

Synthesis, Characterization and Biological Evaluation of Dipicolylamine Sulfonamide Derivatized Platinum Complexes as Potential Anticancer Agents

Supporting Information

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1. Selected bond distances for N(SO₂(2-nap))dpa

Table S1. Selected bond distances for N(SO₂(2-nap))dpa

	Bond length (Å)			Bond length (Å)	
	Actual	Calculated		Actual	Calculated
S1-O1	1.4350 (6)	1.4324	S1-C13	1.7692 (6)	1.7688
S1-O2	1.4352 (6)	1.4333	C13-C22	1.4191 (9)	1.4140
S1-N2	1.6277 (6)	1.6314	N2-C7	1.4712 (9)	1.4584
S1-C13	1.7692 (6)	1.7653	N2-C6	1.4752 (9)	1.4613
N1-C5	1.3359 (10)	1.3306	N3-C8	1.3401 (10)	1.3313
N1-C1	1.3462 (11)	1.3317	N3-C12	1.3412 (11)	1.3303

2. Selected bond angles for N(SO₂(2-nap))dpa

Table S2. Selected bond angles for N(SO₂(2-nap))dpa

	Bond angle (deg)			Bond angle (deg)	
	Actual	Calculated		Actual	Calculated
O2-S1-O1	119.64 (4)	119.83	C5-N1-C1	117.09 (7)	117.98
O2-S1-N2	106.94 (3)	107.10	C7-N2-C6	117.13 (6)	116.42
O1-S1-N2	106.83 (3)	106.95	C7-N2-S1	115.64 (5)	117.96
O2-S1-C13	107.29 (3)	108.11	C6-N2-S1	119.61 (5)	119.67
O1-S1-C13	107.43 (3)	107.99	C8-N3-C12	117.61 (7)	118.16
N2-S1-C13	108.30 (3)	106.05	N1-C1-C2	123.93 (8)	123.38

3. Experimental emission (Em) wavelengths of compounds

Table S3. Experimental emission (Em) wavelengths of N(SO₂(2-nap))dpa, [PtCl₂(N(SO₂(2-nap))dpa)], N(SO₂(1-nap))dpa, [PtCl₂(N(SO₂(1-nap))dpa)] and [PtCl₂(NSO₂pipdpa)] in methanol.

Test sample	Em (nm)
N(SO ₂ (2-nap))dpa	343
[PtCl ₂ (N(SO ₂ (2-nap))dpa)]	612
N(SO ₂ (1-nap))dpa	342
[PtCl ₂ (N(SO ₂ (1-nap))dpa)]	615
[PtCl ₂ (N(SO ₂ pip)dpa)]	611

4. Emission spectra of Pt complexes in methanol excited at 275 nm

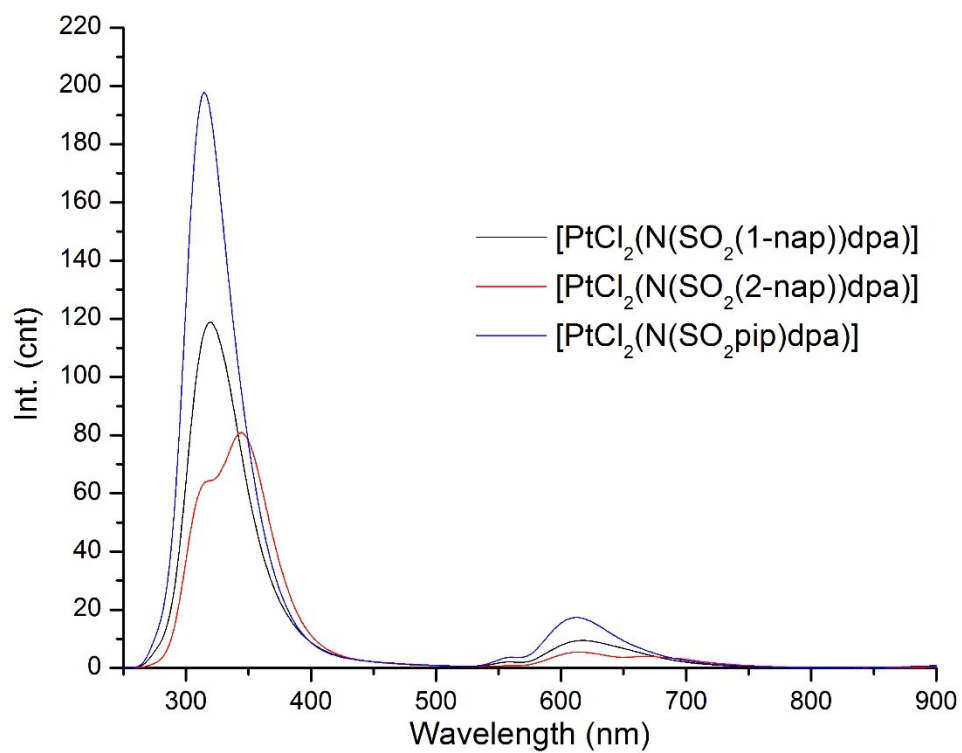


Figure S1: Emission spectra of Pt complexes in methanol excited at 275nm

5. Kohn-Sham frontier molecular orbitals of the optimized ground state structures of $[\text{PtCl}_2(\text{N}(\text{SO}_2(1\text{-nap})\text{dpa}))]$ and $[\text{PtCl}_2(\text{N}(\text{SO}_2\text{pip})\text{dpa})]$ complexes

