
N(2)-C(5)-C(4)	121.4(3)
N(2)-C(5)-H(019)	119.3
C(4)-C(5)-H(019)	119.3

Table C.1.1. continued…

N(2)-C(6)-C(7)	111.6(2)
N(2)-C(6)-H(02D)	109.3
C(7)-C(6)-H(02D)	109.3
N(2)-C(6)-H(02E)	109.3
C(7)-C(6)-H(02E)	109.3
H(02D)-C(6)-H(02E)	108.0
C(23)-C(7)-C(22)	110.1(2)
C(23)-C(7)-C(8)	107.0(2)
C(22)-C(7)-C(8)	110.7(2)
C(23)-C(7)-C(6)	107.8(2)
C(22)-C(7)-C(6)	109.7(2)
C(8)-C(7)-C(6)	111.5(2)
N(3)-C(8)-C(7)	111.9(2)
N(3)-C(8)-H(02F)	109.2
C(7)-C(8)-H(02F)	109.2
N(3)-C(8)-H(02G)	109.2
C(7)-C(8)-H(02G)	109.2
H(02F)-C(8)-H(02G)	107.9
N(3)-C(9)-C(10)	122.5(3)
N(3)-C(9)-H(013)	118.8
C(10)-C(9)-H(013)	118.8
N(4)-C(10)-C(9)	121.1(3)
N(4)-C(10)-C(11)	110.9(2)
C(9)-C(10)-C(11)	128.0(3)
C(12)-C(11)-C(10)	106.0(2)
C(12)-C(11)-H(024)	127.0
C(10)-C(11)-H(024)	127.0
C(11)-C(12)-C(13)	106.8(2)
C(11)-C(12)-H(016)	126.6
C(13)-C(12)-H(016)	126.6
N(4)-C(13)-C(12)	110.5(2)
N(4)-C(13)-C(14)	126.1(2)
C(12)-C(13)-C(14)	123.4(2)
N(5)-C(14)-C(21)	119.9(2)
N(5)-C(14)-C(13)	110.5(2)
C(21)-C(14)-C(13)	129.7(2)
N(5)-C(15)-C(16)	119.0(2)

Table C.1.1. continued…

N(5)-C(15)-C(20)	120.9(2)
C(16)-C(15)-C(20)	120.1(2)
C(17)-C(16)-C(15)	119.1(3)
C(17)-C(16)-H(018)	120.5
C(15)-C(16)-H(018)	120.5
C(16)-C(17)-C(18)	120.9(3)
C(16)-C(17)-H(022)	119.6
C(18)-C(17)-H(022)	119.6
C(19)-C(18)-C(17)	121.2(3)
C(19)-C(18)-H(027)	119.4
C(17)-C(18)-H(027)	119.4
C(18)-C(19)-C(20)	118.9(3)
C(18)-C(19)-H(015)	120.6
C(20)-C(19)-H(015)	120.6
N(6)-C(20)-C(15)	121.0(2)
N(6)-C(20)-C(19)	119.2(2)
C(15)-C(20)-C(19)	119.8(2)
N(6)-C(21)-C(1)	111.0(2)
N(6)-C(21)-C(14)	120.6(2)
C(1)-C(21)-C(14)	128.4(2)
C(7)-C(22)-H(02H)	109.5
C(7)-C(22)-H(02I)	109.5
H(02H)-C(22)-H(02I)	109.5
C(7)-C(22)-H(02J)	109.5
H(02H)-C(22)-H(02J)	109.5
H(02I)-C(22)-H(02J)	109.5
C(7)-C(23)-H(02A)	109.5
C(7)-C(23)-H(02B)	109.5
H(02A)-C(23)-H(02B)	109.5
C(7)-C(23)-H(02C)	109.5
H(02A)-C(23)-H(02C)	109.5
H(02B)-C(23)-H(02C)	109.5
C(1)-N(1)-C(4)	108.8(2)
C(1)-N(1)-H(101)	127(2)
C(4)-N(1)-H(101)	124(2)
C(5)-N(2)-C(6)	120.6(2)
C(9)-N(3)-C(8)	127.3(2)

Table C.1.1. continued…

C(9)-N(3)-H(102)	119(2)
C(8)-N(3)-H(102)	114(2)
C(13)-N(4)-C(10)	105.8(2)
C(14)-N(5)-C(15)	119.0(2)
C(21)-N(6)-C(20)	118.7(2)

Table C.1.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L2. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(2)	18(2)	22(2)	0(1)	1(1)	-2(1)
C(2)	24(2)	27(2)	22(2)	1(1)	1(1)	2(1)
C(3)	20(2)	28(2)	28(2)	-1(1)	0(1)	2(1)
C(4)	24(2)	20(2)	22(2)	-1(1)	5(1)	-2(1)
C(5)	25(2)	21(2)	27(2)	1(1)	3(1)	1(1)
C(6)	32(2)	29(2)	25(2)	1(1)	6(1)	3(1)
C(7)	28(2)	26(2)	23(2)	3(1)	6(1)	4(1)
C(8)	33(2)	29(2)	19(2)	3(1)	3(1)	2(1)
C(9)	28(2)	24(2)	23(2)	1(1)	-4(1)	0(1)
C(10)	25(2)	21(2)	23(2)	2(1)	-3(1)	1(1)
C(11)	29(2)	27(2)	26(2)	5(1)	-1(1)	3(1)
C(12)	25(2)	30(2)	26(2)	-1(1)	4(1)	5(1)
C(13)	24(2)	17(2)	22(2)	-4(1)	1(1)	-4(1)
C(14)	20(2)	16(2)	22(2)	-2(1)	-2(1)	-2(1)
C(15)	26(2)	18(2)	21(2)	-4(1)	3(1)	-3(1)
C(16)	23(2)	31(2)	25(2)	-3(1)	3(1)	0(1)
C(17)	33(2)	32(2)	26(2)	-1(1)	12(1)	2(2)
C(18)	38(2)	26(2)	27(2)	4(1)	8(2)	4(1)
C(19)	32(2)	23(2)	23(2)	0(1)	0(1)	4(1)
C(20)	22(2)	15(2)	24(2)	-2(1)	2(1)	-2(1)
C(21)	22(2)	18(2)	21(2)	-3(1)	-3(1)	-4(1)
C(22)	34(2)	30(2)	34(2)	2(1)	4(1)	0(2)
C(23)	38(2)	38(2)	28(2)	6(1)	7(1)	4(2)
N(1)	25(1)	23(1)	17(1)	-1(1)	0(1)	1(1)
N(2)	32(1)	22(1)	21(1)	3(1)	5(1)	1(1)
N(3)	26(1)	35(2)	19(1)	5(1)	3(1)	3(1)
N(4)	22(1)	23(1)	21(1)	1(1)	2(1)	3(1)
N(5)	21(1)	22(1)	22(1)	-2(1)	4(1)	-1(1)
N(6)	25(1)	22(1)	19(1)	-1(1)	-1(1)	-2(1)

Table C.1.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L2.

	x	y	z	U(eq)
H(021)	6889	2085	-50	29
H(026)	5111	1981	867	30
H(019)	5476	1369	2348	29
H(02D)	5860	883	3506	34
H(02E)	7235	1598	3852	34
H(02F)	9590	465	4331	32
H(02G)	9624	-927	4281	32
H(013)	11690	-1008	3542	30
H(024)	13721	-1187	2582	33
H(016)	13766	-410	1341	32
H(018)	14318	1083	-533	32
H(022)	14022	1872	-1674	36
H(027)	11738	2598	-2176	36
H(015)	9743	2532	-1549	32
H(02H)	5953	-1352	3435	49
H(02I)	7403	-2037	3703	49
H(02J)	7311	-1266	3001	49
H(02A)	6002	-372	4621	52
H(02B)	7344	410	4932	52
H(02C)	7488	-979	4921	52
H(101)	9080(30)	1030(30)	1818(14)	61(11)
H(102)	9350(30)	330(20)	3017(14)	51(11)

Table C.1.4: Torsion angles [°] for H_2L2.

N(1)-C(1)-C(2)-C(3)	-1.5(3)
C(21)-C(1)-C(2)-C(3)	177.8(2)
C(1)-C(2)-C(3)-C(4)	1.1(3)
C(2)-C(3)-C(4)-N(1)	-0.3(3)
C(2)-C(3)-C(4)-C(5)	178.9(3)
N(1)-C(4)-C(5)-N(2)	4.3(4)
C(3)-C(4)-C(5)-N(2)	-174.9(3)
N(2)-C(6)-C(7)-C(23)	178.0(2)
N(2)-C(6)-C(7)-C(22)	-62.2(3)
N(2)-C(6)-C(7)-C(8)	60.8(3)
C(23)-C(7)-C(8)-N(3)	-178.9(2)
C(22)-C(7)-C(8)-N(3)	61.1(3)
C(6)-C(7)-C(8)-N(3)	-61.3(3)
N(3)-C(9)-C(10)-N(4)	-1.5(4)
N(3)-C(9)-C(10)-C(11)	-180.0(3)
N(4)-C(10)-C(11)-C(12)	0.2(3)
C(9)-C(10)-C(11)-C(12)	178.8(3)
C(10)-C(11)-C(12)-C(13)	-0.8(3)
C(11)-C(12)-C(13)-N(4)	1.1(3)
C(11)-C(12)-C(13)-C(14)	-178.7(2)
N(4)-C(13)-C(14)-N(5)	170.6(2)
C(12)-C(13)-C(14)-N(5)	-9.7(4)
N(4)-C(13)-C(14)-C(21)	-11.3(4)
C(12)-C(13)-C(14)-C(21)	168.4(3)
N(5)-C(15)-C(16)-C(17)	-179.4(2)
C(20)-C(15)-C(16)-C(17)	0.4(4)
C(15)-C(16)-C(17)-C(18)	-1.2(4)
C(16)-C(17)-C(18)-C(19)	0.0(4)
C(17)-C(18)-C(19)-C(20)	2.0(4)
N(5)-C(15)-C(20)-N(6)	2.6(4)
C(16)-C(15)-C(20)-N(6)	-177.2(2)
N(5)-C(15)-C(20)-C(19)	-178.6(2)
C(16)-C(15)-C(20)-C(19)	1.6(4) C(18)-C(19)-C(20)-N(6)
C(18)-C(19)-C(20)-C(15)	-2.8(4)
N(1)-C(1)-C(21)-N(6)	-171.3(2)
C(2)-C(1)-C(21)-N(6)	9.5(4)

Table C.1.4. continued…

N(1)-C(1)-C(21)-C(14)	9.0(4)
C(2)-C(1)-C(21)-C(14)	-170.2(3)
N(5)-C(14)-C(21)-N(6)	1.5(4)
C(13)-C(14)-C(21)-N(6)	-176.5(2)
N(5)-C(14)-C(21)-C(1)	-178.8(2)
C(13)-C(14)-C(21)-C(1)	3.2(4)
C(2)-C(1)-N(1)-C(4)	1.3(3)
C(21)-C(1)-N(1)-C(4)	-178.0(2)
C(3)-C(4)-N(1)-C(1)	-0.6(3)
C(5)-C(4)-N(1)-C(1)	-179.9(2)
C(4)-C(5)-N(2)-C(6)	179.3(2)
C(7)-C(6)-N(2)-C(5)	130.7(3)
C(10)-C(9)-N(3)-C(8)	-174.5(3)
C(7)-C(8)-N(3)-C(9)	-149.9(3)
C(12)-C(13)-N(4)-C(10)	-0.9(3)
C(14)-C(13)-N(4)-C(10)	178.8(2)
C(9)-C(10)-N(4)-C(13)	-178.2(2)
C(11)-C(10)-N(4)-C(13)	0.5(3)
C(21)-C(14)-N(5)-C(15)	-1.0(4)
C(13)-C(14)-N(5)-C(15)	177.3(2)
C(16)-C(15)-N(5)-C(14)	178.9(2)
C(20)-C(15)-N(5)-C(14)	-0.9(4)
C(1)-C(21)-N(6)-C(20)	-179.6(2)
C(14)-C(21)-N(6)-C(20)	0.1(4)
C(15)-C(20)-N(6)-C(21)	-2.1(4)
C(19)-C(20)-N(6)-C(21)	179.1(2)

C.2: Full crystallographic Data Tables of H_2L5

Table C.2.1: Bond lengths [Å] and angles [°] for H_2L1

N(001)-C(010)	1.3489(18)
N(001)-C(024)	1.3767(18)
N(002)-C(008)	1.3579(17)
N(002)-C(025)	1.3670(18)
N(002)-H(101)	0.894(10)
N(003)-C(007)	1.3285(17)
N(003)-C(013)	1.3566(18)
N(004)-C(019)	1.2775(19)
N(004)-C(027)	1.4675(18)
N(005)-C(012)	1.3320(18)
N(005)-C(017)	1.3586(18)
N(006)-C(014)	1.292(2)
N(006)-C(021)	1.4609(19)
N(006)-H(102)	0.883(9)
C(007)-C(012)	1.4562(19)
C(007)-C(008)	1.4724(19)
C(008)-C(018)	1.3988(19)
C(009)-C(011)	1.366(2)
C(009)-C(013)	1.411(2)
C(009)-H(009)	0.9500
C(010)-C(015)	1.4197(19)
C(010)-C(012)	1.4715(19)
C(011)-C(023)	1.434(2)
C(011)-C(016)	1.505(2)
C(013)-C(017)	1.411(2)
C(014)-C(024)	1.405(2)
C(014)-H(014)	0.9500
C(015)-C(026)	1.372(2)
C(015)-H(015)	0.9500
C(016)-H(01A)	0.9800
C(016)-H(01B)	0.9800 C(016)-H(01C)
C(017)-C(029)	1.419(2)
C(018)-C(020)	1.388(2)
C(018)-H(018)	0.9500

Table C.2.1. continued…

C(019)-C(025)	1.429(2)
C(019)-H(019)	0.9500
C(020)-C(025)	1.394(2)
C(020)-H(020)	0.9500
C(021)-C(028)	1.523(2)
C(021)-H(02A)	0.9900
C(021)-H(02B)	0.9900
C(023)-C(029)	1.364(2)
C(023)-C(030)	1.506(2)
C(024)-C(026)	1.403(2)
C(026)-H(026)	0.9500
C(027)-C(028)	1.526(2)
C(027)-H(02C)	0.9900
C(027)-H(02D)	0.9900
C(028)-H(02E)	0.9900
C(028)-H(02F)	0.9900
C(029)-H(029)	0.9500
C(030)-H(03A)	0.9800
C(030)-H(03B)	0.9800
C(030)-H(03C)	0.9800

C(010)-N(001)-C(024)	106.94(12)
C(008)-N(002)-C(025)	108.98(12)
C(008)-N(002)-H(101)	117.3(14)
C(025)-N(002)-H(101)	130.4(15)
C(007)-N(003)-C(013)	119.26(12)
C(019)-N(004)-C(027)	121.41(14)
C(012)-N(005)-C(017)	119.03(12)
C(014)-N(006)-C(021)	124.69(13)
C(014)-N(006)-H(102)	122.3(14)
C(021)-N(006)-H(102)	112.6(14)
N(003)-C(007)-C(012)	120.18(12)
N(003)-C(007)-C(008)	111.95(12)
C(012)-C(007)-C(008)	127.84(12)
N(002)-C(008)-C(018)	108.22(12)
N(002)-C(008)-C(007)	125.25(12)
C(018)-C(008)-C(007)	126.33(13)

