Synthesis and Anticancer Activities of a Novel Class of Mono and Dimetallic Pt(II)(Salicylaldiminato) (DMSO or Picolino)Cl Complexes

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Contents

I. Spectroscopic Data

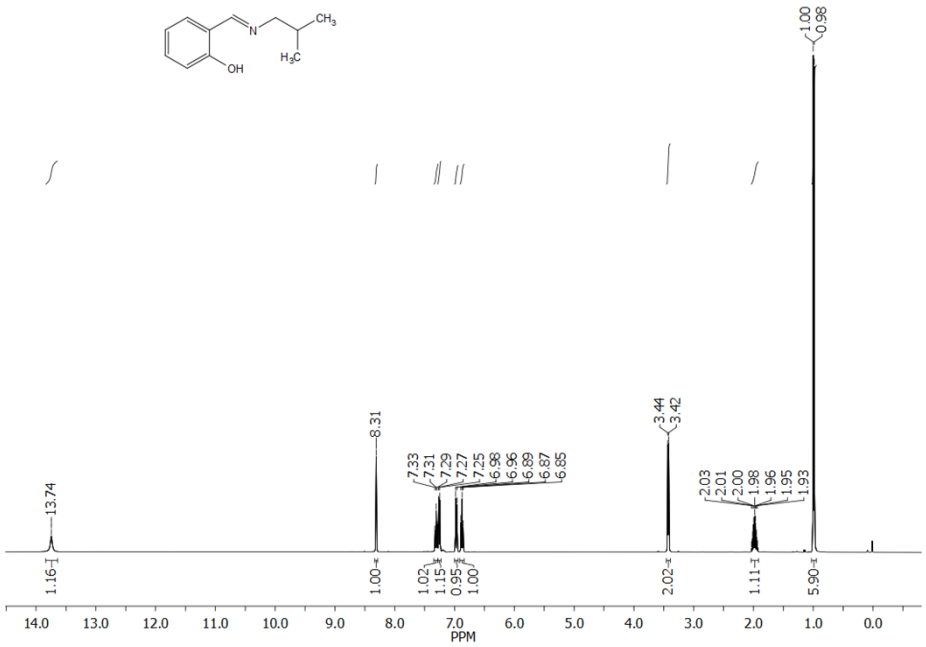