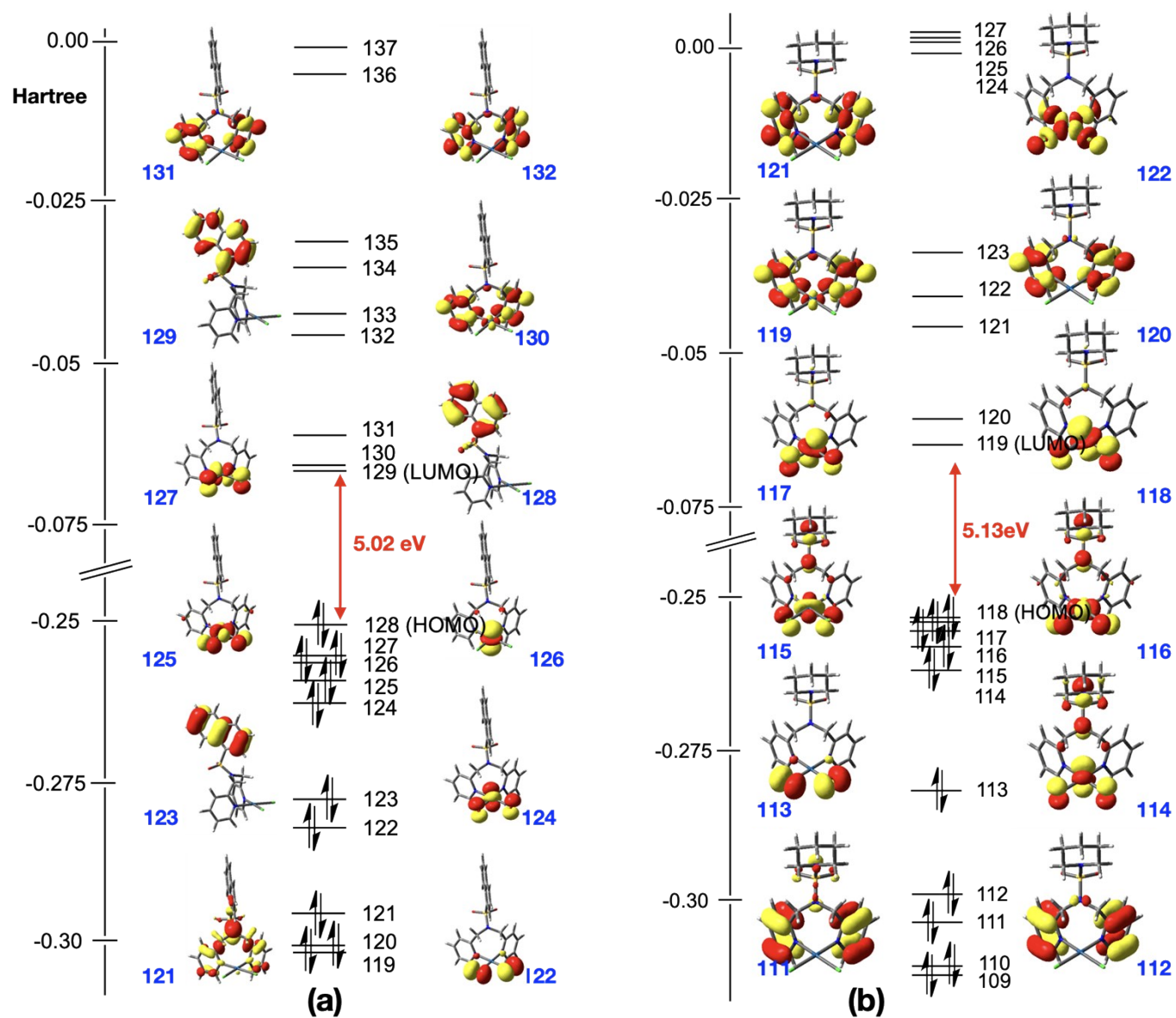


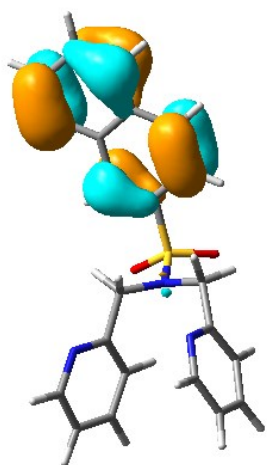
Figure S2. Kohn-Sham frontier molecular orbitals of the optimized structures of (a) $[\text{PtCl}_2(\text{N}(\text{SO}_2(1\text{-nap})\text{dpa}))]$ and (b) $[\text{PtCl}_2(\text{N}(\text{SO}_2\text{pip})\text{dpa})]$.

6. TDDFT results for N(SO₂(2-nap))dpa and [PtCl₂(N(SO₂(2-nap))dpa)] systems

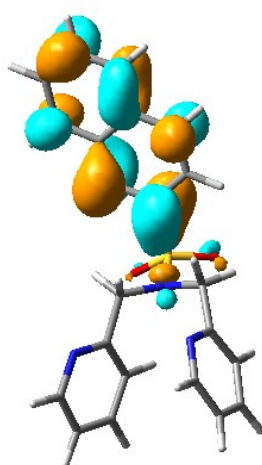
N(SO₂(2-nap))dpa system

Excited State 1: Singlet-?Sym 4.2868 eV 289.23 nm f=0.0651 <S**2>=0.000

101 ->103	0.16166
102 ->103	0.63276
102 ->104	-0.13264
102 ->105	0.11826



HOMO



LUMO

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-DFT) = -1561.53864624

Copying the excited state density for this state as the 1-particle RhoCl density.

Excited state symmetry could not be determined.

Excited State 2: Singlet-?Sym 4.4607 eV 277.95 nm f=0.0170 <S**2>=0.000

97 ->103	-0.10183
99 ->103	0.13310
100 ->103	0.16912
101 ->103	0.37935
102 ->103	-0.26780
102 ->104	-0.37215
102 ->105	0.25788

Excited state symmetry could not be determined.

Excited State 3: Singlet-?Sym 4.9643 eV 249.75 nm f=0.1671 <S**2>=0.000

98 ->103	-0.16725
98 ->104	0.22833
98 ->105	0.26700
98 ->106	0.13534
98 ->107	-0.18253
99 ->103	0.11099
99 ->104	-0.14775
99 ->105	-0.11032
99 ->106	0.12858
101 ->103	-0.24534
101 ->104	0.18181
101 ->105	0.14153
102 ->104	-0.25931

Excited state symmetry could not be determined.

Excited State 4: Singlet-?Sym 5.0036 eV 247.79 nm f=0.0083 <S**2>=0.000

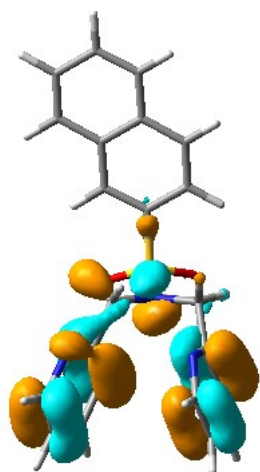
98 ->103	0.11255
98 ->104	-0.24101
98 ->105	-0.27832
99 ->104	-0.26691
99 ->105	-0.20012
99 ->106	0.28264
99 ->107	-0.21859
101 ->104	0.11553
101 ->106	-0.15157
101 ->107	0.11551

Excited state symmetry could not be determined.