Table C.2.1. continued…

C(011)-C(009)-C(013)	121.53(14)
C(011)-C(009)-H(009)	119.2
C(013)-C(009)-H(009)	119.2
N(001)-C(010)-C(015)	109.98(12)
N(001)-C(010)-C(012)	124.72(13)
C(015)-C(010)-C(012)	125.28(13)
C(009)-C(011)-C(023)	119.47(13)
C(009)-C(011)-C(016)	120.16(14)
C(023)-C(011)-C(016)	120.37(13)
N(005)-C(012)-C(007)	120.23(12)
N(005)-C(012)-C(010)	113.00(12)
C(007)-C(012)-C(010)	126.72(12)
N(003)-C(013)-C(017)	120.65(13)
N(003)-C(013)-C(009)	120.13(13)
C(017)-C(013)-C(009)	119.21(13)
N(006)-C(014)-C(024)	124.14(14)
N(006)-C(014)-H(014)	117.9
C(024)-C(014)-H(014)	117.9
C(026)-C(015)-C(010)	106.40(13)
C(026)-C(015)-H(015)	126.8
C(010)-C(015)-H(015)	126.8
C(011)-C(016)-H(01A)	109.5
C(011)-C(016)-H(01B)	109.5
H(01A)-C(016)-H(01B)	109.5
C(011)-C(016)-H(01C)	109.5
H(01A)-C(016)-H(01C)	109.5
H(01B)-C(016)-H(01C)	109.5
N(005)-C(017)-C(013)	120.66(13)
N(005)-C(017)-C(029)	120.66(13)
C(013)-C(017)-C(029)	118.68(13)
C(020)-C(018)-C(008)	107.33(13)
C(020)-C(018)-H(018)	126.3
C(008)-C(018)-H(018)	126.3
N(004)-C(019)-C(025)	121.62(14)
N(004)-C(019)-H(019)	119.2
C(025)-C(019)-H(019)	119.2
C(018)-C(020)-C(025)	107.25(13)

Table C.2.1. continued…

C(018)-C(020)-H(020)	126.4
C(025)-C(020)-H(020)	126.4
N(006)-C(021)-C(028)	110.77(13)
N(006)-C(021)-H(02A)	109.5
C(028)-C(021)-H(02A)	109.5
N(006)-C(021)-H(02B)	109.5
C(028)-C(021)-H(02B)	109.5
H(02A)-C(021)-H(02B)	108.1
C(029)-C(023)-C(011)	119.63(13)
C(029)-C(023)-C(030)	120.57(15)
C(011)-C(023)-C(030)	119.80(14)
N(001)-C(024)-C(026)	109.37(13)
N(001)-C(024)-C(014)	121.94(14)
C(026)-C(024)-C(014)	128.48(13)
N(002)-C(025)-C(020)	108.22(12)
N(002)-C(025)-C(019)	121.69(13)
C(020)-C(025)-C(019)	130.02(14)
C(015)-C(026)-C(024)	107.30(13)
C(015)-C(026)-H(026)	126.4
C(024)-C(026)-H(026)	126.4
N(004)-C(027)-C(028)	109.28(13)
N(004)-C(027)-H(02C)	109.8
C(028)-C(027)-H(02C)	109.8
N(004)-C(027)-H(02D)	109.8
C(028)-C(027)-H(02D)	109.8
H(02C)-C(027)-H(02D)	108.3
C(021)-C(028)-C(027)	114.79(14)
C(021)-C(028)-H(02E)	108.6
C(027)-C(028)-H(02E)	108.6
C(021)-C(028)-H(02F)	108.6
C(027)-C(028)-H(02F)	108.6
H(02E)-C(028)-H(02F)	107.5
C(023)-C(029)-C(017)	121.48(14)
C(023)-C(029)-H(029)	119.3
C(017)-C(029)-H(029)	119.3
C(023)-C(030)-H(03A)	109.5
C(023)-C(030)-H(03B)	109.5

Table C.2.1. continued…

H(03A)-C(030)-H(03B)	109.5
C(023)-C(030)-H(03C)	109.5
H(03A)-C(030)-H(03C)	109.5
H(03B)-C(030)-H(03C)	109.5

Table C.2.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L5. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(001)	32(1)	20(1)	17(1)	-1(1)	14(1)	-3(1)
N(002)	22(1)	27(1)	17(1)	3(1)	11(1)	0(1)
N(003)	22(1)	23(1)	17(1)	1(1)	11(1)	0(1)
N(004)	28(1)	30(1)	18(1)	2(1)	6(1)	-2(1)
N(005)	24(1)	20(1)	23(1)	-1(1)	15(1)	-1(1)
N(006)	36(1)	29(1)	18(1)	1(1)	12(1)	-6(1)
C(007)	20(1)	18(1)	18(1)	0(1)	10(1)	-3(1)
C(008)	21(1)	22(1)	17(1)	3(1)	11(1)	-1(1)
C(009)	26(1)	26(1)	19(1)	-1(1)	11(1)	-1(1)
C(010)	29(1)	17(1)	20(1)	-2(1)	15(1)	-2(1)
C(011)	24(1)	21(1)	21(1)	1(1)	6(1)	-4(1)
C(012)	23(1)	18(1)	19(1)	-1(1)	12(1)	-4(1)
C(013)	19(1)	19(1)	20(1)	-1(1)	9(1)	-2(1)
C(014)	43(1)	23(1)	20(1)	-3(1)	20(1)	-7(1)
C(015)	29(1)	29(1)	26(1)	-1(1)	18(1)	-2(1)
C(016)	32(1)	31(1)	23(1)	3(1)	6(1)	0(1)
C(017)	22(1)	18(1)	22(1)	-1(1)	12(1)	-4(1)
C(018)	23(1)	25(1)	16(1)	1(1)	10(1)	-1(1)
C(019)	24(1)	28(1)	27(1)	4(1)	12(1)	0(1)
C(020)	25(1)	26(1)	24(1)	2(1)	16(1)	2(1)
C(021)	38(1)	32(1)	16(1)	1(1)	7(1)	-9(1)
C(023)	20(1)	19(1)	28(1)	1(1)	7(1)	-3(1)
C(024)	39(1)	22(1)	19(1)	-3(1)	19(1)	-5(1)
C(025)	22(1)	26(1)	23(1)	5(1)	12(1)	2(1)
C(026)	41(1)	28(1)	26(1)	-3(1)	25(1)	-4(1)
C(027)	29(1)	36(1)	22(1)	0(1)	4(1)	-2(1)
C(028)	36(1)	30(1)	19(1)	4(1)	3(1)	-3(1)
C(029)	23(1)	21(1)	32(1)	-2(1)	16(1)	-1(1)
C(030)	23(1)	29(1)	37(1)	3(1)	9(1)	0(1)

Table C.2.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L5.

	x	y	z	U(eq)
H(009)	4407	-1270	5272	29
H(014)	2747	-218	-1082	33
H(015)	4370	-900	1532	32
H(01A)	5059	-2204	6577	50
H(01B)	5608	-2090	6724	50
H(01C)	5331	-3918	6548	50
H(018)	3191	1803	3442	26
H(019)	1609	1888	652	32
H(020)	2285	2639	2376	29
H(02A)	1629	-943	-1771	40
H(02B)	1896	691	-1883	40
H(026)	3778	-616	-33	34
H(02C)	1120	1440	-738	41
H(02D)	1176	-491	-979	41
H(02E)	1181	1603	-1902	42
H(02F)	1683	2434	-1114	42
H(029)	5226	-3164	3987	30
H(03A)	5768	-4944	5841	51
H(03B)	6034	-3088	6074	51
H(03C)	5928	-4087	5257	51
H(101)	2823(8)	-150(30)	1277(11)	91(8)
H(102)	2257(8)	-350(30)	-279(10)	80(7)

Table C.2.4: Torsion angles [°] for H_2L5.

C(013)-N(003)-C(007)-C(012)	0.13(19)
C(013)-N(003)-C(007)-C(008)	-178.35(11)
C(025)-N(002)-C(008)-C(018)	0.30(15)
C(025)-N(002)-C(008)-C(007)	175.34(12)
N(003)-C(007)-C(008)-N(002)	-152.96(13)
C(012)-C(007)-C(008)-N(002)	28.7(2)
N(003)-C(007)-C(008)-C(018)	21.19(19)
C(012)-C(007)-C(008)-C(018)	-157.14(14)
C(024)-N(001)-C(010)-C(015)	-1.15(15)
C(024)-N(001)-C(010)-C(012)	179.76(12)
C(013)-C(009)-C(011)-C(023)	0.7(2)
C(013)-C(009)-C(011)-C(016)	-179.80(13)
C(017)-N(005)-C(012)-C(007)	0.29(19)
C(017)-N(005)-C(012)-C(010)	177.66(11)
N(003)-C(007)-C(012)-N(005)	-0.41(19)
C(008)-C(007)-C(012)-N(005)	177.80(12)
N(003)-C(007)-C(012)-C(010)	-177.39(12)
C(008)-C(007)-C(012)-C(010)	0.8(2)
N(001)-C(010)-C(012)-N(005)	155.09(13)
C(015)-C(010)-C(012)-N(005)	-23.85(19)
N(001)-C(010)-C(012)-C(007)	-27.7(2)
C(015)-C(010)-C(012)-C(007)	153.31(14)
C(007)-N(003)-C(013)-C(017)	0.24(19)
C(007)-N(003)-C(013)-C(009)	-178.48(12)
C(011)-C(009)-C(013)-N(003)	178.74(13)
C(011)-C(009)-C(013)-C(017)	0.0(2)
C(021)-N(006)-C(014)-C(024)	175.43(14)
N(001)-C(010)-C(015)-C(026)	0.68(16)
C(012)-C(010)-C(015)-C(026)	179.76(13)
C(012)-N(005)-C(017)-C(013)	0.07(19)
C(012)-N(005)-C(017)-C(029)	179.01(12)
N(003)-C(013)-C(017)-N(005)	-0.4(2)
C(009)-C(013)-C(017)-N(005)	178.38(12)
N(003)-C(013)-C(017)-C(029)	-179.31(12)
C(009)-C(013)-C(017)-C(029)	-0.6(2)
N(002)-C(008)-C(018)-C(020)	-0.64(15)

Table C.2.4. continued…

C(007)-C(008)-C(018)-C(020)	-175.62(13)
C(027)-N(004)-C(019)-C(025)	-173.81(13)
C(008)-C(018)-C(020)-C(025)	0.74(16)
C(014)-N(006)-C(021)-C(028)	-138.36(15)
C(009)-C(011)-C(023)-C(029)	-0.7(2)
C(016)-C(011)-C(023)-C(029)	179.74(13)
C(009)-C(011)-C(023)-C(030)	179.46(13)
C(016)-C(011)-C(023)-C(030)	-0.1(2)
C(010)-N(001)-C(024)-C(026)	1.20(15)
C(010)-N(001)-C(024)-C(014)	-174.04(13)
N(006)-C(014)-C(024)-N(001)	-2.8(2)
N(006)-C(014)-C(024)-C(026)	-177.01(15)
C(008)-N(002)-C(025)-C(020)	0.17(16)
C(008)-N(002)-C(025)-C(019)	177.55(12)
C(018)-C(020)-C(025)-N(002)	-0.57(16)
C(018)-C(020)-C(025)-C(019)	-177.66(14)
N(004)-C(019)-C(025)-N(002)	2.3(2)
N(004)-C(019)-C(025)-C(020)	179.06(15)
C(010)-C(015)-C(026)-C(024)	0.07(16)
N(001)-C(024)-C(026)-C(015)	-0.78(17)
C(014)-C(024)-C(026)-C(015)	174.05(14)
C(019)-N(004)-C(027)-C(028)	119.06(16)
N(006)-C(021)-C(028)-C(027)	-58.89(18)
N(004)-C(027)-C(028)-C(021)	64.20(17)
C(011)-C(023)-C(029)-C(017)	0.1(2)
C(030)-C(023)-C(029)-C(017)	179.95(13)
N(005)-C(017)-C(029)-C(023)	-178.44(13)
C(013)-C(017)-C(029)-C(023)	0.5(2)

C.3: Full crystallographic Data Tables of H_2L6

Table C.3.1: Bond lengths [Å] and angles [°] for H_2L6.

N(5)-C(007)	1.331(3)
N(5)-C(014)	1.358(3)
N(4)-C(013)	1.350(3)
N(4)-C(016)	1.376(3)
N(1)-C(009)	1.353(3)
N(1)-C(017)	1.372(3)
N(1)-H(101)	0.934(19)
N(6)-C(010)	1.332(3)
N(6)-C(011)	1.358(3)
N(3)-C(022)	1.284(3)
N(3)-C(029)	1.461(3)
N(3)-H(102)	0.90(2)
C(007)-C(010)	1.456(3)
C(007)-C(013)	1.468(3)
N(2)-C(019)	1.294(3)
N(2)-C(028)	1.458(3)
C(009)-C(012)	1.417(3)
C(009)-C(010)	1.465(3)
C(011)-C(014)	1.406(3)
C(011)-C(015)	1.415(3)
C(012)-C(020)	1.379(3)
C(012)-H(012)	0.9500
C(013)-C(024)	1.410(3)
C(014)-C(018)	1.413(3)
C(015)-C(021)	1.368(3)
C(015)-H(015)	0.9500
C(016)-C(025)	1.395(3)
C(016)-C(022)	1.410(3)
C(017)-C(020)	1.399(3)
C(017)-C(019)	1.409(3)
C(018)-C(023)	1.366(3)
C(018)-H(018)	0.9500
C(019)-H(019)	0.9500
C(020)-H(020)	0.9500

Table C.3.1. continued…

C(021)-C(023)	1.422(4)
C(021)-C(030)	1.450(6)
C(022)-H(022)	0.9500
C(023)-C(026)	1.412(5)
C(024)-C(025)	1.374(4)
C(024)-H(024)	0.9500
C(025)-H(025)	0.9500
C(026)-H(26C)	0.9800
C(026)-H(26B)	0.9800
C(026)-H(26A)	0.9800
C(027)-C(029)	1.515(4)
C(027)-C(028)	1.532(4)
C(027)-H(02A)	0.9900
C(027)-H(02B)	0.9900
C(028)-H(02C)	0.9900
C(028)-H(02D)	0.9900
C(029)-H(02E)	0.9900
C(029)-H(02F)	0.9900
C(030)-H(03A)	0.9800
C(030)-H(03B)	0.9800
C(030)-H(03C)	0.9800
O(1W)-H(1W)	1.000(10)
C(007)-N(5)-C(014)	119.00(19)
C(013)-N(4)-C(016)	108.03(18)
C(009)-N(1)-C(017)	107.90(18)
C(009)-N(1)-H(101)	114(3)
C(017)-N(1)-H(101)	137(3)
C(010)-N(6)-C(011)	119.20(18)
C(022)-N(3)-C(029)	123.5(2)
C(022)-N(3)-H(102)	136(4)
C(029)-N(3)-H(102)	96(4)
N(5)-C(007)-C(010)	120.58(19)
N(5)-C(007)-C(013)	112.46(18)
C(010)-C(007)-C(013)	126.92(19)
C(019)-N(2)-C(028)	122.7(2)
N(1)-C(009)-C(012)	109.02(18)