Figure S1. ^{1}H NMR spectrum of $\mathbf{L_1}$ in $CDCl_3$ at 25 °C

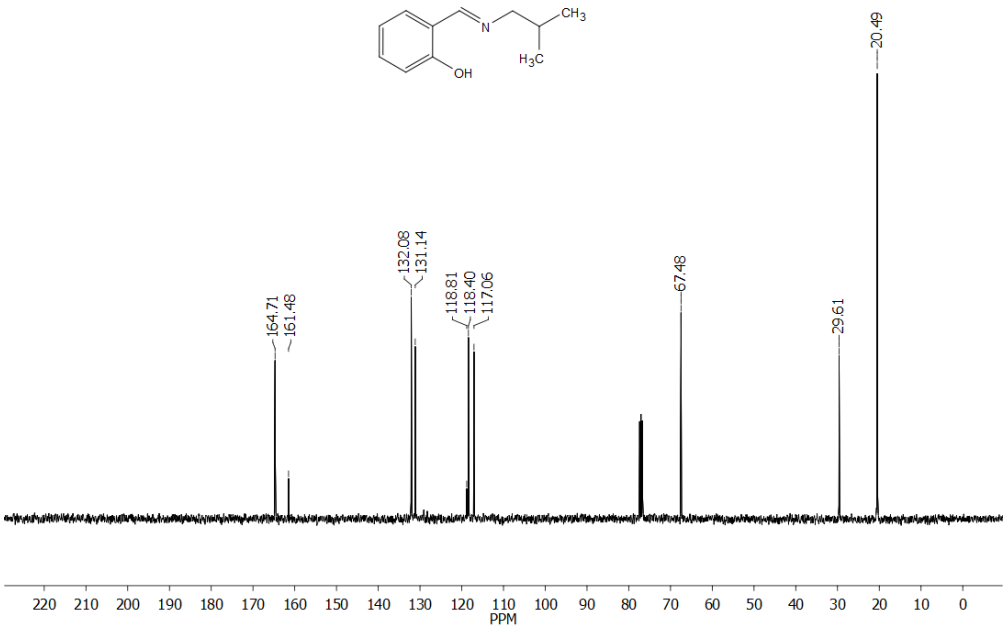

Figure S2. ^{13}C NMR spectrum of $\mathbf{L_1}$ in $CDCl_3$ at 25 °C

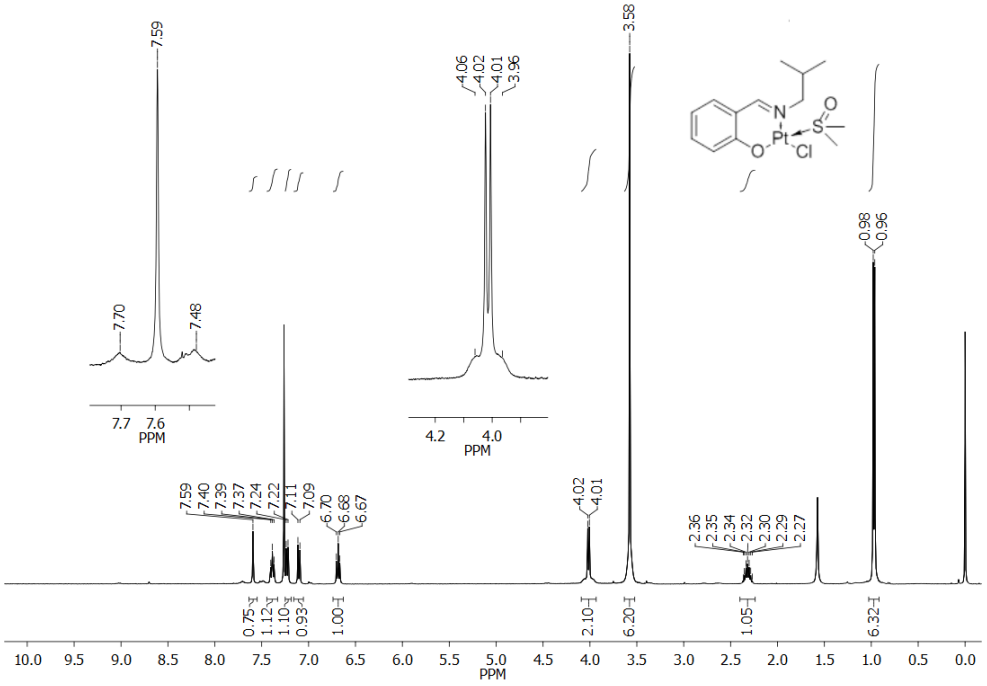