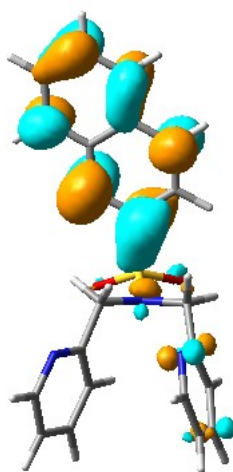
Excited State 5: Singlet-?Sym 5.0776 eV 244.18 nm f=0.2415 <S**2>=0.000

96 ->103	0.10542
99 ->104	-0.12325

99 ->105	-0.10136
99 ->106	0.11893
100 ->103	-0.38470
100 ->104	0.10280
101 ->103	0.43933
102 ->104	0.13514



HOTO

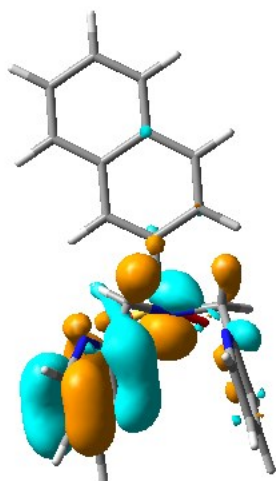


LUTO

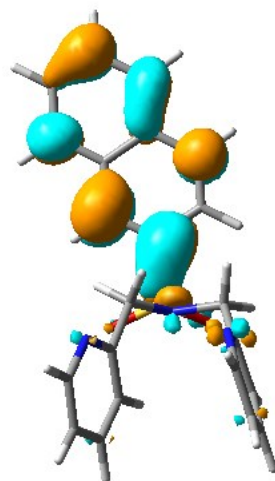
Excited state symmetry could not be determined.

Excited State 6: Singlet-?Sym 5.1089 eV 242.68 nm f=0.2962 <S**2>=0.000

96 ->103	0.12567
97 ->103	0.11427
98 ->104	0.12184
98 ->105	0.17995
98 ->106	0.12539
99 ->103	-0.10048
100 ->103	0.49784
101 ->103	0.11447
102 ->104	0.25705



HOTO



LUTO

Excited state symmetry could not be determined.

Excited State 7: Singlet-?Sym 5.2126 eV 237.86 nm f=0.0031 <S**2>=0.000

98 ->103	-0.13284
99 ->103	0.18435
100 ->103	-0.14726
102 ->104	0.34330
102 ->105	0.50265

Excited state symmetry could not be determined.

Excited State 8: Singlet-?Sym 5.2607 eV 235.68 nm f=0.0044 <S**2>=0.000

98 ->104	-0.10312
98 ->105	0.11165
98 ->106	0.35890
98 ->107	0.37067
98 ->108	-0.17284
99 ->103	0.13565
100 ->105	0.12211
100 ->107	0.10377
101 ->104	-0.10232
101 ->106	0.12306
101 ->107	0.11776
102 ->106	-0.16523
102 ->107	-0.13352

Excited state symmetry could not be determined.

Excited State 9: Singlet-?Sym 5.3032 eV 233.79 nm f=0.0306 <S**2>=0.000

95 ->106	-0.10350
100 ->103	0.15625
100 ->104	0.37669
100 ->105	0.32562
100 ->106	-0.11139
101 ->104	-0.21416
101 ->105	-0.22494
102 ->106	0.11737

Excited state symmetry could not be determined.

Excited State 10: Singlet-?Sym 5.3772 eV 230.58 nm f=0.1415 <S**2>=0.000

98 ->106	0.17101
98 ->107	0.16086
99 ->103	-0.30685
99 ->105	0.10291
99 ->106	0.14851
99 ->107	0.11380
99 ->108	0.23771
101 ->104	0.13725
101 ->108	-0.12633
102 ->105	0.22599
102 ->106	0.31474

Excited state symmetry could not be determined.

Excited State 11: Singlet-?Sym 5.4255 eV 228.52 nm f=0.1441 <S**2>=0.000

97 ->103	0.11312
98 ->103	0.10344
99 ->103	0.41816
99 ->105	0.10043
99 ->106	0.13598

99 ->107	0.17871
99 ->108	0.25353
100 ->104	-0.11156
100 ->107	-0.10820
101 ->106	-0.15049
101 ->108	-0.11848
102 ->105	-0.12361
102 ->107	0.15587

Excited state symmetry could not be determined.

Excited State 12: Singlet-?Sym 5.4390 eV 227.95 nm f=0.0082 <S**2>=0.000

99 ->103	0.20135
99 ->106	-0.16286
99 ->108	-0.22272
102 ->106	0.52072
102 ->107	-0.12024

Excited state symmetry could not be determined.

Excited State 13: Singlet-?Sym 5.4691 eV 226.70 nm f=0.0469 <S**2>=0.000

98 ->103	0.46091
100 ->104	0.16426
101 ->104	0.17124
101 ->107	-0.10530
102 ->105	0.13361
102 ->107	0.35507

Excited state symmetry could not be determined.

Excited State 14: Singlet-?Sym 5.4963 eV 225.58 nm f=0.0258 <S**2>=0.000

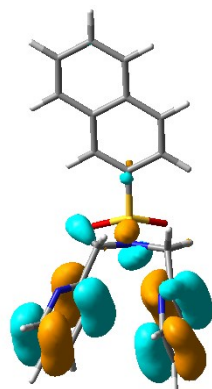
97 ->105	-0.10049
98 ->103	-0.20123
99 ->103	-0.16593
99 ->108	-0.12099
100 ->106	0.19496

100 ->107 -0.10315
101 ->104 -0.16319
102 ->107 0.46401

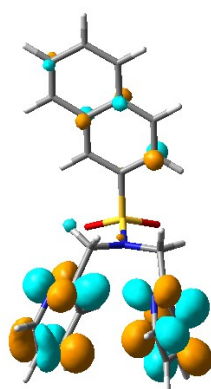
Excited state symmetry could not be determined.

Excited State 15: Singlet-?Sym 5.5432 eV 223.67 nm f=0.1390 <S**2>=0.000

94 ->107 0.12480
95 ->108 0.13849
97 ->104 -0.11111
97 ->105 -0.13658
98 ->103 0.21419
99 ->103 -0.12563
100 ->106 0.34110
100 ->107 -0.10003
101 ->104 0.19453
101 ->105 -0.19620
101 ->106 -0.15902
102 ->107 -0.22615



HOMO



LUMO

Excited state symmetry could not be determined.