Table C.3.1. continued…

N(1)-C(009)-C(010)	124.65(18)
C(012)-C(009)-C(010)	126.3(2)
N(6)-C(010)-C(007)	119.75(19)
N(6)-C(010)-C(009)	113.24(18)
C(007)-C(010)-C(009)	126.97(19)
N(6)-C(011)-C(014)	120.9(2)
N(6)-C(011)-C(015)	120.1(2)
C(014)-C(011)-C(015)	118.9(2)
C(020)-C(012)-C(009)	106.8(2)
C(020)-C(012)-H(012)	126.6
C(009)-C(012)-H(012)	126.6
N(4)-C(013)-C(024)	108.8(2)
N(4)-C(013)-C(007)	125.26(19)
C(024)-C(013)-C(007)	125.8(2)
N(5)-C(014)-C(011)	120.5(2)
N(5)-C(014)-C(018)	119.5(2)
C(011)-C(014)-C(018)	120.0(2)
C(021)-C(015)-C(011)	120.3(2)
C(021)-C(015)-H(015)	119.8
C(011)-C(015)-H(015)	119.8
N(4)-C(016)-C(025)	108.7(2)
N(4)-C(016)-C(022)	121.3(2)
C(025)-C(016)-C(022)	130.0(2)
N(1)-C(017)-C(020)	109.0(2)
N(1)-C(017)-C(019)	121.8(2)
C(020)-C(017)-C(019)	129.0(2)
C(023)-C(018)-C(014)	120.3(2)
C(023)-C(018)-H(018)	119.8 C(014)-C(018)-H(018)
N(2)-C(019)-C(017)	123.4(2)
N(2)-C(019)-H(019)	118.3
C(017)-C(019)-H(019)	118.3
C(012)-C(020)-C(017)	107.22(19)
C(012)-C(020)-H(020)	126.4
C(017)-C(020)-H(020)	126.4
C(015)-C(021)-C(023)	120.6(2)
C(015)-C(021)-C(030)	128.0(3)
C(023)-C(021)-C(030)	111.4(3)

Table C.3.1. continued…

N(3)-C(022)-C(016)	122.1(2)
N(3)-C(022)-H(022)	119.0
C(016)-C(022)-H(022)	119.0
C(018)-C(023)-C(026)	126.6(3)
C(018)-C(023)-C(021)	119.8(2)
C(026)-C(023)-C(021)	113.6(3)
C(025)-C(024)-C(013)	107.2(2)
C(025)-C(024)-H(024)	126.4
C(013)-C(024)-H(024)	126.4
C(024)-C(025)-C(016)	107.3(2)
C(024)-C(025)-H(025)	126.3
C(016)-C(025)-H(025)	126.3
C(023)-C(026)-H(26C)	109.5
C(023)-C(026)-H(26B)	109.5
H(26C)-C(026)-H(26B)	109.5
C(023)-C(026)-H(26A)	109.5
H(26C)-C(026)-H(26A)	109.5
H(26B)-C(026)-H(26A)	109.5
C(029)-C(027)-C(028)	114.1(2)
C(029)-C(027)-H(02A)	108.7
C(028)-C(027)-H(02A)	108.7
C(029)-C(027)-H(02B)	108.7
C(028)-C(027)-H(02B)	108.7
H(02A)-C(027)-H(02B)	107.6
N(2)-C(028)-C(027)	110.4(2)
N(2)-C(028)-H(02C)	109.6
C(027)-C(028)-H(02C)	109.6
N(2)-C(028)-H(02D)	109.6
C(027)-C(028)-H(02D)	109.6
H(02C)-C(028)-H(02D)	108.1
N(3)-C(029)-C(027)	110.3(2)
N(3)-C(029)-H(02E)	109.6
C(027)-C(029)-H(02E)	109.6
N(3)-C(029)-H(02F)	109.6
C(027)-C(029)-H(02F)	109.6
H(02E)-C(029)-H(02F)	108.1
C(021)-C(030)-H(03A)	109.5

Table C.3.1. continued…

C(021)-C(030)-H(03B)	109.5
H(03A)-C(030)-H(03B)	109.5
C(021)-C(030)-H(03C)	109.5
H(03A)-C(030)-H(03C)	109.5
H(03B)-C(030)-H(03C)	109.5

Table C.3.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L6. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(5)	43(1)	38(1)	36(1)	0(1)	27(1)	5(1)
N(4)	34(1)	33(1)	41(1)	-6(1)	28(1)	-2(1)
N(1)	37(1)	28(1)	37(1)	4(1)	27(1)	3(1)
N(6)	35(1)	32(1)	42(1)	0(1)	25(1)	5(1)
N(3)	37(1)	41(1)	63(2)	-6(1)	24(1)	-2(1)
C(007)	36(1)	27(1)	35(1)	2(1)	25(1)	8(1)
N(2)	42(1)	31(1)	45(1)	2(1)	20(1)	6(1)
C(009)	38(1)	27(1)	37(1)	4(1)	28(1)	4(1)
C(010)	32(1)	27(1)	38(1)	2(1)	25(1)	7(1)
C(011)	34(1)	30(1)	40(1)	1(1)	20(1)	9(1)
C(012)	40(1)	42(1)	46(1)	-1(1)	33(1)	1(1)
C(013)	42(1)	30(1)	40(1)	-3(1)	32(1)	2(1)
C(014)	37(1)	35(1)	38(1)	0(1)	20(1)	9(1)
C(015)	36(1)	36(1)	54(2)	-2(1)	23(1)	6(1)
C(016)	47(1)	36(1)	57(2)	-12(1)	41(1)	-9(1)
C(017)	46(1)	29(1)	35(1)	5(1)	30(1)	2(1)
C(018)	50(2)	45(1)	38(1)	0(1)	22(1)	10(1)
C(019)	52(2)	31(1)	36(1)	4(1)	27(1)	4(1)
C(020)	51(2)	45(1)	44(1)	1(1)	38(1)	-2(1)
C(021)	37(1)	35(1)	53(2)	-1(1)	14(1)	12(1)
C(022)	44(2)	38(1)	72(2)	-12(1)	41(2)	-11(1)
C(023)	49(2)	39(1)	42(1)	-1(1)	17(1)	15(1)
C(024)	70(2)	41(1)	45(2)	-6(1)	43(1)	-15(1)
C(025)	78(2)	46(1)	64(2)	-12(1)	59(2)	-22(1)
C(026)	54(3)	44(3)	24(2)	1(2)	17(2)	17(2)
C(027)	47(2)	39(1)	60(2)	-9(1)	15(1)	-4(1)
C(028)	47(2)	37(1)	48(2)	-4(1)	14(1)	7(1)
C(029)	37(2)	51(2)	73(2)	-6(1)	22(2)	-5(1)
C(030)	49(3)	49(3)	63(3)	11(3)	33(3)	9(2)
O(1W)	72(2)	61(2)	87(2)	0	55(2)	0

Table C.3.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L6.

	x	y	z	U(eq)
H(012)	4474	732	6690	46
H(015)	5366	3273	9159	52
H(018)	4529	1547	10446	55
H(019)	2768	83	3993	46
H(020)	3848	377	5093	49
H(022)	1639	-1818	5739	57
H(024)	3280	-1674	8586	56
H(025)	2346	-2532	7490	63
H(26C)	5296	2571	11794	66
H(26B)	5481	4353	11621	66
H(26A)	5824	2635	11839	66
H(02A)	1151	-1535	3136	69
H(02B)	1670	-2388	3950	69
H(02C)	1897	-703	3179	62
H(02D)	1630	973	3270	62
H(02E)	1183	638	4060	71
H(02F)	1102	-1269	4295	71
H(03A)	6129	3375	11405	80
H(03B)	5856	5214	11019	80
H(03C)	6119	4200	10627	80
H(1W)	4779(18)	3360(60)	7580(40)	220(30)
H(101)	3050(14)	680(60)	6190(30)	158(19)
H(102)	2029(19)	110(80)	4990(30)	210(30)

Table C.3.4: Torsion angles [°] for H_2L6.

C(014)-N(5)-C(007)-C(010)	0.0(3)
C(014)-N(5)-C(007)-C(013)	178.01(18)
C(017)-N(1)-C(009)-C(012)	0.8(2)
C(017)-N(1)-C(009)-C(010)	179.12(18)
C(011)-N(6)-C(010)-C(007)	0.0(3)
C(011)-N(6)-C(010)-C(009)	-177.70(17)
N(5)-C(007)-C(010)-N(6)	-0.1(3)
C(013)-C(007)-C(010)-N(6)	-177.79(18)
N(5)-C(007)-C(010)-C(009)	177.30(18)
C(013)-C(007)-C(010)-C(009)	-0.4(3)
N(1)-C(009)-C(010)-N(6)	-153.11(19)
C(012)-C(009)-C(010)-N(6)	24.9(3)
N(1)-C(009)-C(010)-C(007)	29.3(3)
C(012)-C(009)-C(010)-C(007)	-152.7(2)
C(010)-N(6)-C(011)-C(014)	0.1(3)
C(010)-N(6)-C(011)-C(015)	-178.88(18)
N(1)-C(009)-C(012)-C(020)	-0.8(2)
C(010)-C(009)-C(012)-C(020)	-179.01(19)
C(016)-N(4)-C(013)-C(024)	-0.7(2)
C(016)-N(4)-C(013)-C(007)	-175.91(19)
N(5)-C(007)-C(013)-N(4)	151.23(19)
C(010)-C(007)-C(013)-N(4)	-30.9(3)
N(5)-C(007)-C(013)-C(024)	-23.2(3)
C(010)-C(007)-C(013)-C(024)	154.6(2)
C(007)-N(5)-C(014)-C(011)	0.1(3)
C(007)-N(5)-C(014)-C(018)	178.94(19)
N(6)-C(011)-C(014)-N(5)	-0.2(3)
C(015)-C(011)-C(014)-N(5)	178.79(19)
N(6)-C(011)-C(014)-C(018)	-178.99(19)
C(015)-C(011)-C(014)-C(018)	0.0(3)
N(6)-C(011)-C(015)-C(021)	178.74(19)
C(014)-C(011)-C(015)-C(021)	-0.3(3)
C(013)-N(4)-C(016)-C(025)	0.4(2)
C(013)-N(4)-C(016)-C(022)	-178.82(19)
C(009)-N(1)-C(017)-C(020)	-0.6(2)
C(009)-N(1)-C(017)-C(019)	174.34(18)

Table C.3.4. continued…

N(5)-C(014)-C(018)-C(023)	-178.5(2)
C(011)-C(014)-C(018)-C(023)	0.3(3)
C(028)-N(2)-C(019)-C(017)	-175.4(2)
N(1)-C(017)-C(019)-N(2)	3.3(3)
C(020)-C(017)-C(019)-N(2)	177.1(2)
C(009)-C(012)-C(020)-C(017)	0.4(2)
N(1)-C(017)-C(020)-C(012)	0.1(2)
C(019)-C(017)-C(020)-C(012)	-174.3(2)
C(011)-C(015)-C(021)-C(023)	0.2(3)
C(011)-C(015)-C(021)-C(030)	-177.8(3)
C(029)-N(3)-C(022)-C(016)	173.5(2)
N(4)-C(016)-C(022)-N(3)	-2.0(3)
C(025)-C(016)-C(022)-N(3)	178.9(2)
C(014)-C(018)-C(023)-C(026)	179.3(3)
C(014)-C(018)-C(023)-C(021)	-0.4(3)
C(015)-C(021)-C(023)-C(018)	0.1(3)
C(030)-C(021)-C(023)-C(018)	178.4(3)
C(015)-C(021)-C(023)-C(026)	-179.6(3)
C(030)-C(021)-C(023)-C(026)	-1.2(4)
N(4)-C(013)-C(024)-C(025)	0.7(3)
C(007)-C(013)-C(024)-C(025)	175.9(2)
C(013)-C(024)-C(025)-C(016)	-0.4(3)
N(4)-C(016)-C(025)-C(024)	0.0(3)
C(022)-C(016)-C(025)-C(024)	179.2(2)
C(019)-N(2)-C(028)-C(027)	137.0(2)
C(029)-C(027)-C(028)-N(2)	58.3(3)
C(022)-N(3)-C(029)-C(027)	-115.7(3)
C(028)-C(027)-C(029)-N(3)	-65.5(3)

C.4: Full crystallographic Data Tables of H_2L7

Table C.4.1: Bond lengths [Å] and angles [°] for H_2L7

N(4)-C(008)	1.349(3)
N(4)-C(023)	1.377(3)
F(2)-C(015)	1.323(3)
N(1)-C(012)	1.361(3)
N(1)-C(014)	1.362(3)
N(1)-H(101)	0.893(10)
N(2)-C(022)	1.280(3)
N(2)-C(027)	1.467(3)
N(5)-C(009)	1.336(2)
N(5)-C(017)	1.358(3)
N(6)-C(011)	1.329(3)
N(6)-C(016)	1.360(2)
N(3)-C(024)	1.298(3)
N(3)-C(028)	1.471(3)
N(3)-H(102)	0.882(10)
C(008)-C(026)	1.424(3)
C(008)-C(009)	1.479(3)
C(009)-C(011)	1.464(3)
C(010)-C(020)	1.390(3)
C(010)-C(012)	1.395(3)
C(010)-H(010)	0.9500
C(011)-C(014)	1.469(3)
C(012)-C(022)	1.430(3)
C(013)-F(1)	1.298(5)
C(013)-C(019)	1.369(3)
C(013)-C(015)	1.403(3)
C(014)-C(020)	1.397(3)
C(015)-C(018)	1.352(3)
C(016)-C(017)	1.410(3)
C(016)-C(018)	1.414(3)
C(017)-C(019)	1.420(3)
C(018)-H(018)	0.9500
C(019)-H(019)	0.9500
C(020)-H(020)	0.9500

Table C.4.1. continued…

C(021)-C(028)	1.519(3)
C(021)-C(027)	1.524(3)
C(021)-H(02A)	0.9900
C(021)-H(02B)	0.9900
C(022)-H(022)	0.9500
C(023)-C(024)	1.397(3)
C(023)-C(025)	1.414(3)
C(024)-H(024)	0.9500
C(025)-C(026)	1.363(3)
C(025)-H(025)	0.9500
C(026)-H(026)	0.9500
C(027)-H(02C)	0.9900
C(027)-H(02D)	0.9900
C(028)-H(02E)	0.9900
C(028)-H(02F)	0.9900
C(008)-N(4)-C(023)	105.67(16)
C(012)-N(1)-C(014)	108.87(17)
C(012)-N(1)-H(101)	134.0(18)
C(014)-N(1)-H(101)	116.2(17)
C(022)-N(2)-C(027)	120.98(18)
C(009)-N(5)-C(017)	119.02(17)
C(011)-N(6)-C(016)	118.80(17)
C(024)-N(3)-C(028)	126.2(2)
C(024)-N(3)-H(102)	121(2)
C(028)-N(3)-H(102)	112(2)
N(4)-C(008)-C(026)	110.64(19)
N(4)-C(008)-C(009)	125.17(17)
C(026)-C(008)-C(009)	124.17(19)
N(5)-C(009)-C(011)	120.16(18)
N(5)-C(009)-C(008)	110.93(16)
C(011)-C(009)-C(008)	128.90(18)
C(020)-C(010)-C(012)	106.36(17)
C(020)-C(010)-H(010)	126.8
C(012)-C(010)-H(010)	126.8
N(6)-C(011)-C(009)	120.14(18)
N(6)-C(011)-C(014)	110.89(17)

Table C.4.1. continued…

C(009)-C(011)-C(014)	128.92(18)
N(1)-C(012)-C(010)	108.95(19)
N(1)-C(012)-C(022)	121.58(19)
C(010)-C(012)-C(022)	129.45(18)
F(1)-C(013)-C(019)	129.2(3)
F(1)-C(013)-C(015)	111.5(3)
C(019)-C(013)-C(015)	118.8(2)
N(1)-C(014)-C(020)	107.79(18)
N(1)-C(014)-C(011)	126.02(18)
C(020)-C(014)-C(011)	126.18(19)
F(2)-C(015)-C(018)	119.7(2)
F(2)-C(015)-C(013)	115.38(19)
C(018)-C(015)-C(013)	124.9(2)
N(6)-C(016)-C(017)	121.17(19)
N(6)-C(016)-C(018)	118.77(18)
C(017)-C(016)-C(018)	120.02(18)
N(5)-C(017)-C(016)	120.45(18)
N(5)-C(017)-C(019)	119.10(17)
C(016)-C(017)-C(019)	120.45(19)
C(015)-C(018)-C(016)	116.90(19)
C(015)-C(018)-H(018)	121.5
C(016)-C(018)-H(018)	121.5
C(013)-C(019)-C(017)	118.90(19)
C(013)-C(019)-H(019)	120.5
C(017)-C(019)-H(019)	120.5
C(010)-C(020)-C(014)	108.03(19)
C(010)-C(020)-H(020)	126.0
C(014)-C(020)-H(020)	126.0
C(028)-C(021)-C(027)	114.4(2)
C(028)-C(021)-H(02A)	108.6
C(027)-C(021)-H(02A)	108.6
C(028)-C(021)-H(02B)	108.6
C(027)-C(021)-H(02B)	108.6
H(02A)-C(021)-H(02B)	107.6
N(2)-C(022)-C(012)	120.67(19)
N(2)-C(022)-H(022)	119.7
C(012)-C(022)-H(022)	119.7