Figure S3. ^{1}H NMR spectrum of **C-1**-*cis* in $CDCl_3$ at 25 °C

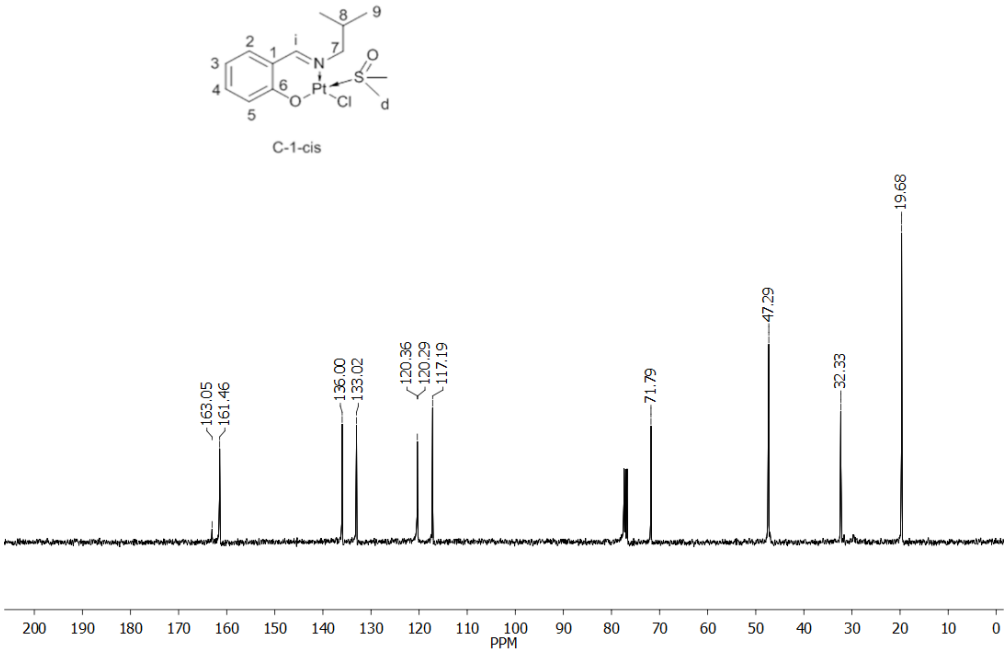

Figure S4. ^{13}C NMR spectrum of **C-1**-*cis* in $CDCl_3$ at 25 °C

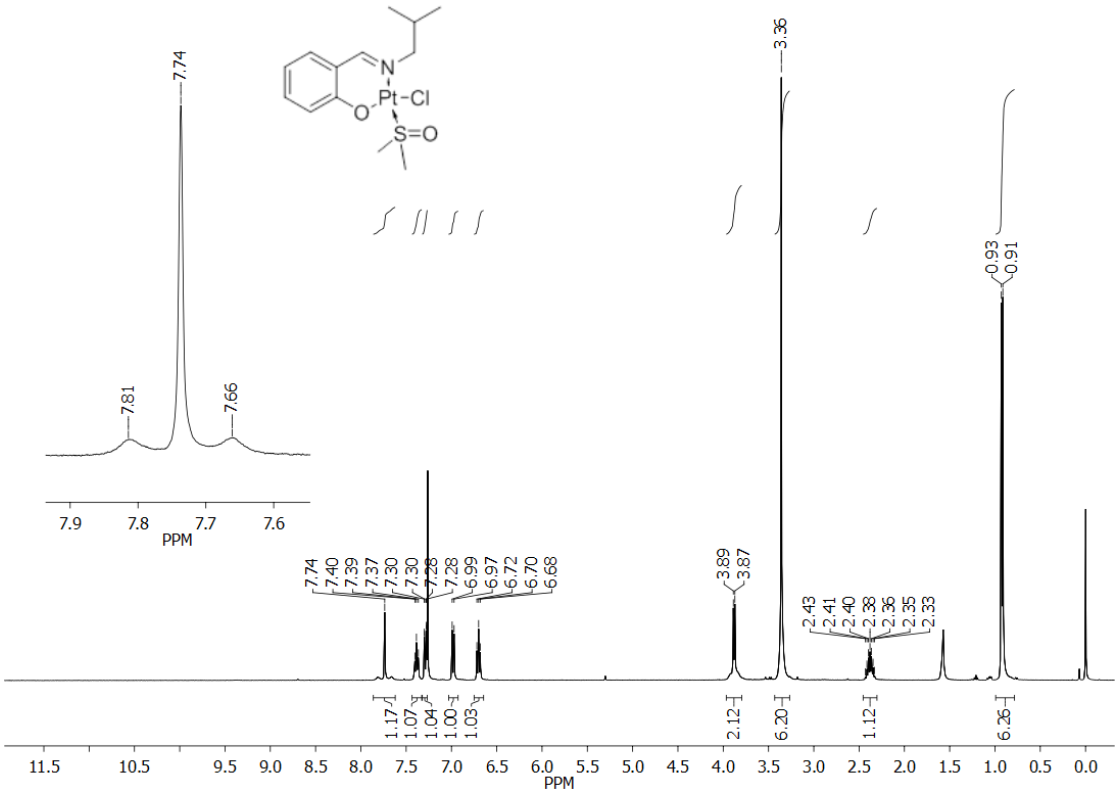

Figure S5. ^{1}H NMR spectrum of **C-1**-*trans* in $CDCl_3$ at 25 °C