Excited State 16: Singlet-?Sym 5.5691 eV 222.63 nm f=0.0291 <S**2>=0.000

97 ->103 0.51715
98 ->103 -0.25483
98 ->107 0.12523

101 ->104 0.28321

Excited state symmetry could not be determined.

Excited State 17: Singlet-?Sym 5.6325 eV 220.12 nm f=0.3422 <S**2>=0.000

97 ->103 0.26505
98 ->103 0.15067
98 ->107 -0.10013
99 ->106 0.10228
99 ->107 -0.10401
100 ->104 -0.12267
100 ->105 -0.25727
100 ->106 -0.17153
100 ->107 0.14791
101 ->104 -0.25454
101 ->105 -0.20783
101 ->106 0.10792
102 ->104 -0.17950
102 ->106 -0.12352

Excited state symmetry could not be determined.

Excited State 18: Singlet-?Sym 5.7063 eV 217.28 nm f=0.1358 <S**2>=0.000

96 ->103 -0.18879
96 ->105 0.11145
97 ->103 0.24773
100 ->105 0.11517
100 ->107 -0.11027
101 ->104 -0.22353
101 ->105 0.46062
102 ->105 0.12804

Excited state symmetry could not be determined.

Excited State 19: Singlet-?Sym 5.7256 eV 216.54 nm f=0.0154 <S**2>=0.000

100 ->104 -0.36421

100 ->105 0.32171
100 ->107 0.40300
101 ->107 -0.23555

Excited state symmetry could not be determined.

Excited State 20: Singlet-?Sym 5.7737 eV 214.74 nm f=0.1385 <S**2>=0.000

93 ->103 -0.23409
96 ->103 0.39177
97 ->104 0.14998
99 ->105 0.10048
101 ->106 -0.13230
102 ->108 -0.13241
102 ->109 0.38003

Excited state symmetry could not be determined.

Excited State 21: Singlet-?Sym 5.7927 eV 214.03 nm f=0.0061 <S**2>=0.000

96 ->103 0.22175
97 ->106 0.10403
99 ->104 -0.23466
99 ->105 -0.12896
100 ->106 0.17102
101 ->106 0.41577
101 ->107 -0.24871
102 ->106 0.10264
102 ->107 -0.10198

Excited state symmetry could not be determined.

Excited State 22: Singlet-?Sym 5.8145 eV 213.23 nm f=0.0210 <S**2>=0.000

93 ->103 0.12667
97 ->103 0.10945
97 ->104 0.20418
97 ->105 0.25967
97 ->106 0.11386

99 ->105	0.10717
99 ->106	0.11966
99 ->107	-0.11588
100 ->105	0.20934
100 ->106	0.16295
101 ->106	0.17584
101 ->107	0.21508
102 ->108	0.18885
102 ->109	-0.16894

Excited state symmetry could not be determined.

Excited State 23: Singlet-?Sym 5.8324 eV 212.58 nm f=0.0160 <S**2>=0.000

93 ->103	0.10303
96 ->103	0.12172
100 ->104	0.24820
100 ->105	-0.24250
100 ->106	0.30841
100 ->107	0.35195
101 ->104	-0.11678
101 ->105	0.12471
101 ->106	-0.14329
101 ->107	-0.10376
102 ->108	0.18408
102 ->109	-0.11908

Excited state symmetry could not be determined.

Excited State 24: Singlet-?Sym 5.8608 eV 211.55 nm f=0.0223 <S**2>=0.000

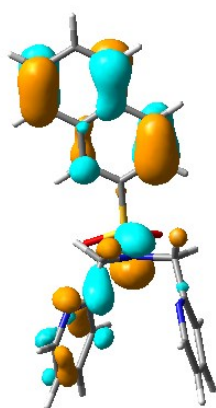
96 ->103	0.19093
97 ->104	-0.17662
97 ->105	-0.16147
97 ->107	0.10984
98 ->106	-0.14097
99 ->108	0.12392

100 ->106	-0.12193
100 ->107	0.10901
101 ->105	0.13757
101 ->106	0.14126
101 ->107	0.30626
101 ->108	-0.10301
102 ->108	0.27833

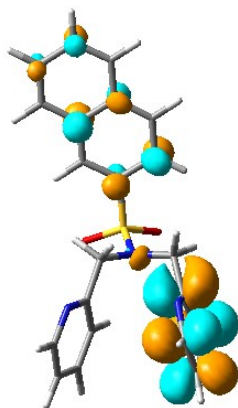
Excited state symmetry could not be determined.

Excited State 25: Singlet-?Sym 5.8898 eV 210.51 nm f=0.1247 <S**2>=0.000

96 ->103	0.22552
99 ->105	-0.10836
99 ->108	-0.10793
100 ->104	-0.10129
100 ->106	-0.17044
100 ->107	-0.21447
101 ->106	-0.19519
101 ->107	-0.25541
102 ->108	0.35906



HOMO



LUMO

Excited state symmetry could not be determined.

Excited State 26: Singlet-?Sym 5.9254 eV 209.24 nm f=0.0849 <S**2>=0.000

93 ->103	-0.24565
96 ->103	-0.27757

97 ->104	0.10287
98 ->104	0.10845
99 ->104	-0.15420
102 ->108	0.38867
102 ->109	0.29626

Excited state symmetry could not be determined.

Excited State 27: Singlet-?Sym 5.9708 eV 207.65 nm f=0.0906 <S**2>=0.000

93 ->103	-0.12878
97 ->104	-0.14813
98 ->104	-0.31343
98 ->106	0.22397
98 ->107	-0.28428
99 ->104	0.31667
99 ->106	0.11622
99 ->107	-0.12309
101 ->104	0.11537
102 ->108	0.10084
102 ->109	0.13354

Excited state symmetry could not be determined.

Excited State 28: Singlet-?Sym 5.9857 eV 207.14 nm f=0.0108 <S**2>=0.000

97 ->104	0.27469
97 ->106	-0.26678
97 ->107	0.19965
98 ->104	-0.16654
98 ->106	0.17415
98 ->107	-0.21082
99 ->104	-0.18311
99 ->105	-0.10650
99 ->106	-0.22837
99 ->107	0.19096
101 ->107	0.12036

Excited state symmetry could not be determined.

Excited State 29: Singlet-?Sym 6.0560 eV 204.73 nm f=0.0728 <S**2>=0.000

96 ->104	0.16803
97 ->105	-0.10400
98 ->106	0.12610
99 ->104	-0.27945
99 ->105	0.50735
99 ->108	-0.14096
101 ->105	0.10374
101 ->108	0.11374

Excited state symmetry could not be determined.