Table C.4.1. continued…

N(4)-C(023)-C(024)	120.89(18)
N(4)-C(023)-C(025)	110.53(19)
C(024)-C(023)-C(025)	128.55(19)
N(3)-C(024)-C(023)	124.0(2)
N(3)-C(024)-H(024)	118.0
C(023)-C(024)-H(024)	118.0
C(026)-C(025)-C(023)	106.36(18)
C(026)-C(025)-H(025)	126.8
C(023)-C(025)-H(025)	126.8
C(025)-C(026)-C(008)	106.78(19)
C(025)-C(026)-H(026)	126.6
C(008)-C(026)-H(026)	126.6
N(2)-C(027)-C(021)	109.50(18)
N(2)-C(027)-H(02C)	109.8
C(021)-C(027)-H(02C)	109.8
N(2)-C(027)-H(02D)	109.8
C(021)-C(027)-H(02D)	109.8
H(02C)-C(027)-H(02D)	108.2
N(3)-C(028)-C(021)	110.65(19)
N(3)-C(028)-H(02E)	109.5
C(021)-C(028)-H(02E)	109.5
N(3)-C(028)-H(02F)	109.5
C(021)-C(028)-H(02F)	109.5
H(02E)-C(028)-H(02F)	108.1

Table C.4.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L7. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(4)	18(1)	28(1)	36(1)	-2(1)	-3(1)	0(1)
F(2)	27(1)	45(1)	44(1)	7(1)	-16(1)	-1(1)
N(1)	20(1)	28(1)	33(1)	3(1)	-2(1)	1(1)
N(2)	27(1)	38(1)	38(1)	5(1)	-11(1)	5(1)
N(5)	23(1)	25(1)	33(1)	-1(1)	0(1)	-1(1)
N(6)	21(1)	30(1)	32(1)	-1(1)	-1(1)	2(1)
N(3)	26(1)	43(1)	41(1)	0(1)	-10(1)	0(1)
C(008)	20(1)	25(1)	35(1)	0(1)	0(1)	-1(1)
C(009)	21(1)	22(1)	33(1)	-5(1)	-1(1)	0(1)
C(010)	24(1)	33(1)	37(1)	4(1)	3(1)	-4(1)
C(011)	18(1)	26(1)	30(1)	-4(1)	-1(1)	2(1)
C(012)	22(1)	29(1)	35(1)	2(1)	-1(1)	1(1)
C(013)	36(1)	30(1)	39(1)	0(1)	-7(1)	5(1)
C(014)	19(1)	27(1)	32(1)	-3(1)	-4(1)	1(1)
C(015)	32(1)	30(1)	42(1)	1(1)	-11(1)	5(1)
C(016)	24(1)	24(1)	31(1)	-1(1)	-3(1)	2(1)
C(017)	22(1)	25(1)	32(1)	-2(1)	-1(1)	3(1)
C(018)	24(1)	31(1)	35(1)	0(1)	-3(1)	2(1)
C(019)	32(1)	30(1)	39(1)	4(1)	3(1)	-1(1)
C(020)	19(1)	36(1)	37(1)	2(1)	-2(1)	-3(1)
C(021)	36(1)	46(2)	49(1)	4(1)	-18(1)	5(1)
C(022)	31(1)	28(1)	36(1)	5(1)	-2(1)	1(1)
C(023)	18(1)	27(1)	45(1)	-4(1)	-3(1)	-2(1)
C(024)	20(1)	32(1)	51(1)	-8(1)	-8(1)	-2(1)
C(025)	19(1)	35(1)	50(1)	0(1)	1(1)	-4(1)
C(026)	24(1)	34(1)	42(1)	3(1)	2(1)	-1(1)
C(027)	39(1)	43(1)	42(1)	8(1)	-14(1)	-1(1)
C(028)	30(1)	53(2)	43(1)	-2(1)	-16(1)	2(1)
F(1)	36(3)	35(3)	27(3)	20(3)	4(3)	2(3)

Table C.4.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L7.

	x	y	z	U(eq)
H(010)	2059	-1215	7865	38
H(018)	681	1253	4449	36
H(019)	5066	2490	3336	40
H(020)	1686	-412	6501	37
H(02A)	8773	-789	9709	52
H(02B)	8280	-1330	8883	52
H(022)	4346	-995	8924	38
H(024)	10167	1069	7433	41
H(025)	10088	1771	5890	42
H(026)	8085	1990	4936	40
H(02C)	6286	-885	9688	49
H(02D)	6742	563	9716	49
H(02E)	9194	1196	9142	50
H(02F)	10127	139	8720	50
H(101)	5503(15)	680(30)	7135(15)	69(9)
H(102)	7558(12)	650(30)	8058(18)	89(11)

Table C.4.4: Torsion angles [°] for H_2L7.

C(023)-N(4)-C(008)-C(026)	-1.3(2)
C(023)-N(4)-C(008)-C(009)	176.90(19)
C(017)-N(5)-C(009)-C(011)	-1.2(3)
C(017)-N(5)-C(009)-C(008)	177.43(17)
N(4)-C(008)-C(009)-N(5)	173.63(18)
C(026)-C(008)-C(009)-N(5)	-8.4(3)
N(4)-C(008)-C(009)-C(011)	-7.8(3)
C(026)-C(008)-C(009)-C(011)	170.2(2)
C(016)-N(6)-C(011)-C(009)	4.9(3)
C(016)-N(6)-C(011)-C(014)	-172.64(17)
N(5)-C(009)-C(011)-N(6)	-3.5(3)
C(008)-C(009)-C(011)-N(6)	178.13(19)
N(5)-C(009)-C(011)-C(014)	173.65(19)
C(008)-C(009)-C(011)-C(014)	-4.8(3)
C(014)-N(1)-C(012)-C(010)	0.2(2)
C(014)-N(1)-C(012)-C(022)	179.12(18)
C(020)-C(010)-C(012)-N(1)	-0.4(2)
C(020)-C(010)-C(012)-C(022)	-179.3(2)
C(012)-N(1)-C(014)-C(020)	0.1(2)
C(012)-N(1)-C(014)-C(011)	-178.61(18)
N(6)-C(011)-C(014)-N(1)	-167.19(19)
C(009)-C(011)-C(014)-N(1)	15.5(3)
N(6)-C(011)-C(014)-C(020)	14.3(3)
C(009)-C(011)-C(014)-C(020)	-163.0(2)
F(1)-C(013)-C(015)-F(2)	-4.9(4)
C(019)-C(013)-C(015)-F(2)	-178.5(2)
F(1)-C(013)-C(015)-C(018)	173.5(3)
C(019)-C(013)-C(015)-C(018)	-0.1(4)
C(011)-N(6)-C(016)-C(017)	-2.0(3)
C(011)-N(6)-C(016)-C(018)	175.85(19)
C(009)-N(5)-C(017)-C(016)	4.2(3)
C(009)-N(5)-C(017)-C(019)	-175.76(18)
N(6)-C(016)-C(017)-N(5)	-2.7(3)
C(018)-C(016)-C(017)-N(5)	179.46(19)
N(6)-C(016)-C(017)-C(019)	177.26(19)
C(018)-C(016)-C(017)-C(019)	-0.6(3)

Table C.4.4. continued…

F(2)-C(015)-C(018)-C(016)	176.9(2)
C(013)-C(015)-C(018)-C(016)	-1.4(3)
N(6)-C(016)-C(018)-C(015)	-176.23(19)
C(017)-C(016)-C(018)-C(015)	1.7(3)
F(1)-C(013)-C(019)-C(017)	-171.0(4)
C(015)-C(013)-C(019)-C(017)	1.3(3)
N(5)-C(017)-C(019)-C(013)	179.0(2)
C(016)-C(017)-C(019)-C(013)	-0.9(3)
C(012)-C(010)-C(020)-C(014)	0.5(2)
N(1)-C(014)-C(020)-C(010)	-0.4(2)
C(011)-C(014)-C(020)-C(010)	178.34(19)
C(027)-N(2)-C(022)-C(012)	-178.47(19)
N(1)-C(012)-C(022)-N(2)	3.3(3)
C(010)-C(012)-C(022)-N(2)	-178.0(2)
C(008)-N(4)-C(023)-C(024)	-176.90(19)
C(008)-N(4)-C(023)-C(025)	1.0(2)
C(028)-N(3)-C(024)-C(023)	178.0(2)
N(4)-C(023)-C(024)-N(3)	-3.7(3)
C(025)-C(023)-C(024)-N(3)	178.8(2)
N(4)-C(023)-C(025)-C(026)	-0.3(2)
C(024)-C(023)-C(025)-C(026)	177.4(2)
C(023)-C(025)-C(026)-C(008)	-0.5(2)
N(4)-C(008)-C(026)-C(025)	1.2(2)
C(009)-C(008)-C(026)-C(025)	-177.1(2)
C(022)-N(2)-C(027)-C(021)	131.0(2)
C(028)-C(021)-C(027)-N(2)	63.2(3)
C(024)-N(3)-C(028)-C(021)	-142.8(2)
C(027)-C(021)-C(028)-N(3)	-60.2(3)

C.5: Full crystallographic Data Tables of H_2L8a

Table C.5.1: Bond lengths [Å] and angles [°] for H_2L8a

N(1)-C(1)	1.293(5)
N(1)-C(2')	1.457(6)
N(2)-C(3)	1.355(5)
N(2)-C(2)	1.364(5)
N(2)-H(103)	0.873(11)
N(3)-C(6)	1.355(5)
N(3)-C(7)	1.370(5)
N(4)-C(8)	1.285(5)
N(4)-C(9)	1.462(5)
N(4)-H(104)	0.873(11)
N(5)-C(13)	1.334(5)
N(5)-C(4)	1.337(5)
N(6)-C(15)	1.323(5)
N(6)-C(5)	1.354(5)
N(7)-C(21)	1.295(5)
N(7)-C(20)	1.463(5)
N(8)-C(23)	1.340(5)
N(8)-C(22)	1.372(5)
N(8)-H(102)	0.874(11)
N(9)-C(26)	1.320(5)
N(9)-C(25)	1.346(5)
N(10)-C(31)	1.328(5)
N(10)-C(24)	1.352(5)
N(15)-C(33)	1.363(5)
N(15)-C(32)	1.366(5)
N(16)-C(34)	1.276(5)
N(16)-C(35)	1.469(5)
N(16)-H(101)	0.870(12)
C(1)-C(2)	1.410(6)
C(1)-H(1)	0.9300
C(2)-C(12)	1.403(5)
C(3)-C(11)	1.420(5)
C(3)-C(4)	1.464(5)
C(4)-C(5)	1.456(5)

Table C.5.1. continued…

C(5)-C(6)	1.459(5)
C(6)-C(17)	1.416(5)
C(7)-C(16)	1.400(6)
C(7)-C(8)	1.419(6)
C(8)-H(8)	0.9300
C(9)-C(10)	1.481(7)
C(9)-H(6)	0.9700
C(9)-H(7)	0.9700
C(10)-C(2')	1.474(7)
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(11)-C(12)	1.383(5)
C(11)-H(2)	0.9300
C(12)-H(3)	0.9300
C(13)-C(15)	1.390(5)
C(13)-C(14)	1.444(6)
C(14)-N(13)	1.141(5)
C(15)-C(18)	1.450(6)
C(16)-C(17)	1.370(6)
C(16)-H(5)	0.9300
C(17)-H(4)	0.9300
C(18)-N(14)	1.139(5)
C(20)-C(1')	1.521(6)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(21)-C(22)	1.413(5)
C(21)-H(14)	0.9300
C(22)-C(37)	1.414(5)
C(23)-C(36)	1.437(5)
C(23)-C(24)	1.458(5)
C(24)-C(25)	1.461(5)
C(25)-C(32)	1.445(5)
C(26)-C(31)	1.392(5)
C(26)-C(27)	1.459(6)
C(27)-N(12)	1.140(5)
N(11)-C(30)	1.148(5)
C(30)-C(31)	1.448(6)

Table C.5.1. continued…

C(32)-C(39)	1.397(5)
C(33)-C(38)	1.386(6)
C(33)-C(34)	1.433(6)
C(34)-H(15)	0.9300
C(35)-C(1')	1.519(6)
C(35)-H(35A)	0.9700
C(35)-H(35B)	0.9700
C(35)-H(101)	1.5(3)
C(36)-C(37)	1.368(5)
C(36)-H(13)	0.9300
C(37)-H(12)	0.9300
C(38)-C(39)	1.385(6)
C(38)-H(17)	0.9300
C(39)-H(16)	0.9300
C(1')-H(1'1)	0.9700
C(1')-H(1'2)	0.9700
C(2')-H(2'1)	0.9700
C(2')-H(2'2)	0.9700
C(1)-N(1)-C(2')	123.9(4)
C(3)-N(2)-C(2)	108.0(3)
C(3)-N(2)-H(103)	113(6)
C(2)-N(2)-H(103)	139(6)
C(6)-N(3)-C(7)	107.2(3)
C(8)-N(4)-C(9)	124.2(4)
C(8)-N(4)-H(104)	127(8)
C(9)-N(4)-H(104)	108(8)
C(13)-N(5)-C(4)	119.2(3)
C(15)-N(6)-C(5)	119.2(3)
C(21)-N(7)-C(20)	126.6(3)
C(23)-N(8)-C(22)	106.3(3)
C(23)-N(8)-H(102)	115(10)
C(22)-N(8)-H(102)	138(10)
C(26)-N(9)-C(25)	119.0(3)
C(31)-N(10)-C(24)	119.7(3)
C(33)-N(15)-C(32)	109.0(3)
C(34)-N(16)-C(35)	120.7(3)

Table C.5.1. continued…

C(34)-N(16)-H(101)	158(10)
C(35)-N(16)-H(101)	77(10)
N(1)-C(1)-C(2)	122.1(4)
N(1)-C(1)-H(1)	118.9
C(2)-C(1)-H(1)	118.9
N(2)-C(2)-C(12)	109.4(4)
N(2)-C(2)-C(1)	121.6(3)
C(12)-C(2)-C(1)	129.0(4)
N(2)-C(3)-C(11)	108.9(3)
N(2)-C(3)-C(4)	126.1(3)
C(11)-C(3)-C(4)	124.9(3)
N(5)-C(4)-C(5)	120.0(3)
N(5)-C(4)-C(3)	111.2(3)
C(5)-C(4)-C(3)	128.8(3)
N(6)-C(5)-C(4)	118.7(3)
N(6)-C(5)-C(6)	111.0(3)
C(4)-C(5)-C(6)	130.2(3)
N(3)-C(6)-C(17)	109.4(3)
N(3)-C(6)-C(5)	125.3(3)
C(17)-C(6)-C(5)	125.2(4)
N(3)-C(7)-C(16)	109.3(4)
N(3)-C(7)-C(8)	121.1(4)
C(16)-C(7)-C(8)	129.6(4)
N(4)-C(8)-C(7)	122.1(4)
N(4)-C(8)-H(8)	119.0
C(7)-C(8)-H(8)	119.0
N(4)-C(9)-C(10)	111.3(4)
N(4)-C(9)-H(6)	109.4
C(10)-C(9)-H(6)	109.4
N(4)-C(9)-H(7)	109.4
C(10)-C(9)-H(7)	109.4
H(6)-C(9)-H(7)	108.0
C(2')-C(10)-C(9)	118.1(5)
C(2')-C(10)-H(10A)	107.8
C(9)-C(10)-H(10A)	107.8
C(2')-C(10)-H(10B)	107.8
C(9)-C(10)-H(10B)	107.8