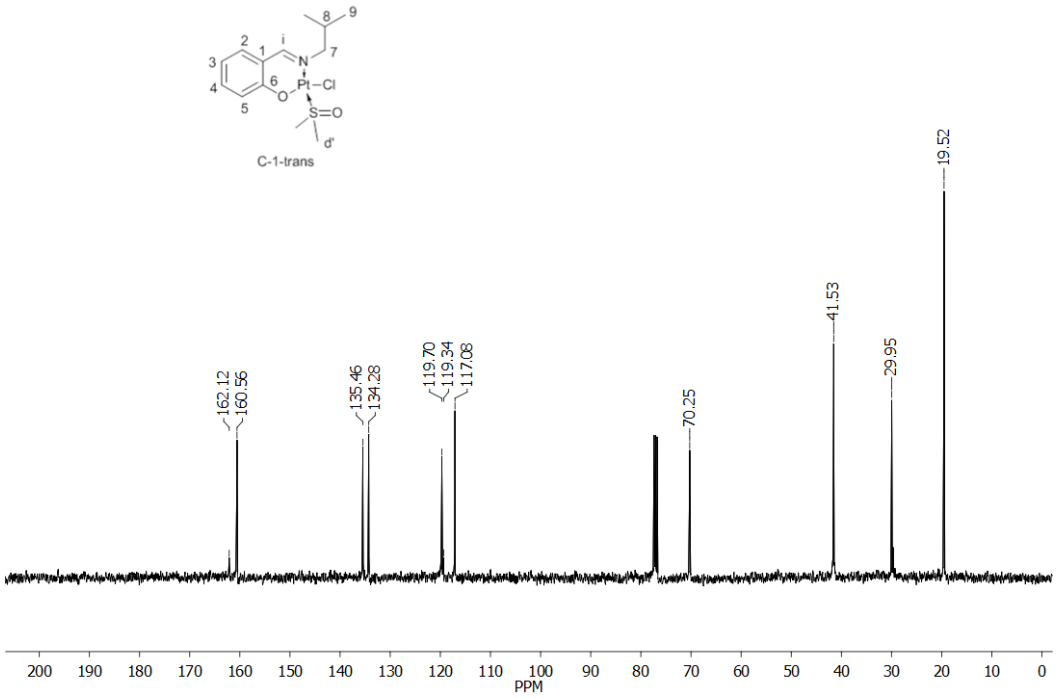

Figure S6. ^{13}C NMR spectrum of **C-1**-*trans* in $CDCl_3$ at 25 °C

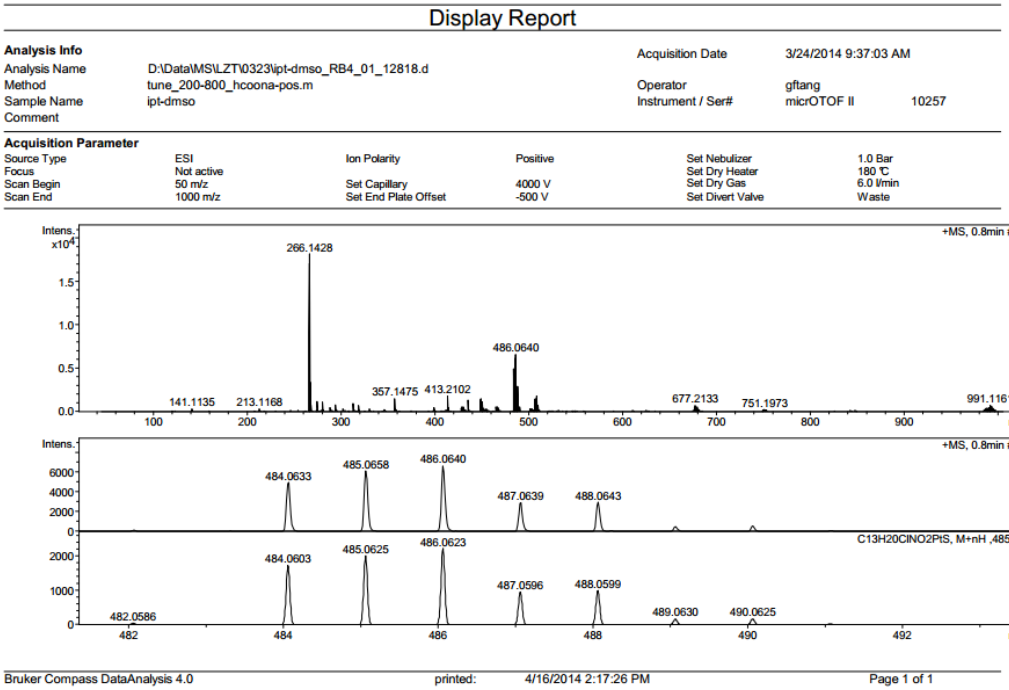

Figure S7. ESI-MS Spectrum of **C-1**-*cis/trans,* experimental (top) and calculated (bottom) peaks.