Excited State 30: Singlet-?Sym 6.0776 eV 204.00 nm f=0.0062 <S**2>=0.000

95 ->103	0.66679
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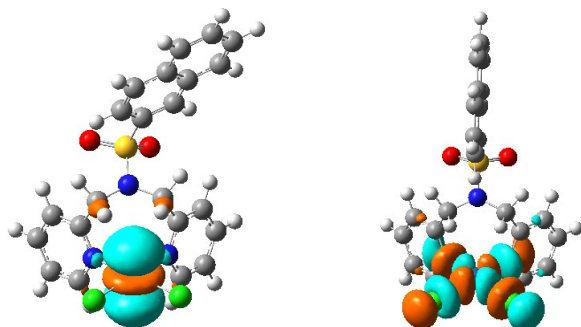
[PtCl₂(N(SO₂(2-nap))dpa)] system

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: Singlet-?Sym 3.6564 eV 339.08 nm f=0.0002 <S**2>=0.000

126 -> 133	0.64213
126 -> 134	0.14491
127 -> 133	-0.17437
128 -> 133	0.13091



HOTO**LUTO**

Excited State 2: Singlet-?Sym 3.7971 eV 326.52 nm f=0.0007 <S**2>=0.000

124 -> 133 0.15356

125 -> 133 0.64762

125 -> 134 0.14541

Excited State 3: Singlet-?Sym 3.8400 eV 322.87 nm f=0.0003 <S**2>=0.000

115 -> 133 0.12577

126 -> 133 0.16908

127 -> 133 0.64223

127 -> 134 0.14403

Excited state symmetry could not be determined.

Excited State 4: Singlet-?Sym 3.9452 eV 314.26 nm f=0.0006 <S**2>=0.000

114 -> 133 -0.11033

124 -> 133 0.60912

124 -> 134 0.13579

125 -> 133 -0.13554

127 -> 129 -0.16861

127 -> 130 0.14689

Excited State 5: Singlet-?Sym 3.9979 eV 310.12 nm f=0.0003 <S**2>=0.000

126 -> 129 0.49463

126 -> 130 -0.43537

127 -> 129 -0.13272

127 -> 130 0.11942

128 -> 129 0.12138

128 -> 130 -0.10163

Excited State 6: Singlet-?Sym 4.1498 eV 298.77 nm f=0.0002 <S**2>=0.000

126 -> 129	0.14560
126 -> 130	0.11171
126 -> 131	0.54325
127 -> 129	0.22058
127 -> 130	-0.25888
127 -> 131	-0.11840
128 -> 131	0.13382

Excited State 7: Singlet-?Sym 4.1561 eV 298.32 nm f=0.0004 <S**2>=0.000

124 -> 133	0.18358
126 -> 130	-0.19505
126 -> 131	-0.30113
127 -> 129	0.42928
127 -> 130	-0.32986
127 -> 131	0.13647

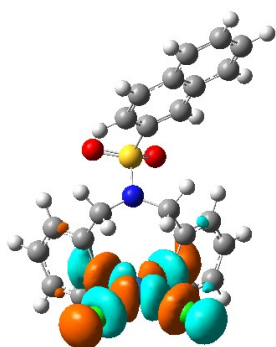
Excited State 8: Singlet-?Sym 4.2545 eV 291.42 nm f=0.0094 <S**2>=0.000

124 -> 129	0.39745
124 -> 130	-0.36024
125 -> 129	-0.14635
125 -> 130	0.13510
127 -> 131	-0.30099
128 -> 129	-0.20146

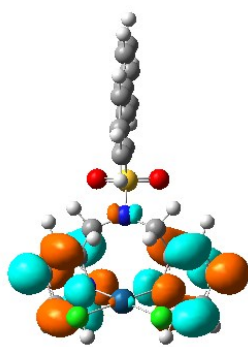
Excited State 9: Singlet-?Sym 4.2665 eV 290.60 nm f=0.0472 <S**2>=0.000

123 -> 129	0.11884
123 -> 130	0.12685
123 -> 132	0.11165

124 -> 129 0.12759
 127 -> 131 -0.12942
 128 -> 129 0.44555
 128 -> 130 0.36584
 128 -> 131 -0.11746
 128 -> 134 0.15196



HOTO



LUTO

Excited State 10: Singlet-?Sym 4.2821 eV 289.54 nm f=0.0005 <S**2>=0.000

124 -> 129 0.27186
 124 -> 130 -0.22822
 126 -> 131 0.14721
 127 -> 130 0.18073
 127 -> 131 0.54097

Excited State 11: Singlet-?Sym 4.3982 eV 281.89 nm f=0.0139 <S**2>=0.000

124 -> 130 0.17764
 124 -> 131 0.50464
 125 -> 129 -0.11139
 125 -> 131 -0.39154
 128 -> 131 -0.12723

Excited State 12: Singlet-?Sym 4.4081 eV 281.27 nm f=0.0562 <S**2>=0.000

124 -> 129 0.17263

124 -> 130 -0.10635

125 -> 129 0.49304

125 -> 130 -0.43023

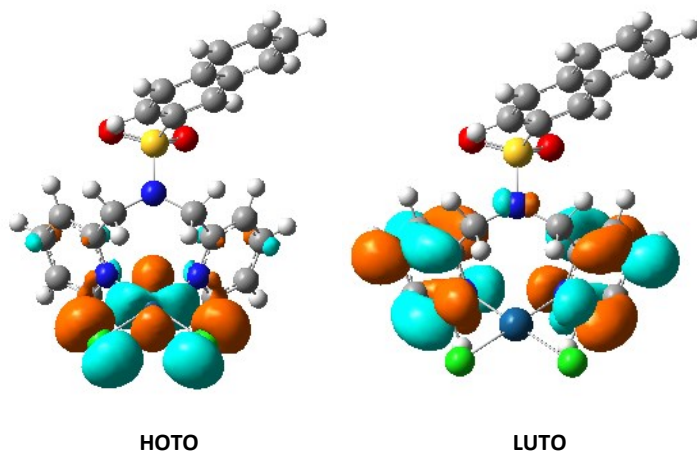
Excited State 13: Singlet-?Sym 4.4514 eV 278.53 nm f=0.0536 <S**2>=0.000