Table C.5.1. continued…

H(10A)-C(10)-H(10B)	107.1
C(12)-C(11)-C(3)	106.8(3)
C(12)-C(11)-H(2)	126.6
C(3)-C(11)-H(2)	126.6
C(11)-C(12)-C(2)	106.9(3)
C(11)-C(12)-H(3)	126.6
C(2)-C(12)-H(3)	126.6
N(5)-C(13)-C(15)	121.0(4)
N(5)-C(13)-C(14)	118.2(4)
C(15)-C(13)-C(14)	120.8(4)
N(13)-C(14)-C(13)	176.5(5)
N(6)-C(15)-C(13)	121.8(3)
N(6)-C(15)-C(18)	118.0(3)
C(13)-C(15)-C(18)	120.2(4)
C(17)-C(16)-C(7)	107.4(4)
C(17)-C(16)-H(5)	126.3
C(7)-C(16)-H(5)	126.3
C(16)-C(17)-C(6)	106.7(4)
C(16)-C(17)-H(4)	126.7
C(6)-C(17)-H(4)	126.7
N(14)-C(18)-C(15)	176.7(5)
N(7)-C(20)-C(1')	109.7(3)
N(7)-C(20)-H(20A)	109.7
C(1')-C(20)-H(20A)	109.7
N(7)-C(20)-H(20B)	109.7
C(1')-C(20)-H(20B)	109.7
H(20A)-C(20)-H(20B)	108.2
N(7)-C(21)-C(22)	122.8(3)
N(7)-C(21)-H(14)	118.6
C(22)-C(21)-H(14)	118.6
N(8)-C(22)-C(21)	120.9(3)
N(8)-C(22)-C(37)	110.6(3)
C(21)-C(22)-C(37)	128.5(3)
N(8)-C(23)-C(36)	110.4(3)
N(8)-C(23)-C(24)	126.4(3)
C(36)-C(23)-C(24)	123.2(3)
N(10)-C(24)-C(23)	111.3(3)

Table C.5.1. continued…

N(10)-C(24)-C(25)	118.7(3)
C(23)-C(24)-C(25)	130.0(3)
N(9)-C(25)-C(32)	111.6(3)
N(9)-C(25)-C(24)	119.5(3)
C(32)-C(25)-C(24)	128.8(3)
N(9)-C(26)-C(31)	122.2(3)
N(9)-C(26)-C(27)	117.6(4)
C(31)-C(26)-C(27)	120.2(4)
N(12)-C(27)-C(26)	178.3(4)
N(11)-C(30)-C(31)	179.4(5)
N(10)-C(31)-C(26)	120.8(4)
N(10)-C(31)-C(30)	117.7(4)
C(26)-C(31)-C(30)	121.5(3)
N(15)-C(32)-C(39)	107.5(3)
N(15)-C(32)-C(25)	125.3(3)
C(39)-C(32)-C(25)	127.1(4)
N(15)-C(33)-C(38)	108.4(4)
N(15)-C(33)-C(34)	120.7(4)
C(38)-C(33)-C(34)	130.9(4)
N(16)-C(34)-C(33)	121.2(4)
N(16)-C(34)-H(15)	119.4
C(33)-C(34)-H(15)	119.4
N(16)-C(35)-C(1')	110.9(3)
N(16)-C(35)-H(35A)	109.5
C(1')-C(35)-H(35A)	109.5
N(16)-C(35)-H(35B)	109.5
C(1')-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	108.0
N(16)-C(35)-H(101)	34(5)
C(1')-C(35)-H(101)	80(9)
H(35A)-C(35)-H(101)	110.1
H(35B)-C(35)-H(101)	134.6
C(37)-C(36)-C(23)	106.4(3)
C(37)-C(36)-H(13)	126.8
C(23)-C(36)-H(13)	126.8
C(36)-C(37)-C(22)	106.3(3)
C(36)-C(37)-H(12)	126.9

Table C.5.1. continued…

C(22)-C(37)-H(12)	126.9
C(39)-C(38)-C(33)	107.3(3)
C(39)-C(38)-H(17)	126.3
C(33)-C(38)-H(17)	126.3
C(38)-C(39)-C(32)	107.7(4)
C(38)-C(39)-H(16)	126.1
C(32)-C(39)-H(16)	126.1
C(35)-C(1')-C(20)	113.0(4)
C(35)-C(1')-H(1'1)	109.0
C(20)-C(1')-H(1'1)	109.0
C(35)-C(1')-H(1'2)	109.0
C(20)-C(1')-H(1'2)	109.0
H(1'1)-C(1')-H(1'2)	107.8
N(1)-C(2')-C(10)	111.2(4)
N(1)-C(2')-H(2'1)	109.4
C(10)-C(2')-H(2'1)	109.4
N(1)-C(2')-H(2'2)	109.4
C(10)-C(2')-H(2'2)	109.4
H(2'1)-C(2')-H(2'2)	108.0

Table C.5.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L8a. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	47(3)	34(2)	28(2)	-1(2)	-7(2)	4(2)
N(2)	18(2)	28(2)	26(2)	2(2)	1(1)	5(1)
N(3)	21(2)	24(2)	27(2)	0(1)	2(2)	6(1)
N(4)	37(2)	33(2)	25(2)	-1(2)	0(2)	4(2)
N(5)	19(2)	29(2)	32(2)	-4(1)	4(2)	2(1)
N(6)	24(2)	29(2)	28(2)	2(1)	-2(2)	3(1)
N(7)	30(2)	29(2)	22(2)	3(1)	1(2)	0(2)
N(8)	20(2)	27(2)	23(2)	-3(1)	-1(1)	4(1)
N(9)	26(2)	27(2)	24(2)	-2(1)	0(2)	4(1)
N(10)	20(2)	28(2)	24(2)	1(1)	0(1)	3(1)
N(15)	18(2)	22(2)	30(2)	-1(1)	2(1)	3(1)
N(16)	25(2)	26(2)	32(2)	2(2)	4(2)	5(1)
C(1)	32(2)	29(2)	24(2)	7(2)	3(2)	6(2)
C(2)	18(2)	31(2)	29(2)	4(2)	0(2)	6(2)
C(3)	20(2)	25(2)	28(2)	-1(2)	1(2)	5(2)
C(4)	14(2)	29(2)	25(2)	1(2)	0(2)	5(2)
C(5)	17(2)	26(2)	26(2)	1(2)	0(2)	4(1)
C(6)	19(2)	26(2)	25(2)	1(2)	1(2)	4(2)
C(7)	20(2)	29(2)	29(2)	1(2)	5(2)	2(2)
C(8)	25(2)	23(2)	36(2)	0(2)	1(2)	1(2)
C(9)	61(4)	38(2)	32(3)	-11(2)	-1(2)	-2(2)
C(10)	79(4)	44(3)	32(3)	-7(2)	-2(3)	-12(3)
C(11)	23(2)	26(2)	32(2)	2(2)	-1(2)	0(2)
C(12)	23(2)	32(2)	30(2)	8(2)	3(2)	1(2)
C(13)	23(2)	28(2)	28(2)	-3(2)	-1(2)	4(2)
C(14)	31(2)	32(2)	26(2)	-3(2)	-1(2)	5(2)
C(15)	23(2)	29(2)	25(2)	2(2)	-3(2)	5(2)
C(16)	27(2)	22(2)	30(2)	4(2)	4(2)	2(2)
C(17)	29(2)	34(2)	27(2)	6(2)	3(2)	3(2)
C(18)	38(3)	32(2)	28(2)	2(2)	-4(2)	0(2)
N(14)	73(3)	49(2)	32(2)	6(2)	-12(2)	0(2)
C(20)	44(3)	33(2)	22(2)	4(2)	-2(2)	2(2)
C(21)	29(2)	27(2)	24(2)	-4(2)	-2(2)	2(2)
C(22)	19(2)	29(2)	23(2)	-3(2)	2(2)	4(2)

Table C.5.2. continued…

C(23)	18(2)	25(2)	24(2)	-1(2)	1(2)	1(2)
C(24)	15(2)	28(2)	26(2)	-3(2)	2(2)	7(2)
C(25)	19(2)	27(2)	25(2)	-1(2)	2(2)	5(2)
C(26)	27(2)	32(2)	22(2)	0(2)	2(2)	9(2)
C(27)	40(3)	28(2)	25(2)	-6(2)	3(2)	5(2)
N(12)	76(3)	35(2)	28(2)	-5(2)	2(2)	-3(2)
N(11)	58(3)	38(2)	27(2)	7(2)	5(2)	0(2)
C(30)	39(3)	32(2)	21(2)	-3(2)	2(2)	3(2)
C(31)	22(2)	30(2)	24(2)	1(2)	3(2)	3(2)
C(32)	15(2)	28(2)	26(2)	-4(2)	1(2)	5(2)
C(33)	17(2)	26(2)	33(2)	-1(2)	2(2)	2(2)
C(34)	22(2)	19(2)	38(3)	-4(2)	5(2)	1(2)
C(35)	34(2)	30(2)	32(2)	6(2)	6(2)	-1(2)
C(36)	23(2)	26(2)	26(2)	-1(2)	1(2)	1(2)
C(37)	21(2)	26(2)	27(2)	-6(2)	3(2)	3(2)
C(38)	26(2)	25(2)	35(2)	-7(2)	2(2)	1(2)
C(39)	22(2)	39(2)	26(2)	-8(2)	-2(2)	2(2)
C(1')	41(3)	30(2)	28(2)	6(2)	5(2)	2(2)
C(2')	78(4)	39(3)	32(3)	1(2)	-11(3)	-1(3)
N(13)	49(3)	43(2)	38(2)	-7(2)	-2(2)	-3(2)

Table C.5.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L8a.

	x	y	z	U(eq)
H(1)	6563	9189	5608	34
H(8)	4678	6361	6954	34
H(6)	3263	6874	5885	52
H(7)	4991	6360	5952	52
H(10A)	7041	7120	5545	62
H(10B)	5316	6975	5146	62
H(2)	7820	10499	7276	32
H(3)	7470	10330	6253	34
H(5)	5255	6415	8103	31
H(4)	6152	7359	8747	36
H(20A)	11749	8134	9710	40
H(20B)	13335	7659	9444	40
H(14)	12505	9199	9224	32
H(15)	9921	6483	7858	32
H(35A)	12310	6612	8877	39
H(35B)	10109	6454	8799	39
H(13)	12669	10631	7590	30
H(12)	12831	10401	8606	29
H(17)	9563	6641	6688	34
H(16)	10049	7643	6058	35
H(1'1)	10507	7023	9641	40
H(1'2)	9339	7504	9240	40
H(2'1)	6178	8113	5121	60
H(2'2)	4042	8033	5325	60
H(102)	11700(300)	8650(40)	7760(60)	390(100)
H(101)	11300(700)	7520(130)	8540(110)	1000(300)
H(103)	6320(150)	8580(20)	7080(30)	170(40)
H(104)	5650(170)	7550(30)	6430(50)	250(60)

Table C.5.4: Torsion angles [°] for H_2L8a.

C(2')-N(1)-C(1)-C(2)	177.3(5)
C(3)-N(2)-C(2)-C(12)	-1.2(4)
C(3)-N(2)-C(2)-C(1)	179.0(4)
N(1)-C(1)-C(2)-N(2)	2.6(6)
N(1)-C(1)-C(2)-C(12)	-177.1(4)
C(2)-N(2)-C(3)-C(11)	1.4(4)
C(2)-N(2)-C(3)-C(4)	-178.4(4)
C(13)-N(5)-C(4)-C(5)	-1.4(6)
C(13)-N(5)-C(4)-C(3)	-179.9(4)
N(2)-C(3)-C(4)-N(5)	178.5(4)
C(11)-C(3)-C(4)-N(5)	-1.1(6)
N(2)-C(3)-C(4)-C(5)	0.2(7)
C(11)-C(3)-C(4)-C(5)	-179.5(4)
C(15)-N(6)-C(5)-C(4)	-2.6(6)
C(15)-N(6)-C(5)-C(6)	178.7(3)
N(5)-C(4)-C(5)-N(6)	4.0(6)
C(3)-C(4)-C(5)-N(6)	-177.7(4)
N(5)-C(4)-C(5)-C(6)	-177.6(4)
C(3)-C(4)-C(5)-C(6)	0.7(7)
C(7)-N(3)-C(6)-C(17)	0.1(4)
C(7)-N(3)-C(6)-C(5)	-180.0(4)
N(6)-C(5)-C(6)-N(3)	175.5(4)
C(4)-C(5)-C(6)-N(3)	-3.0(7)
N(6)-C(5)-C(6)-C(17)	-4.6(6)
C(4)-C(5)-C(6)-C(17)	176.9(4)
C(6)-N(3)-C(7)-C(16)	-0.1(4)
C(6)-N(3)-C(7)-C(8)	-179.9(4)
C(9)-N(4)-C(8)-C(7)	-178.9(4)
N(3)-C(7)-C(8)-N(4)	2.1(6)
C(16)-C(7)-C(8)-N(4)	-177.7(4)
C(8)-N(4)-C(9)-C(10)	-153.3(5)
N(4)-C(9)-C(10)-C(2')	-57.6(7)
N(2)-C(3)-C(11)-C(12)	-1.0(5)
C(4)-C(3)-C(11)-C(12)	178.7(4)
C(3)-C(11)-C(12)-C(2)	0.3(5)
N(2)-C(2)-C(12)-C(11)	0.5(5)

Table C.5.4. continued…

C(1)-C(2)-C(12)-C(11)	-179.7(4)
C(4)-N(5)-C(13)-C(15)	-2.5(6)
C(4)-N(5)-C(13)-C(14)	175.6(4)
N(5)-C(13)-C(14)-N(13)	-138(8)
C(15)-C(13)-C(14)-N(13)	40(8)
C(5)-N(6)-C(15)-C(13)	-1.3(6)
C(5)-N(6)-C(15)-C(18)	177.1(4)
N(5)-C(13)-C(15)-N(6)	4.0(6)
C(14)-C(13)-C(15)-N(6)	-174.0(4)
N(5)-C(13)-C(15)-C(18)	-174.3(4)
C(14)-C(13)-C(15)-C(18)	7.7(6)
N(3)-C(7)-C(16)-C(17)	0.0(5)
C(8)-C(7)-C(16)-C(17)	179.8(4)
C(7)-C(16)-C(17)-C(6)	0.1(5)
N(3)-C(6)-C(17)-C(16)	-0.1(5)
C(5)-C(6)-C(17)-C(16)	180.0(4)
N(6)-C(15)-C(18)-N(14)	-138(9)
C(13)-C(15)-C(18)-N(14)	40(10)
C(21)-N(7)-C(20)-C(1')	142.1(4)
C(20)-N(7)-C(21)-C(22)	-179.3(4)
C(23)-N(8)-C(22)-C(21)	-179.3(4)
C(23)-N(8)-C(22)-C(37)	0.8(4)
N(7)-C(21)-C(22)-N(8)	1.9(6)
N(7)-C(21)-C(22)-C(37)	-178.3(4)
C(22)-N(8)-C(23)-C(36)	-0.4(4)
C(22)-N(8)-C(23)-C(24)	179.0(4)
C(31)-N(10)-C(24)-C(23)	-178.5(4)
C(31)-N(10)-C(24)-C(25)	1.8(5)
N(8)-C(23)-C(24)-N(10)	-171.1(4)
C(36)-C(23)-C(24)-N(10)	8.3(5)
N(8)-C(23)-C(24)-C(25)	8.6(7)
C(36)-C(23)-C(24)-C(25)	-172.0(4)
C(26)-N(9)-C(25)-C(32)	-178.9(3)
C(26)-N(9)-C(25)-C(24)	2.5(6)
N(10)-C(24)-C(25)-N(9)	-3.8(5)
C(23)-C(24)-C(25)-N(9)	176.5(4)
N(10)-C(24)-C(25)-C(32)	177.8(4)