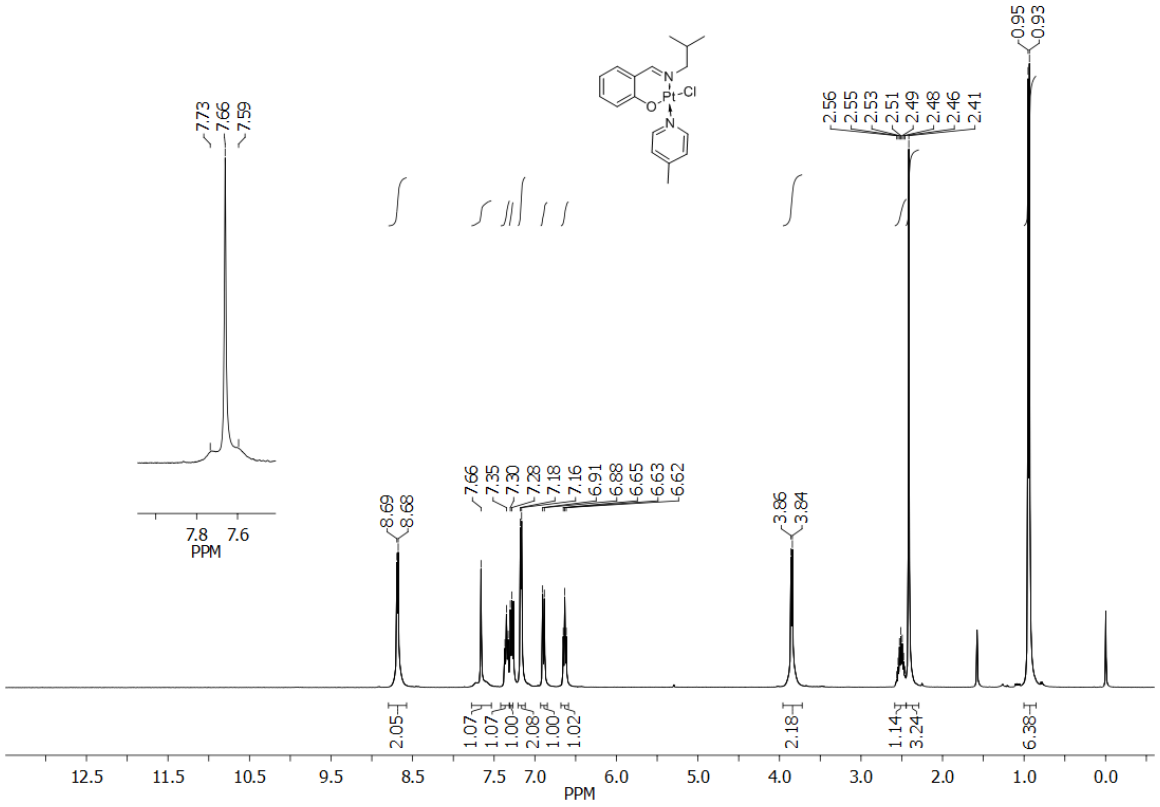

Figure S8. ^{1}H NMR spectrum of **C-2** in $CDCl_3$ at 25 °C