124 -> 130 0.12096

124 -> 131 0.40352

125 -> 130 0.16800

125 -> 131 0.51053



Excited State 14: Singlet-?Sym 4.4760 eV 277.00 nm f=0.0291 <S**2>=0.000

123 -> 129 0.32742

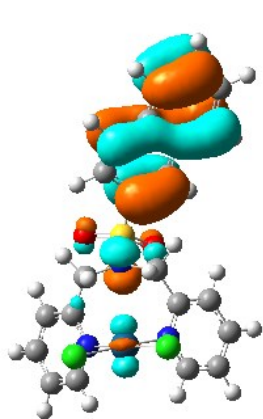
123 -> 130 0.24047

128 -> 129 -0.26463

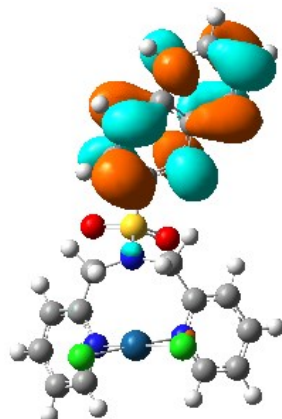
128 -> 130 -0.10373

128 -> 132 -0.28380

128 -> 134 0.31203



HOTO



LUTO

Excited State 15: Singlet-?Sym 4.5467 eV 272.69 nm f=0.0021 <S**2>=0.000

126 -> 129 0.14316

128 -> 129 -0.34901

128 -> 130 0.55483

Excited State 16: Singlet-?Sym 4.5806 eV 270.68 nm f=0.0028 <S**2>=0.000

126 -> 129 0.35480

126 -> 130 0.39542

126 -> 131 -0.17077

126 -> 132 -0.28295

126 -> 134 -0.16242

127 -> 129 -0.10737

127 -> 130 -0.11712

128 -> 132 -0.14148

Excited State 17: Singlet-?Sym 4.6428 eV 267.05 nm f=0.0001 <S**2>=0.000

126 -> 129 0.11558

126 -> 130 0.12562

127 -> 129 0.40305

127 -> 130 0.43365

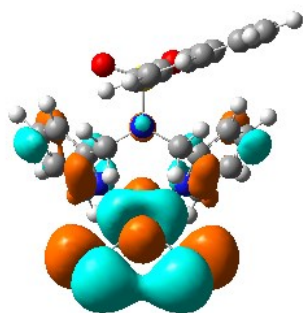
127 -> 131 -0.20934
127 -> 132 -0.22334
127 -> 134 -0.10870

Excited State 18: Singlet-?Sym 4.6563 eV 266.27 nm f=0.0025 <S**2>=0.000

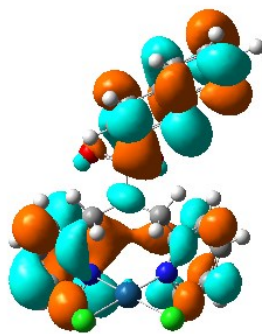
123 -> 131 -0.10342
126 -> 131 -0.15117
128 -> 129 0.16085
128 -> 131 0.64099

Excited State 19: Singlet-?Sym 4.7503 eV 261.00 nm f=0.0123 <S**2>=0.000

125 -> 129 0.39151
125 -> 130 0.43218
125 -> 131 -0.21108
125 -> 132 -0.25900
125 -> 134 -0.13206



HOTO



LUTO

Excited State 20: Singlet-?Sym 4.7970 eV 258.46 nm f=0.0067 <S**2>=0.000

124 -> 129 -0.24169
124 -> 130 -0.24892
124 -> 131 0.12264
124 -> 132 0.15029

126 -> 129	0.17427
126 -> 130	0.18947
126 -> 132	0.38417
126 -> 134	0.23626
127 -> 132	-0.12200
128 -> 134	0.10105

7. IC₅₀ graphs of compounds against MCF-7 human breast cancer cells

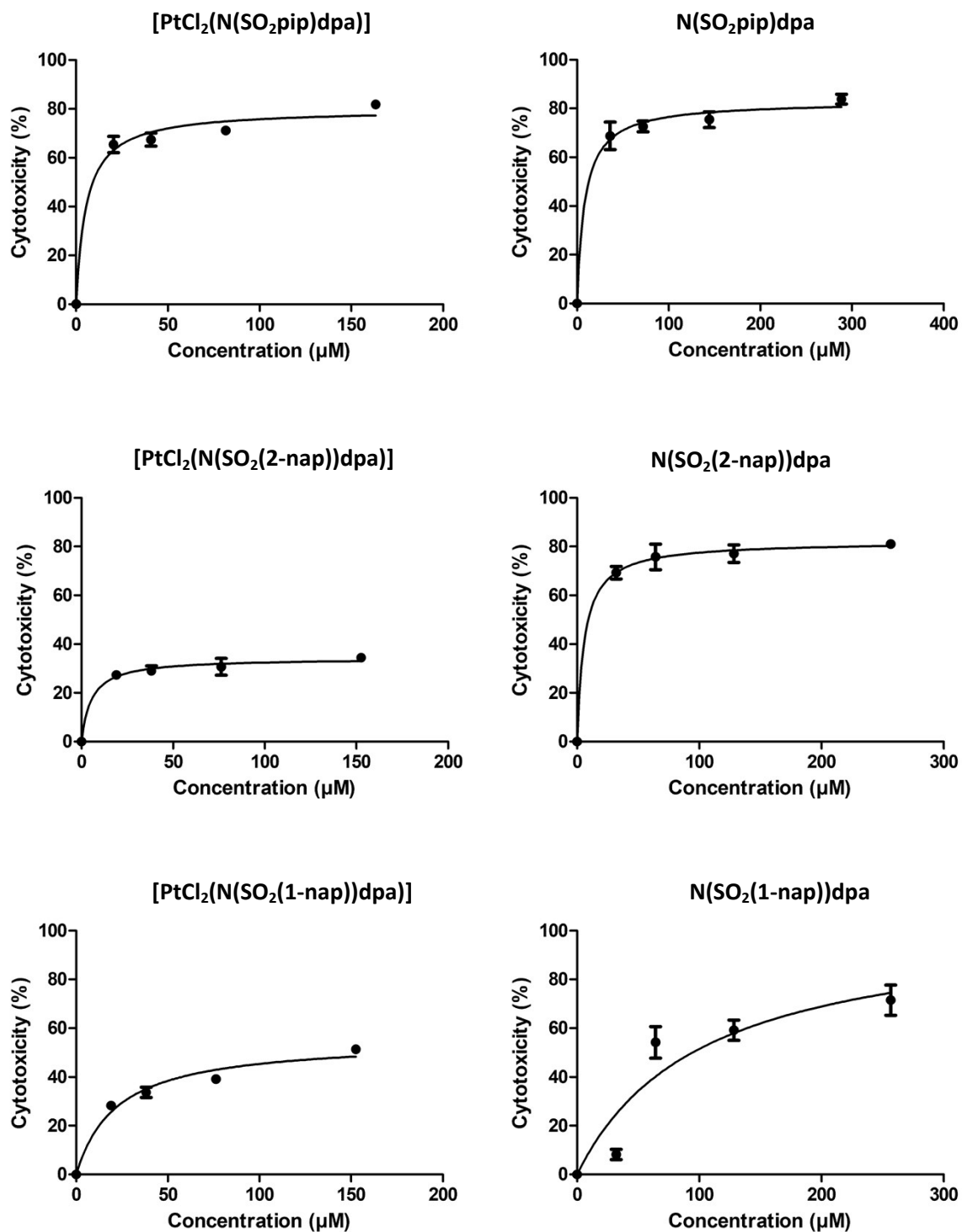
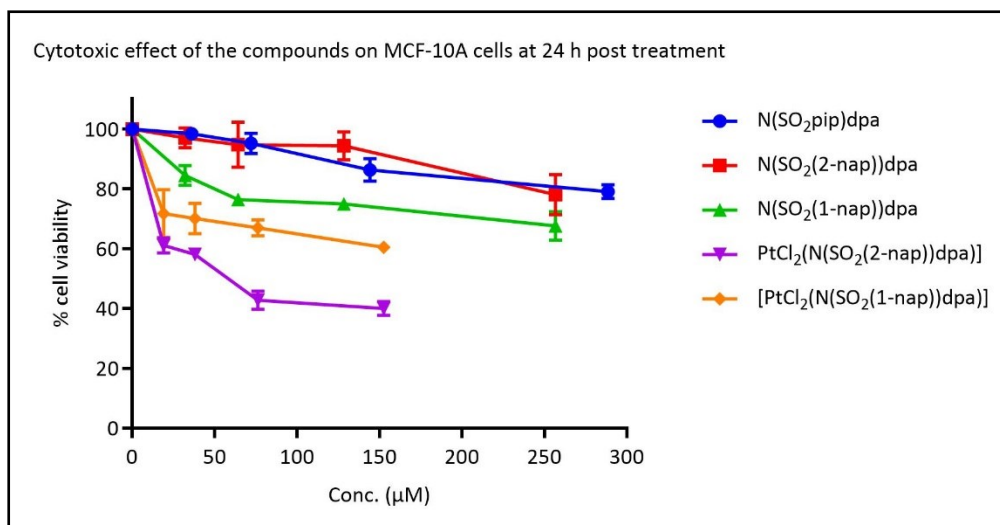