Table C.5.4. continued…

C(23)-C(24)-C(25)-C(32)	-1.9(7)
C(25)-N(9)-C(26)-C(31)	0.8(6)
C(25)-N(9)-C(26)-C(27)	-177.7(4)
N(9)-C(26)-C(27)-N(12)	144(19)
C(31)-C(26)-C(27)-N(12)	-35(19)
C(24)-N(10)-C(31)-C(26)	1.5(6)
C(24)-N(10)-C(31)-C(30)	-176.8(4)
N(9)-C(26)-C(31)-N(10)	-3.0(7)
C(27)-C(26)-C(31)-N(10)	175.5(4)
N(9)-C(26)-C(31)-C(30)	175.3(4)
C(27)-C(26)-C(31)-C(30)	-6.2(6)
N(11)-C(30)-C(31)-N(10)	45(49)
N(11)-C(30)-C(31)-C(26)	-134(48)
C(33)-N(15)-C(32)-C(39)	-0.1(4)
C(33)-N(15)-C(32)-C(25)	179.6(4)
N(9)-C(25)-C(32)-N(15)	177.0(4)
C(24)-C(25)-C(32)-N(15)	-4.6(6)
N(9)-C(25)-C(32)-C(39)	-3.4(6)
C(24)-C(25)-C(32)-C(39)	175.1(4)
C(32)-N(15)-C(33)-C(38)	0.6(4)
C(32)-N(15)-C(33)-C(34)	-179.7(3)
C(35)-N(16)-C(34)-C(33)	-178.7(4)
N(15)-C(33)-C(34)-N(16)	-5.3(6)
C(38)-C(33)-C(34)-N(16)	174.4(4)
C(34)-N(16)-C(35)-C(1')	-142.7(4)
N(8)-C(23)-C(36)-C(37)	-0.1(4)
C(24)-C(23)-C(36)-C(37)	-179.5(4)
C(23)-C(36)-C(37)-C(22)	0.5(4)
N(8)-C(22)-C(37)-C(36)	-0.8(5)
C(21)-C(22)-C(37)-C(36)	179.3(4)
N(15)-C(33)-C(38)-C(39)	-0.9(5)
C(34)-C(33)-C(38)-C(39)	179.4(4)
C(33)-C(38)-C(39)-C(32)	0.8(5)
N(15)-C(32)-C(39)-C(38)	-0.5(5)
C(25)-C(32)-C(39)-C(38)	179.8(4)
N(16)-C(35)-C(1')-C(20)	-62.5(5)
N(7)-C(20)-C(1')-C(35)	62.5(5)

Table C.5.4. continued…

C(1)-N(1)-C(2')-C(10)	153.6(5)
C(9)-C(10)-C(2')-N(1)	56.5(7)

C.6: Full crystallographic Data Tables of H_2L8b

Table C.6.1: Bond lengths [Å] and angles [°] for H_2L8b

O(1)-C(16)	1.342(6)
O(1)-C(19)	1.423(7)
C(16)-N(6)	1.328(7)
C(16)-C(17)	1.383(7)
N(5)-C(17)	1.317(7)
N(5)-C(14)	1.350(7)
N(4)-C(13)	1.346(7)
N(4)-C(10)	1.391(7)
N(1)-C(4)	1.356(7)
N(1)-C(1)	1.369(7)
N(1)-H(101)	0.95(2)
C(1)-C(2)	1.399(7)
C(1)-C(15)	1.446(7)
C(15)-N(6)	1.364(7)
C(15)-C(14)	1.430(7)
C(19)-H(19C)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19A)	0.9800
C(17)-C(18)	1.438(8)
C(14)-C(13)	1.473(7)
C(13)-C(12)	1.414(8)
C(10)-C(9)	1.399(8)
C(10)-C(11)	1.402(9)
C(9)-N(3)	1.300(8)
C(9)-H(9)	0.9500
N(3)-C(8)	1.465(8)
N(3)-H(103)	0.94(2)
C(8)-C(7)	1.503(11)
C(8)-H(8A)	0.9900
C(8)-H(8B)	0.9900
C(7)-C(6)	1.489(11)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(6)-N(2)	1.470(8)

Table C.6.1. continued…

C(6)-H(6B)	0.9900
C(6)-H(6A)	0.9900
N(2)-C(5)	1.286(8)
C(5)-C(4)	1.426(8)
C(5)-H(5)	0.9500
C(4)-C(3)	1.385(9)
C(11)-C(12)	1.369(9)
C(11)-H(11)	0.9500
C(12)-H(12)	0.9500
C(18)-N(7)	1.119(8)
C(2)-C(3)	1.393(9)
C(2)-H(2)	0.9500
C(3)-H(3)	0.9500
C(16)-O(1)-C(19)	118.4(5)
N(6)-C(16)-O(1)	119.9(4)
N(6)-C(16)-C(17)	122.0(5)
O(1)-C(16)-C(17)	118.1(5)
C(17)-N(5)-C(14)	120.2(5)
C(13)-N(4)-C(10)	106.3(4)
C(4)-N(1)-C(1)	109.2(5)
C(4)-N(1)-H(101)	139(8)
C(1)-N(1)-H(101)	111(8)
N(1)-C(1)-C(2)	107.9(5)
N(1)-C(1)-C(15)	125.9(5)
C(2)-C(1)-C(15)	126.2(5)
N(6)-C(15)-C(14)	119.1(5)
N(6)-C(15)-C(1)	110.8(5)
C(14)-C(15)-C(1)	130.2(5)
C(16)-N(6)-C(15)	118.7(4)
O(1)-C(19)-H(19C)	109.5
O(1)-C(19)-H(19B)	109.5
H(19C)-C(19)-H(19B)	109.5
O(1)-C(19)-H(19A)	109.5
H(19C)-C(19)-H(19A)	109.5
H(19B)-C(19)-H(19A)	109.5
N(5)-C(17)-C(16)	120.6(5)

Table C.6.1. continued…

N(5)-C(17)-C(18)	118.7(5)
C(16)-C(17)-C(18)	120.8(5)
N(5)-C(14)-C(15)	119.4(5)
N(5)-C(14)-C(13)	111.2(5)
C(15)-C(14)-C(13)	129.4(5)
N(4)-C(13)-C(12)	110.7(5)
N(4)-C(13)-C(14)	125.3(5)
C(12)-C(13)-C(14)	123.9(5)
N(4)-C(10)-C(9)	121.6(5)
N(4)-C(10)-C(11)	109.1(5)
C(9)-C(10)-C(11)	129.3(5)
N(3)-C(9)-C(10)	122.5(6)
N(3)-C(9)-H(9)	118.8
C(10)-C(9)-H(9)	118.8
C(9)-N(3)-C(8)	125.6(6)
C(9)-N(3)-H(103)	120(5)
C(8)-N(3)-H(103)	114(5)
N(3)-C(8)-C(7)	110.5(6)
N(3)-C(8)-H(8A)	109.6
C(7)-C(8)-H(8A)	109.6
N(3)-C(8)-H(8B)	109.6
C(7)-C(8)-H(8B)	109.6
H(8A)-C(8)-H(8B)	108.1
C(6)-C(7)-C(8)	117.5(7)
C(6)-C(7)-H(7A)	107.9
C(8)-C(7)-H(7A)	107.9
C(6)-C(7)-H(7B)	107.9
C(8)-C(7)-H(7B)	107.9
H(7A)-C(7)-H(7B)	107.2
N(2)-C(6)-C(7)	109.8(6)
N(2)-C(6)-H(6B)	109.7
C(7)-C(6)-H(6B)	109.7
N(2)-C(6)-H(6A)	109.7
C(7)-C(6)-H(6A)	109.7
H(6B)-C(6)-H(6A)	108.2
C(5)-N(2)-C(6)	121.1(6)
N(2)-C(5)-C(4)	120.9(6)

Table C.6.1. continued…

N(2)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
N(1)-C(4)-C(3)	108.3(5)
N(1)-C(4)-C(5)	121.8(6)
C(3)-C(4)-C(5)	129.8(6)
C(12)-C(11)-C(10)	107.6(5)
C(12)-C(11)-H(11)	126.2
C(10)-C(11)-H(11)	126.2
C(11)-C(12)-C(13)	106.3(5)
C(11)-C(12)-H(12)	126.9
C(13)-C(12)-H(12)	126.9
N(7)-C(18)-C(17)	179.1(8)
C(3)-C(2)-C(1)	106.7(5)
C(3)-C(2)-H(2)	126.6
C(1)-C(2)-H(2)	126.6
C(4)-C(3)-C(2)	107.9(5)
C(4)-C(3)-H(3)	126.1
C(2)-C(3)-H(3)	126.1

Table C.6.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L8b. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	57(2)	43(2)	63(2)	-7(2)	8(2)	7(2)
C(16)	31(2)	51(3)	40(3)	-6(3)	-1(2)	8(2)
N(5)	39(2)	43(2)	52(3)	3(2)	2(2)	-2(2)
N(4)	40(2)	44(2)	43(3)	-5(2)	2(2)	3(2)
N(1)	45(2)	36(2)	50(3)	1(2)	2(2)	-5(2)
C(1)	39(3)	39(3)	51(3)	-1(2)	-4(3)	2(2)
C(15)	37(3)	49(3)	38(3)	-1(2)	-5(2)	4(2)
N(6)	40(2)	43(2)	45(2)	-2(2)	-3(2)	4(2)
C(19)	79(4)	48(3)	81(5)	-8(3)	5(4)	4(3)
C(17)	43(3)	43(3)	49(3)	-2(3)	-1(3)	0(2)
C(14)	39(3)	38(3)	40(3)	-4(2)	-4(2)	2(2)
C(13)	35(3)	47(3)	45(3)	-3(2)	-1(3)	1(2)
C(10)	43(3)	48(3)	62(4)	-9(3)	11(3)	8(3)
C(9)	47(3)	52(3)	71(4)	-10(3)	8(3)	4(3)
N(3)	54(3)	72(4)	59(3)	-9(3)	13(3)	2(3)
C(8)	62(4)	87(5)	57(4)	2(4)	23(3)	6(3)
C(7)	96(6)	107(7)	62(5)	-2(4)	28(5)	-6(5)
C(6)	79(5)	73(4)	71(5)	-2(4)	29(4)	-8(4)
N(2)	61(3)	65(3)	63(3)	4(3)	18(3)	-7(3)
C(5)	58(4)	55(4)	65(4)	9(3)	4(3)	-9(3)
C(4)	51(3)	47(3)	61(4)	2(3)	3(3)	-5(3)
C(11)	80(4)	40(3)	109(6)	-13(4)	39(5)	2(3)
C(12)	66(4)	41(3)	84(5)	2(3)	27(4)	-5(3)
C(18)	58(3)	47(3)	59(4)	-1(3)	19(3)	3(3)
N(7)	97(4)	61(4)	94(5)	-3(3)	42(4)	-7(3)
C(2)	63(4)	43(3)	74(5)	1(3)	13(4)	2(3)
C(3)	71(4)	32(3)	108(6)	-3(4)	13(4)	-5(3)

Table C.6.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L8b.

	x	y	z	U(eq)
H(19C)	13554	941	2462	104
H(19B)	13965	1015	978	104
H(19A)	12391	1021	1390	104
H(9)	7051	4553	7578	68
H(8A)	4919	3397	8287	83
H(8B)	5951	3780	9304	83
H(7A)	6869	2567	9779	106
H(7B)	5262	2558	10026	106
H(6B)	5954	1396	9101	89
H(6A)	4923	1841	8155	89
H(5)	7028	739	7395	71
H(11)	8856	5278	5918	92
H(12)	10527	4774	4302	77
H(2)	10666	631	4182	72
H(3)	8950	71	5731	84
H(103)	7090(70)	2950(30)	7260(70)	90(30)
H(101)	8860(110)	2445(19)	5790(140)	170(50)

Table C.6.4: Torsion angles [°] for H_2L8b.

C(19)-O(1)-C(16)-N(6)	5.1(8)
C(19)-O(1)-C(16)-C(17)	-174.2(6)
C(4)-N(1)-C(1)-C(2)	0.7(7)
C(4)-N(1)-C(1)-C(15)	-179.2(5)
N(1)-C(1)-C(15)-N(6)	-178.3(5)
C(2)-C(1)-C(15)-N(6)	1.8(8)
N(1)-C(1)-C(15)-C(14)	1.8(10)
C(2)-C(1)-C(15)-C(14)	-178.0(6)
O(1)-C(16)-N(6)-C(15)	179.5(4)
C(17)-C(16)-N(6)-C(15)	-1.2(8)
C(14)-C(15)-N(6)-C(16)	0.9(8)
C(1)-C(15)-N(6)-C(16)	-178.9(4)
C(14)-N(5)-C(17)-C(16)	1.5(9)
C(14)-N(5)-C(17)-C(18)	179.8(5)
N(6)-C(16)-C(17)-N(5)	0.0(9)
O(1)-C(16)-C(17)-N(5)	179.3(5)
N(6)-C(16)-C(17)-C(18)	-178.3(5)
O(1)-C(16)-C(17)-C(18)	1.0(8)
C(17)-N(5)-C(14)-C(15)	-1.7(8)
C(17)-N(5)-C(14)-C(13)	178.1(5)
N(6)-C(15)-C(14)-N(5)	0.5(8)
C(1)-C(15)-C(14)-N(5)	-179.7(5)
N(6)-C(15)-C(14)-C(13)	-179.3(5)
C(1)-C(15)-C(14)-C(13)	0.5(10)
C(10)-N(4)-C(13)-C(12)	-0.5(6)
C(10)-N(4)-C(13)-C(14)	178.0(5)
N(5)-C(14)-C(13)-N(4)	-180.0(5)
C(15)-C(14)-C(13)-N(4)	-0.2(9)
N(5)-C(14)-C(13)-C(12)	-1.6(8)
C(15)-C(14)-C(13)-C(12)	178.2(6)
C(13)-N(4)-C(10)-C(9)	-178.4(5)
C(13)-N(4)-C(10)-C(11)	0.2(7)
N(4)-C(10)-C(9)-N(3)	-0.4(9)
C(11)-C(10)-C(9)-N(3)	-178.8(7)
C(10)-C(9)-N(3)-C(8)	179.8(6)
C(9)-N(3)-C(8)-C(7)	-153.9(7)

Table C.6.4. continued…

N(3)-C(8)-C(7)-C(6)	-58.7(10)
C(8)-C(7)-C(6)-N(2)	58.8(10)
C(7)-C(6)-N(2)-C(5)	151.4(7)
C(6)-N(2)-C(5)-C(4)	-178.9(6)
C(1)-N(1)-C(4)-C(3)	-0.3(7)
C(1)-N(1)-C(4)-C(5)	177.3(5)
N(2)-C(5)-C(4)-N(1)	-1.0(9)
N(2)-C(5)-C(4)-C(3)	176.1(7)
N(4)-C(10)-C(11)-C(12)	0.2(8)
C(9)-C(10)-C(11)-C(12)	178.7(7)
C(10)-C(11)-C(12)-C(13)	-0.5(8)
N(4)-C(13)-C(12)-C(11)	0.7(7)
C(14)-C(13)-C(12)-C(11)	-177.9(6)
N(1)-C(1)-C(2)-C(3)	-0.7(7)
C(15)-C(1)-C(2)-C(3)	179.1(6)
N(1)-C(4)-C(3)-C(2)	-0.1(8)
C(5)-C(4)-C(3)-C(2)	-177.5(6)
C(1)-C(2)-C(3)-C(4)	0.5(8)

C.7: Full crystallographic Data Tables of H_2L8c

Table C.7.1: Bond lengths [Å] and angles [°] for H_2L8c

O(1)-C(8)	1.360(3)
O(1)-C(9)	1.433(3)
N(1)-C(2)	1.293(3)
N(1)-C(1)	1.469(3)
N(1)-H(15)	0.8800
N(2)-C(4)	1.345(3)
N(2)-C(3)	1.377(3)
N(3)-C(7)	1.333(3)
N(3)-C(6)	1.348(3)
N(5)-C(10)	1.326(3)
N(5)-C(5)	1.344(3)
N(6)-C(15)	1.271(3)
N(6)-C(14)	1.465(3)
N(7)-C(17)	1.361(3)
N(7)-C(16)	1.362(3)
N(7)-H(6)	0.8800
C(1)-C(13)	1.507(4)
C(1)-H(14)	0.9900
C(1)-H(1)	0.9900
C(2)-C(3)	1.402(3)
C(2)-H(16)	0.9500
C(3)-C(20)	1.407(3)
C(4)-C(21)	1.425(3)
C(4)-C(5)	1.468(3)
C(5)-C(6)	1.448(3)
C(6)-C(17)	1.457(3)
C(7)-C(10)	1.390(3)
C(7)-C(8)	1.491(3)
C(8)-N(9)	1.252(3)
C(9)-H(2)	0.9800
C(9)-H(3)	0.9800
C(9)-H(19)	0.9800
C(10)-C(11)	1.461(3)
C(11)-N(8)	1.138(3)

Table C.7.1. continued…

C(13)-C(14)	1.521(4)
C(13)-H(13)	0.9900
C(13)-H(12)	0.9900
C(14)-H(11)	0.9900
C(14)-H(10)	0.9900
C(15)-C(16)	1.444(3)
C(15)-H(9)	0.9500
C(16)-C(19)	1.403(3)
C(17)-C(18)	1.402(3)
C(18)-C(19)	1.380(4)
C(18)-H(8)	0.9500
C(19)-H(7)	0.9500
C(20)-C(21)	1.365(3)
C(20)-H(17)	0.9500
C(21)-H(18)	0.9500
N(9)-H(101)	0.98(4)
C(8)-O(1)-C(9)	115.7(2)
C(2)-N(1)-C(1)	127.6(2)
C(2)-N(1)-H(15)	116.2
C(1)-N(1)-H(15)	116.2
C(4)-N(2)-C(3)	105.87(18)
C(7)-N(3)-C(6)	120.3(2)
C(10)-N(5)-C(5)	120.0(2)
C(15)-N(6)-C(14)	120.8(2)
C(17)-N(7)-C(16)	110.37(19)
C(17)-N(7)-H(6)	124.8
C(16)-N(7)-H(6)	124.8
N(1)-C(1)-C(13)	109.7(2)
N(1)-C(1)-H(14)	109.7
C(13)-C(1)-H(14)	109.7
N(1)-C(1)-H(1)	109.7
C(13)-C(1)-H(1)	109.7
H(14)-C(1)-H(1)	108.2
N(1)-C(2)-C(3)	122.8(2)
N(1)-C(2)-H(16)	118.6
C(3)-C(2)-H(16)	118.6

Table C.7.1. continued…

N(2)-C(3)-C(2)	122.4(2)
N(2)-C(3)-C(20)	110.69(19)
C(2)-C(3)-C(20)	126.9(2)
N(2)-C(4)-C(21)	110.35(19)
N(2)-C(4)-C(5)	126.52(19)
C(21)-C(4)-C(5)	123.1(2)
N(5)-C(5)-C(6)	119.1(2)
N(5)-C(5)-C(4)	111.08(19)
C(6)-C(5)-C(4)	129.7(2)
N(3)-C(6)-C(5)	118.8(2)
N(3)-C(6)-C(17)	112.3(2)
C(5)-C(6)-C(17)	128.9(2)
N(3)-C(7)-C(10)	120.2(2)
N(3)-C(7)-C(8)	115.5(2)
C(10)-C(7)-C(8)	124.3(2)
N(9)-C(8)-O(1)	122.4(2)
N(9)-C(8)-C(7)	128.0(2)
O(1)-C(8)-C(7)	109.6(2)
O(1)-C(9)-H(2)	109.5
O(1)-C(9)-H(3)	109.5
H(2)-C(9)-H(3)	109.5
O(1)-C(9)-H(19)	109.5
H(2)-C(9)-H(19)	109.5
H(3)-C(9)-H(19)	109.5
N(5)-C(10)-C(7)	121.4(2)
N(5)-C(10)-C(11)	114.9(2)
C(7)-C(10)-C(11)	123.6(2)
N(8)-C(11)-C(10)	176.6(3)
C(1)-C(13)-C(14)	114.2(2)
C(1)-C(13)-H(13)	108.7
C(14)-C(13)-H(13)	108.7
C(1)-C(13)-H(12)	108.7
C(14)-C(13)-H(12)	108.7
H(13)-C(13)-H(12)	107.6
N(6)-C(14)-C(13)	111.3(2)
N(6)-C(14)-H(11)	109.4
C(13)-C(14)-H(11)	109.4

Table C.7.1. continued…

N(6)-C(14)-H(10)	109.4
C(13)-C(14)-H(10)	109.4
H(11)-C(14)-H(10)	108.0
N(6)-C(15)-C(16)	121.3(2)
N(6)-C(15)-H(9)	119.4
C(16)-C(15)-H(9)	119.4
N(7)-C(16)-C(19)	106.9(2)
N(7)-C(16)-C(15)	121.2(2)
C(19)-C(16)-C(15)	131.9(2)
N(7)-C(17)-C(18)	107.2(2)
N(7)-C(17)-C(6)	125.4(2)
C(18)-C(17)-C(6)	127.3(2)
C(19)-C(18)-C(17)	107.6(2)
C(19)-C(18)-H(8)	126.2
C(17)-C(18)-H(8)	126.2
C(18)-C(19)-C(16)	107.9(2)
C(18)-C(19)-H(7)	126.0
C(16)-C(19)-H(7)	126.0
C(21)-C(20)-C(3)	106.2(2)
C(21)-C(20)-H(17)	126.9
C(3)-C(20)-H(17)	126.9
C(20)-C(21)-C(4)	106.9(2)
C(20)-C(21)-H(18)	126.6
C(4)-C(21)-H(18)	126.6
C(8)-N(9)-H(101)	104(2)

Table C.7.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L8c. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	43(1)	42(1)	34(1)	4(1)	-1(1)	0(1)
N(1)	36(1)	34(1)	30(1)	3(1)	-1(1)	2(1)
N(2)	29(1)	25(1)	26(1)	-1(1)	3(1)	2(1)
N(3)	30(1)	37(1)	26(1)	-5(1)	3(1)	6(1)
N(5)	32(1)	31(1)	29(1)	3(1)	6(1)	5(1)
N(6)	45(1)	24(1)	36(1)	1(1)	6(1)	2(1)
N(7)	29(1)	27(1)	28(1)	-4(1)	3(1)	0(1)
C(1)	39(1)	42(1)	32(1)	8(1)	2(1)	7(1)
C(2)	28(1)	36(1)	28(1)	-5(1)	3(1)	2(1)
C(3)	27(1)	30(1)	28(1)	-5(1)	4(1)	2(1)
C(4)	29(1)	25(1)	28(1)	-2(1)	7(1)	4(1)
C(5)	28(1)	28(1)	28(1)	0(1)	8(1)	6(1)
C(6)	29(1)	35(1)	24(1)	-2(1)	6(1)	8(1)
C(7)	36(1)	35(1)	26(1)	1(1)	8(1)	10(1)
C(8)	35(1)	36(1)	31(1)	-1(1)	4(1)	5(1)
C(9)	48(2)	46(2)	37(1)	5(1)	-2(1)	3(1)
C(10)	33(1)	34(1)	28(1)	2(1)	7(1)	5(1)
C(11)	37(1)	37(1)	30(1)	2(1)	3(1)	3(1)
N(8)	51(1)	42(1)	40(1)	8(1)	1(1)	-3(1)
C(13)	43(1)	42(1)	41(1)	13(1)	9(1)	10(1)
C(14)	50(2)	27(1)	46(1)	6(1)	12(1)	5(1)
C(15)	41(1)	23(1)	39(1)	-5(1)	14(1)	-2(1)
C(16)	34(1)	28(1)	34(1)	-6(1)	8(1)	-1(1)
C(17)	28(1)	33(1)	25(1)	-5(1)	5(1)	2(1)
C(18)	32(1)	40(1)	29(1)	-6(1)	3(1)	-1(1)
C(19)	33(1)	38(1)	39(1)	-12(1)	7(1)	-7(1)
C(20)	33(1)	30(1)	37(1)	-5(1)	0(1)	-3(1)
C(21)	39(1)	24(1)	42(1)	0(1)	5(1)	-2(1)
N(9)	45(1)	49(1)	38(1)	-4(1)	6(1)	-5(1)

Table C.7.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L8c.

	x	y	z	U(eq)
H(15)	287	6277	1562	41
H(6)	2066	5977	3559	34
H(14)	-1813	6894	159	46
H(1)	-1286	6434	-979	46
H(16)	-1636	5399	262	37
H(2)	6228	3533	10501	67
H(3)	4685	3414	11113	67
H(19)	5463	4123	11208	67
H(13)	-20	7440	-955	50
H(12)	1187	6867	-551	50
H(11)	1737	7799	842	49
H(10)	112	7731	1343	49
H(9)	3351	7570	2704	40
H(8)	5476	6184	6534	41
H(7)	5307	7200	5134	44
H(17)	-1567	4241	1603	41
H(18)	-4	3830	3700	42
H(101)	6630(50)	4790(20)	8210(40)	83(12)

Table C.7.4: Torsion angles [°] for H_2L8c.

C(2)-N(1)-C(1)-C(13)	-149.4(2)
C(1)-N(1)-C(2)-C(3)	-179.8(2)
C(4)-N(2)-C(3)-C(2)	178.7(2)
C(4)-N(2)-C(3)-C(20)	0.3(2)
N(1)-C(2)-C(3)-N(2)	-2.6(3)
N(1)-C(2)-C(3)-C(20)	175.5(2)
C(3)-N(2)-C(4)-C(21)	-0.6(2)
C(3)-N(2)-C(4)-C(5)	179.87(19)
C(10)-N(5)-C(5)-C(6)	2.1(3)
C(10)-N(5)-C(5)-C(4)	-179.77(18)
N(2)-C(4)-C(5)-N(5)	-179.95(19)
C(21)-C(4)-C(5)-N(5)	0.5(3)
N(2)-C(4)-C(5)-C(6)	-2.0(4)
C(21)-C(4)-C(5)-C(6)	178.5(2)
C(7)-N(3)-C(6)-C(5)	-0.5(3)
C(7)-N(3)-C(6)-C(17)	179.26(18)
N(5)-C(5)-C(6)-N(3)	-1.9(3)
C(4)-C(5)-C(6)-N(3)	-179.65(19)
N(5)-C(5)-C(6)-C(17)	178.4(2)
C(4)-C(5)-C(6)-C(17)	0.6(4)
C(6)-N(3)-C(7)-C(10)	2.7(3)
C(6)-N(3)-C(7)-C(8)	-176.92(19)
C(9)-O(1)-C(8)-N(9)	-4.3(3)
C(9)-O(1)-C(8)-C(7)	177.8(2)
N(3)-C(7)-C(8)-N(9)	-29.7(4)
C(10)-C(7)-C(8)-N(9)	150.7(3)
N(3)-C(7)-C(8)-O(1)	148.1(2)
C(10)-C(7)-C(8)-O(1)	-31.6(3)
C(5)-N(5)-C(10)-C(7)	0.1(3)
C(5)-N(5)-C(10)-C(11)	-176.45(19)
N(3)-C(7)-C(10)-N(5)	-2.6(3)
C(8)-C(7)-C(10)-N(5)	177.0(2)
N(3)-C(7)-C(10)-C(11)	173.7(2)
C(8)-C(7)-C(10)-C(11)	-6.7(4)
N(1)-C(1)-C(13)-C(14)	-60.0(3)
C(15)-N(6)-C(14)-C(13)	139.5(2)

Table C.7.1. continued…

C(1)-C(13)-C(14)-N(6)	62.9(3)
C(14)-N(6)-C(15)-C(16)	177.2(2)
C(17)-N(7)-C(16)-C(19)	-0.8(2)
C(17)-N(7)-C(16)-C(15)	-179.16(19)
N(6)-C(15)-C(16)-N(7)	6.5(3)
N(6)-C(15)-C(16)-C(19)	-171.5(2)
C(16)-N(7)-C(17)-C(18)	0.8(2)
C(16)-N(7)-C(17)-C(6)	-177.6(2)
N(3)-C(6)-C(17)-N(7)	-178.18(19)
C(5)-C(6)-C(17)-N(7)	1.6(3)
N(3)-C(6)-C(17)-C(18)	3.7(3)
C(5)-C(6)-C(17)-C(18)	-176.5(2)
N(7)-C(17)-C(18)-C(19)	-0.5(2)
C(6)-C(17)-C(18)-C(19)	177.9(2)
C(17)-C(18)-C(19)-C(16)	0.1(3)
N(7)-C(16)-C(19)-C(18)	0.4(3)
C(15)-C(16)-C(19)-C(18)	178.6(2)
N(2)-C(3)-C(20)-C(21)	0.0(3)
C(2)-C(3)-C(20)-C(21)	-178.2(2)
C(3)-C(20)-C(21)-C(4)	-0.4(3)
N(2)-C(4)-C(21)-C(20)	0.6(3)
C(5)-C(4)-C(21)-C(20)	-179.8(2)

C.8: Full crystallographic Data Tables of H_2L9

Table C.8.1: Bond lengths [Å] and angles [°] for H_2L9

C(1)-N(1)	1.4600(18)
C(1)-H(1A)	0.9800
C(1)-H(1B)	0.9800
C(1)-H(1C)	0.9800
C(2)-N(1)	1.2788(18)
C(2)-C(3)	1.438(2)
C(2)-H(2)	0.9500
C(3)-N(2)	1.3619(17)
C(3)-C(4)	1.3899(19)
C(4)-C(5)	1.393(2)
C(4)-H(4)	0.9500
C(5)-C(6)	1.3974(19)
C(5)-H(5)	0.9500
C(6)-N(2)	1.3636(18)
C(6)-C(7)	1.4656(19)
C(7)-N(3)	1.3344(17)
C(7)-C(14)	1.4615(19)
C(8)-N(3)	1.3551(18)
C(8)-C(13)	1.4079(19)
C(8)-C(9)	1.419(2)
C(9)-C(10)	1.360(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.414(2)
C(10)-H(10)	0.9500
C(11)-C(12)	1.366(2)
C(11)-H(11)	0.9500
C(12)-C(13)	1.4137(19)
C(12)-H(12)	0.9500
C(13)-N(4)	1.3584(18)
C(14)-N(4)	1.3343(17)
C(14)-C(15)	1.4753(19)
C(15)-N(5)	1.3468(18)
C(15)-C(16)	1.4246(19)