Fig S3. IC₅₀ graphs of compounds

8. IC₅₀ graphs of compounds against MCF-10A human normal breast cells



9. Cartesian coordinates of the optimized structures

N(SO₂(2-nap))dpa system

S 4.54194000 1.71050500 5.13762800
O 4.32082900 0.56066200 4.30771000
O 4.90949300 1.54382500 6.51548200
N 0.69181200 4.46903600 5.99196600
N 3.15920000 2.57659000 5.11818000
N 0.34574800 2.62471000 2.79941700
C -0.59183600 4.43864300 6.34261600
H -1.24542700 5.14048900 5.83295800
C -1.10193600 3.57542200 7.29848900
H -2.15677600 3.59211600 7.54214400
C -0.22820400 2.70485700 7.93206200
H -0.58339500 2.01913000 8.69227500
C 1.10677100 2.72582100 7.57164600
H 1.82254000 2.05441900 8.03112600
C 1.52200500 3.61810000 6.59007800
C 2.95041100 3.62256900 6.11817900
H 3.18378400 4.60332400 5.69244000
H 3.61816700 3.42393200 6.95401800
C 2.49848100 2.76481600 3.83682400
H 3.13092400 2.36542300 3.04002100
H 2.38351800 3.83412600 3.64323000
C 1.14212800 2.11447700 3.73642900
C 0.76705200 1.04810000 4.54143600
H 1.45152900 0.66617800 5.28667100
C -0.49481200 0.50333700 4.37601200
H -0.81973600 -0.32374000 4.99663700
C -1.33270600 1.03290800 3.40764300
H -2.32908000 0.64142300 3.24567400
C -0.86065300 2.08788800 2.64292700
H -1.48554100 2.52789900 1.87082600
C 5.76352000 2.70958400 4.36189600
C 6.09688200 2.47660400 3.05487300

H 5.65573500 1.64523200 2.51849200
C 7.02985500 3.31268600 2.40589000
C 7.40190700 3.10396100 1.05952900
H 6.95702400 2.27801800 0.51567500
C 8.30697200 3.93215700 0.45400600
H 8.58714200 3.76743300 -0.57968800
C 8.88020800 5.00292000 1.16800700
H 9.59602500 5.65052000 0.67537700
C 8.53990500 5.22824100 2.47463300
H 8.98137900 6.05125300 3.02572100
C 7.60835500 4.39304400 3.12763600
C 7.23834800 4.59511500 4.47784400
H 7.68966400 5.41361100 5.02732800
C 6.33561900 3.77527600 5.09060500
H 6.06891200 3.92487300 6.12897000

[PtCl₂(N(SO₂(1-nap))dpa)] complex

Pt 6.77147200 4.57946800 10.39376400
Cl 5.91861200 5.12465400 8.30810400
Cl 4.80423500 5.18225800 11.46251500
N 8.49844600 3.99009300 9.49741000
N 9.76957300 6.22642300 11.41342700
N 7.54559500 4.05072000 12.19891600
C 8.53625600 2.75082100 8.99031600
H 7.63113200 2.16859900 9.09301700
C 9.65596800 2.24459000 8.36582200
H 9.63497400 1.23785700 7.97114600
C 10.77696400 3.04913500 8.25580200
H 11.67319500 2.68806800 7.76689500
C 10.73146200 4.32736900 8.78100300
H 11.58632200 4.98716300 8.72675300
C 9.57991600 4.78048300 9.40374100
C 9.51633000 6.16874100 9.97562600
H 10.25512100 6.78346900 9.46310100
H 8.53123900 6.59914300 9.78379800
C 8.66819300 6.22272400 12.37338400
H 7.78674200 6.64104200 11.88350400
H 8.92641400 6.87230800 13.20882700
C 8.33975200 4.86091100 12.91736700
C 8.83618600 4.45310500 14.14473900
H 9.47677000 5.12764000 14.69579600
C 8.52131300 3.19984200 14.63661400
H 8.90494300 2.87400000 15.59541700
C 7.70628700 2.37443900 13.88138400
H 7.42564700 1.38581900 14.21854300
C 7.23633000 2.83565800 12.67037400
H 6.58737500 2.23500800 12.04824400
S 11.25819000 6.61825500 11.93274100
O 12.19343500 6.13224200 10.95704600
O 11.36715200 6.17313000 13.29392600
C 11.34540600 8.38519100 11.93280400
C 10.26047500 9.11469600 11.52640500
H 9.35253500 8.62068700 11.20771300
C 10.30933300 10.51960300 11.51756300
H 9.44057700 11.07819600 11.19276800
C 11.44466900 11.16413600 11.91630500
H 11.49209700 12.24743000 11.91303200
C 12.58162700 10.44069000 12.34134500
C 13.75462700 11.11029500 12.75337600
H 13.76383800 12.19450100 12.73706200
C 14.85399500 10.40893900 13.16382900

H 15.74959800 10.93134500 13.47829200
C 14.82317000 9.00304900 13.17825700
H 15.69694200 8.45122600 13.50419300
C 13.70232600 8.32195300 12.78562900
H 13.70439300 7.24055100 12.80652200
C 12.54985100 9.01728100 12.35638100

[PtCl₂(N(SO₂(2-nap)dpa))] complex

Pt 18.24248900 4.86333400 7.73597600
Cl 18.93409100 5.44651700 9.86989100
Cl 20.29192600 5.43770700 6.81395300
S 13.87607400 6.71030300 5.77574300
N 16.45112000 4.30614700 8.51993000
N 15.33831800 6.44948200 6.45380900
N 17.62128700 4.29729600 5.88310800
C 16.36450400 3.08196900 9.05606700
H 17.26435100 2.48338700 9.02138800
C 15.20270900 2.60989300 9.62862600
H 15.18424900 1.61389500 10.04976800
C 14.09103900 3.43443000 9.65413200
H 13.16301100 3.10020900 10.10107200
C 14.18685700 4.69658800 9.09741700
H 13.34109300 5.37040100 9.08331800
C 15.37920800 5.11476700 8.52943000
C 15.49364100 6.47590800 7.90263300
H 14.72851100 7.11825200 8.33415400
H 16.47059200 6.90512900 8.13067500
C 16.49590500 6.45197300 5.56891200
H 17.32998000 6.91274200 6.10100800
H 16.27725200 7.08230900 4.70426000
C 16.90019500 5.09172800 5.07545500
C 16.54522200 4.66687700 3.80562700
H 15.96661100 5.32943900 3.17686900
C 16.91890500 3.41083400 3.36508700
H 16.64480900 3.07235000 2.37365000
C 17.64853300 2.59838600 4.21556500
H 17.96773300 1.60704000 3.92382000
C 17.98421100 3.07821100 5.46340100
H 18.56822000 2.49118500 6.15847600
O 12.91977200 6.64967100 6.84495600
O 13.74534400 5.83883600 4.64364500
C 13.93973800 8.35719100 5.16702200
C 14.02165300 8.57699000 3.81920800
H 14.01938300 7.74162100 3.12978900
C 14.09813300 9.89655900 3.32460900
C 14.18004200 10.16545000 1.94105000
H 14.18457800 9.33378300 1.24523200
C 14.25184200 11.45502200 1.48916100
H 14.31426000 11.65552600 0.42616700
C 14.24453300 12.52888500 2.40045300
H 14.30139300 13.54501000 2.02809900
C 14.16591000 12.29769400 3.74776700
H 14.15950700 13.12413500 4.44971500
C 14.09111700 10.97983800 4.24567300
C 14.00550400 10.70571900 5.63176500
H 13.99478100 11.53539700 6.32955200
C 13.93120600 9.42404300 6.09213200
H 13.85346700 9.22235700 7.15293300

[PtCl₂(N(SO₂pip)dpa))] complex

Pt 4.93334600 4.69948400 6.25613400
Cl 2.81452500 4.13415200 5.50621400
Cl 5.90023400 4.20958000 4.20640600
S 6.76864300 2.39638100 10.55346700
O 5.77724600 2.71379900 11.53687000
O 8.09458600 2.92896100 10.64750100
N 4.13273600 5.18897000 8.05827400
N 6.16025400 2.91907900 9.12322700
N 6.75641700 5.25164100 6.96782600
N 6.92325500 0.77472200 10.55437400
C 3.61057900 6.41546800 8.18840700
H 3.63518200 7.03906000 7.30535700
C 3.06462400 6.85997300 9.37344700
H 2.65284000 7.85858800 9.42768000
C 3.05398100 6.00525700 10.46261400
H 2.62919000 6.31811600 11.40833700
C 3.59248700 4.73981300 10.32019500
H 3.61154800 4.04081700 11.14502500
C 4.13239800 4.34814000 9.10540100
C 4.71571100 2.97279500 8.93411300
H 4.23626900 2.31364300 9.65459100
H 4.48304700 2.60137800 7.93423400
C 7.05922800 3.03589400 7.98116100
H 6.55393600 2.64142000 7.09742700
H 7.94060700 2.42254200 8.15779100
C 7.52661300 4.43930600 7.70961800
C 8.74248800 4.88325000 8.20522400
H 9.33609600 4.20626200 8.80391300
C 9.16901900 6.17182500 7.94302000
H 10.11716500 6.52581400 8.32833500
C 8.36300000 6.99602300 7.17648500
H 8.64891900 8.01106600 6.93621700
C 7.16646500 6.49978600 6.70564700
H 6.50487600 7.09954500 6.09616500
C 8.01702200 0.18000400 9.78182300
H 8.88495300 0.83257100 9.85474500
H 7.72881200 0.09566300 8.72411600
C 8.33168200 -1.19911800 10.33055900
H 8.71300500 -1.09448200 11.35136400
H 9.12871600 -1.63992800 9.72671200
C 7.09469700 -2.08252500 10.32600700
H 7.31711900 -3.05464000 10.77220900
H 6.78745400 -2.27022100 9.29022200
C 5.95858600 -1.40308500 11.07288700
H 5.03889500 -1.98895200 11.00191400
H 6.21020000 -1.31581100 12.13468200
C 5.69054600 -0.01545900 10.51993500
H 5.32386700 -0.09096500 9.48604400
H 4.93684600 0.49382000 11.11829100