Table C.8.1. continued…

C(16)-C(17)	1.365(2)
C(16)-H(16)	0.9500
C(17)-C(18)	1.4128(19)
C(17)-H(17)	0.9500
C(18)-N(5)	1.3802(17)
C(18)-C(19)	1.392(2)
C(19)-N(6)	1.3036(18)
C(19)-H(19)	0.9500
C(20)-N(6)	1.4570(19)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
N(2)-H(101)	0.963(19)
N(6)-H(102)	0.923(17)

N(1)-C(1)-H(1A)	109.5
N(1)-C(1)-H(1B)	109.5
H(1A)-C(1)-H(1B)	109.5
N(1)-C(1)-H(1C)	109.5
H(1A)-C(1)-H(1C)	109.5
H(1B)-C(1)-H(1C)	109.5
N(1)-C(2)-C(3)	125.08(13)
N(1)-C(2)-H(2)	117.5
C(3)-C(2)-H(2)	117.5
N(2)-C(3)-C(4)	107.91(12)
N(2)-C(3)-C(2)	123.84(12)
C(4)-C(3)-C(2)	128.24(13)
C(3)-C(4)-C(5)	107.68(12)
C(3)-C(4)-H(4)	126.2
C(5)-C(4)-H(4)	126.2
C(4)-C(5)-C(6)	107.07(12)
C(4)-C(5)-H(5)	126.5
C(6)-C(5)-H(5)	126.5
N(2)-C(6)-C(5)	107.88(12)
N(2)-C(6)-C(7)	125.91(12)
C(5)-C(6)-C(7)	126.14(12)
N(3)-C(7)-C(14)	120.17(12)

Table C.8.1. continued…

N(3)-C(7)-C(6)	111.85(12)
C(14)-C(7)-C(6)	127.94(12)
N(3)-C(8)-C(13)	120.41(12)
N(3)-C(8)-C(9)	120.47(13)
C(13)-C(8)-C(9)	119.10(13)
C(10)-C(9)-C(8)	120.05(14)
C(10)-C(9)-H(9)	120.0
C(8)-C(9)-H(9)	120.0
C(9)-C(10)-C(11)	120.76(13)
C(9)-C(10)-H(10)	119.6
C(11)-C(10)-H(10)	119.6
C(12)-C(11)-C(10)	120.39(14)
C(12)-C(11)-H(11)	119.8
C(10)-C(11)-H(11)	119.8
C(11)-C(12)-C(13)	119.89(14)
C(11)-C(12)-H(12)	120.1
C(13)-C(12)-H(12)	120.1
N(4)-C(13)-C(8)	120.61(12)
N(4)-C(13)-C(12)	119.57(12)
C(8)-C(13)-C(12)	119.80(12)
N(4)-C(14)-C(7)	119.31(12)
N(4)-C(14)-C(15)	111.41(11)
C(7)-C(14)-C(15)	129.25(12)
N(5)-C(15)-C(16)	110.73(11)
N(5)-C(15)-C(14)	126.34(12)
C(16)-C(15)-C(14)	122.93(12)
C(17)-C(16)-C(15)	106.66(12)
C(17)-C(16)-H(16)	126.7
C(15)-C(16)-H(16)	126.7
C(16)-C(17)-C(18)	106.48(13)
C(16)-C(17)-H(17)	126.8
C(18)-C(17)-H(17)	126.8
N(5)-C(18)-C(19)	124.47(12)
N(5)-C(18)-C(17)	110.36(12)
C(19)-C(18)-C(17)	125.15(13)
N(6)-C(19)-C(18)	127.65(13)
N(6)-C(19)-H(19)	116.2

Table C.8.1. continued…

C(18)-C(19)-H(19)	116.2
N(6)-C(20)-H(20A)	109.5
N(6)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
N(6)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(2)-N(1)-C(1)	115.86(12)
C(3)-N(2)-C(6)	109.47(12)
C(3)-N(2)-H(101)	128.2(10)
C(6)-N(2)-H(101)	122.3(10)
C(7)-N(3)-C(8)	119.61(12)
C(14)-N(4)-C(13)	119.85(12)
C(15)-N(5)-C(18)	105.77(11)
C(19)-N(6)-C(20)	121.92(13)
C(19)-N(6)-H(102)	121.2(10)
C(20)-N(6)-H(102)	116.8(10)

Table C.8.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L9. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	27(1)	36(1)	31(1)	-8(1)	10(1)	-2(1)
C(2)	26(1)	25(1)	21(1)	-2(1)	6(1)	-6(1)
C(3)	23(1)	21(1)	21(1)	0(1)	4(1)	-6(1)
C(4)	32(1)	22(1)	22(1)	2(1)	4(1)	-3(1)
C(5)	27(1)	19(1)	24(1)	1(1)	2(1)	2(1)
C(6)	19(1)	17(1)	23(1)	-2(1)	2(1)	-2(1)
C(7)	18(1)	18(1)	22(1)	-4(1)	1(1)	-3(1)
C(8)	20(1)	20(1)	24(1)	-6(1)	2(1)	-3(1)
C(9)	24(1)	21(1)	30(1)	-2(1)	3(1)	1(1)
C(10)	24(1)	28(1)	32(1)	-9(1)	4(1)	4(1)
C(11)	26(1)	35(1)	29(1)	-7(1)	10(1)	1(1)
C(12)	28(1)	30(1)	25(1)	-2(1)	8(1)	1(1)
C(13)	20(1)	22(1)	22(1)	-6(1)	3(1)	-2(1)
C(14)	19(1)	20(1)	19(1)	-4(1)	1(1)	-3(1)
C(15)	20(1)	20(1)	20(1)	-2(1)	2(1)	-1(1)
C(16)	23(1)	24(1)	26(1)	3(1)	7(1)	-1(1)
C(17)	26(1)	20(1)	26(1)	4(1)	4(1)	1(1)
C(18)	22(1)	18(1)	22(1)	0(1)	2(1)	0(1)
C(19)	24(1)	19(1)	24(1)	-1(1)	1(1)	0(1)
C(20)	24(1)	28(1)	43(1)	-1(1)	10(1)	3(1)
N(1)	22(1)	25(1)	24(1)	-5(1)	6(1)	-3(1)
N(2)	20(1)	20(1)	22(1)	2(1)	4(1)	-1(1)
N(3)	20(1)	20(1)	26(1)	-2(1)	2(1)	-1(1)
N(4)	21(1)	23(1)	22(1)	-3(1)	3(1)	0(1)
N(5)	20(1)	20(1)	21(1)	1(1)	3(1)	1(1)
N(6)	22(1)	22(1)	29(1)	-1(1)	7(1)	1(1)

Table C.8.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L9.

	x	y	z	U(eq)
H(1A)	8343	803	-623	46
H(1B)	8182	-89	-244	46
H(1C)	9272	497	778	46
H(2)	6451	1465	-773	29
H(4)	3987	2446	-1124	31
H(5)	1927	2584	-85	30
H(9)	-1470	2863	1527	32
H(10)	-3284	2681	2538	35
H(11)	-3050	1643	3987	36
H(12)	-981	794	4427	33
H(16)	2476	-524	4299	29
H(17)	4740	-1386	4484	30
H(19)	7086	-1301	3620	28
H(20A)	9149	-1352	3009	48
H(20B)	9759	-511	2753	48
H(20C)	8808	-1046	1579	48
H(101)	4710(20)	815(11)	1667(17)	54(5)
H(102)	7149(18)	-101(10)	1989(15)	39(5)

Table C.8.4: Torsion angles [°] for H_2L9.

N(1)-C(2)-C(3)-N(2)	-0.7(2)
N(1)-C(2)-C(3)-C(4)	179.78(14)
N(2)-C(3)-C(4)-C(5)	-0.17(15)
C(2)-C(3)-C(4)-C(5)	179.40(13)
C(3)-C(4)-C(5)-C(6)	0.10(15)
C(4)-C(5)-C(6)-N(2)	0.01(14)
C(4)-C(5)-C(6)-C(7)	-176.93(12)
N(2)-C(6)-C(7)-N(3)	177.51(12)
C(5)-C(6)-C(7)-N(3)	-6.09(18)
N(2)-C(6)-C(7)-C(14)	-4.5(2)
C(5)-C(6)-C(7)-C(14)	171.93(13)
N(3)-C(8)-C(9)-C(10)	177.93(12)
C(13)-C(8)-C(9)-C(10)	-0.63(19)
C(8)-C(9)-C(10)-C(11)	0.5(2)
C(9)-C(10)-C(11)-C(12)	0.2(2)
C(10)-C(11)-C(12)-C(13)	-0.7(2)
N(3)-C(8)-C(13)-N(4)	-0.25(19)
C(9)-C(8)-C(13)-N(4)	178.30(12)
N(3)-C(8)-C(13)-C(12)	-178.44(12)
C(9)-C(8)-C(13)-C(12)	0.11(19)
C(11)-C(12)-C(13)-N(4)	-177.63(13)
C(11)-C(12)-C(13)-C(8)	0.6(2)
N(3)-C(7)-C(14)-N(4)	0.21(18)
C(6)-C(7)-C(14)-N(4)	-177.66(12)
N(3)-C(7)-C(14)-C(15)	178.02(12)
C(6)-C(7)-C(14)-C(15)	0.2(2)
N(4)-C(14)-C(15)-N(5)	-173.68(12)
C(7)-C(14)-C(15)-N(5)	8.4(2)
N(4)-C(14)-C(15)-C(16)	5.90(17)
C(7)-C(14)-C(15)-C(16)	-172.05(13)
N(5)-C(15)-C(16)-C(17)	0.26(15)
C(14)-C(15)-C(16)-C(17)	-179.38(12)
C(15)-C(16)-C(17)-C(18)	-0.10(15)
C(16)-C(17)-C(18)-N(5)	-0.09(16)
C(16)-C(17)-C(18)-C(19)	178.62(13)
N(5)-C(18)-C(19)-N(6)	-2.7(2)

Table C.8.4. continued…

C(17)-C(18)-C(19)-N(6)	178.73(13)
C(3)-C(2)-N(1)-C(1)	179.71(12)
C(4)-C(3)-N(2)-C(6)	0.18(15)
C(2)-C(3)-N(2)-C(6)	-179.41(12)
C(5)-C(6)-N(2)-C(3)	-0.12(14)
C(7)-C(6)-N(2)-C(3)	176.83(12)
C(14)-C(7)-N(3)-C(8)	-1.94(18)
C(6)-C(7)-N(3)-C(8)	176.25(11)
C(13)-C(8)-N(3)-C(7)	1.97(18)
C(9)-C(8)-N(3)-C(7)	-176.56(12)
C(7)-C(14)-N(4)-C(13)	1.50(18)
C(15)-C(14)-N(4)-C(13)	-176.68(11)
C(8)-C(13)-N(4)-C(14)	-1.49(18)
C(12)-C(13)-N(4)-C(14)	176.70(12)
C(16)-C(15)-N(5)-C(18)	-0.31(14)
C(14)-C(15)-N(5)-C(18)	179.32(12)
C(19)-C(18)-N(5)-C(15)	-178.47(12)
C(17)-C(18)-N(5)-C(15)	0.24(14)
C(18)-C(19)-N(6)-C(20)	179.32(13)

C.9: Full crystallographic Data Tables of H_2L12

Table C.9.1: Bond lengths [Å] and angles [°] for H_2L12

C(1)-N(1)	1.3633(12)
C(1)-C(2)	1.3750(15)
C(1)-H(1)	0.9500
C(2)-C(3)	1.4132(14)
C(2)-H(2)	0.9500
C(3)-C(4)	1.3838(13)
C(3)-H(3)	0.9500
C(4)-N(1)	1.3743(14)
C(4)-C(5)	1.4427(13)
C(5)-N(2)	1.2772(12)
C(5)-H(5)	0.9500
C(6)-N(2)	1.4670(11)
C(6)-C(7)	1.5297(13)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(7)#1	1.5265(16)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
N(1)-H(11)	0.927(14)
N(1)-C(1)-C(2)	109.01(8)
N(1)-C(1)-H(1)	125.5
C(2)-C(1)-H(1)	125.5
C(1)-C(2)-C(3)	106.68(9)
C(1)-C(2)-H(2)	126.7
C(3)-C(2)-H(2)	126.7
C(4)-C(3)-C(2)	107.71(9)
C(4)-C(3)-H(3)	126.1
C(2)-C(3)-H(3)	126.1
N(1)-C(4)-C(3)	107.60(8)
N(1)-C(4)-C(5)	125.22(8)
C(3)-C(4)-C(5)	127.14(9)
N(2)-C(5)-C(4)	124.69(9)
N(2)-C(5)-H(5)	117.7

Table C.9.1. continued…

C(4)-C(5)-H(5)	117.7
N(2)-C(6)-C(7)	110.51(8)
N(2)-C(6)-H(6A)	109.5
C(7)-C(6)-H(6A)	109.5
N(2)-C(6)-H(6B)	109.5
C(7)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	108.1
C(7)#1-C(7)-C(6)	112.78(9)
C(7)#1-C(7)-H(7A)	109.0
C(6)-C(7)-H(7A)	109.0
C(7)#1-C(7)-H(7B)	109.0
C(6)-C(7)-H(7B)	109.0
H(7A)-C(7)-H(7B)	107.8
C(1)-N(1)-C(4)	109.00(8)
C(1)-N(1)-H(11)	126.0(8)
C(4)-N(1)-H(11)	124.9(8)
C(5)-N(2)-C(6)	115.99(8)

Table C.9.2: Anisotropic displacement parameters ($Å^2 x\ 10^3$)for H_2L12. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	18(1)	28(1)	28(1)	-2(1)	1(1)	2(1)
C(2)	19(1)	32(1)	24(1)	-2(1)	2(1)	-2(1)
C(3)	20(1)	27(1)	24(1)	-4(1)	6(1)	-1(1)
C(4)	17(1)	22(1)	22(1)	0(1)	6(1)	-2(1)
C(5)	18(1)	21(1)	24(1)	0(1)	8(1)	-1(1)
C(6)	16(1)	20(1)	26(1)	2(1)	4(1)	2(1)
C(7)	16(1)	22(1)	26(1)	5(1)	5(1)	2(1)
N(1)	17(1)	23(1)	25(1)	-3(1)	2(1)	0(1)
N(2)	15(1)	22(1)	25(1)	1(1)	5(1)	0(1)

Table C.9.3: Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for H_2L12.

	x	y	z	U(eq)
H(1)	4337	-3026	6832	30
H(2)	4455	502	8054	30
H(3)	3258	3214	7644	28
H(5)	1984	3041	6253	25
H(6A)	908	1687	4287	24
H(6B)	965	3117	5296	24
H(7A)	483	-2204	4985	25
H(7B)	460	-541	5924	25
H(11)	3123(7)	-2480(30)	5699(9)	34(3)

Table C.9.4: Torsion angles [°] for H_2L12.

N(1)-C(1)-C(2)-C(3)	-0.26(11)
C(1)-C(2)-C(3)-C(4)	0.11(11)
C(2)-C(3)-C(4)-N(1)	0.07(10)
C(2)-C(3)-C(4)-C(5)	178.09(8)
N(1)-C(4)-C(5)-N(2)	3.10(14)
C(3)-C(4)-C(5)-N(2)	-174.59(9)
N(2)-C(6)-C(7)-C(7)#1	-172.89(9)
C(2)-C(1)-N(1)-C(4)	0.32(10)
C(3)-C(4)-N(1)-C(1)	-0.24(10)
C(5)-C(4)-N(1)-C(1)	-178.30(8)
C(4)-C(5)-N(2)-C(6)	176.15(8)
C(7)-C(6)-N(2)-C(5)	-110.86(10)