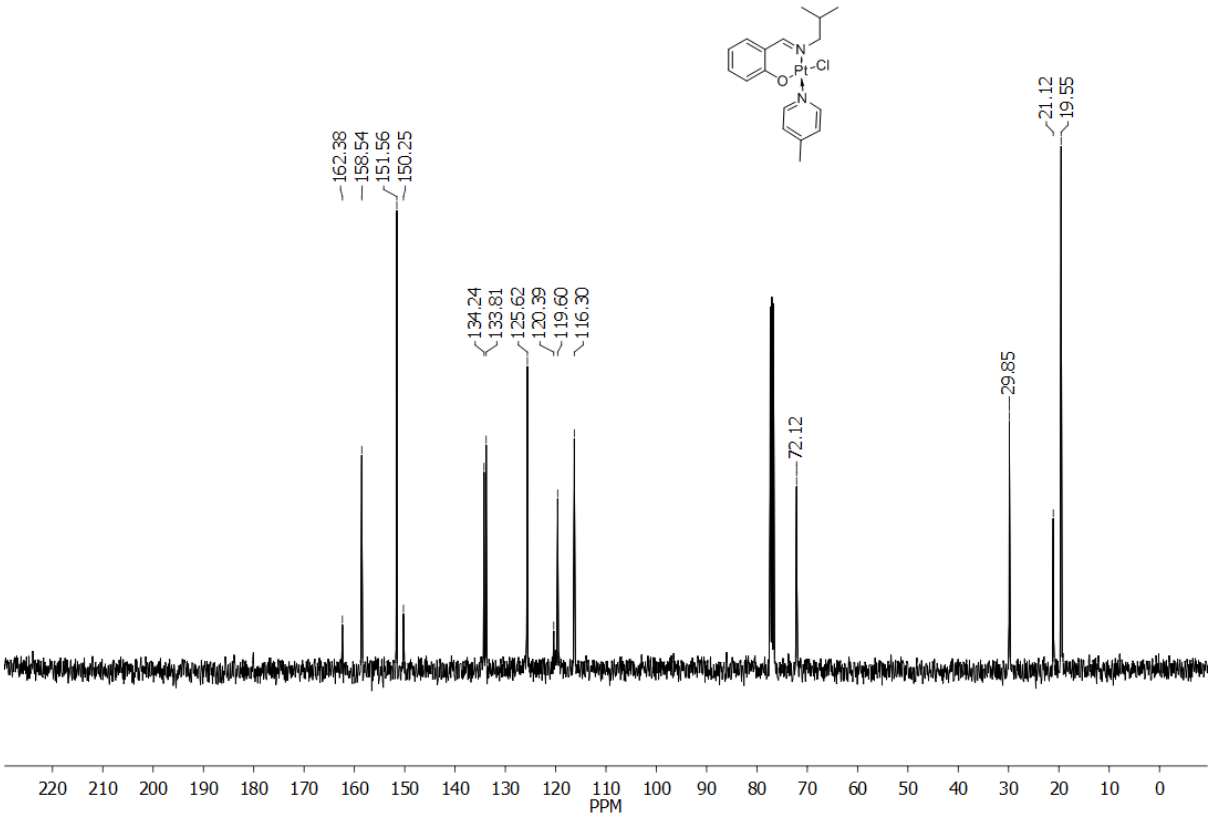

Figure S9. ^{13}C NMR spectrum of **C-2** in $CDCl_3$ at 25 °C

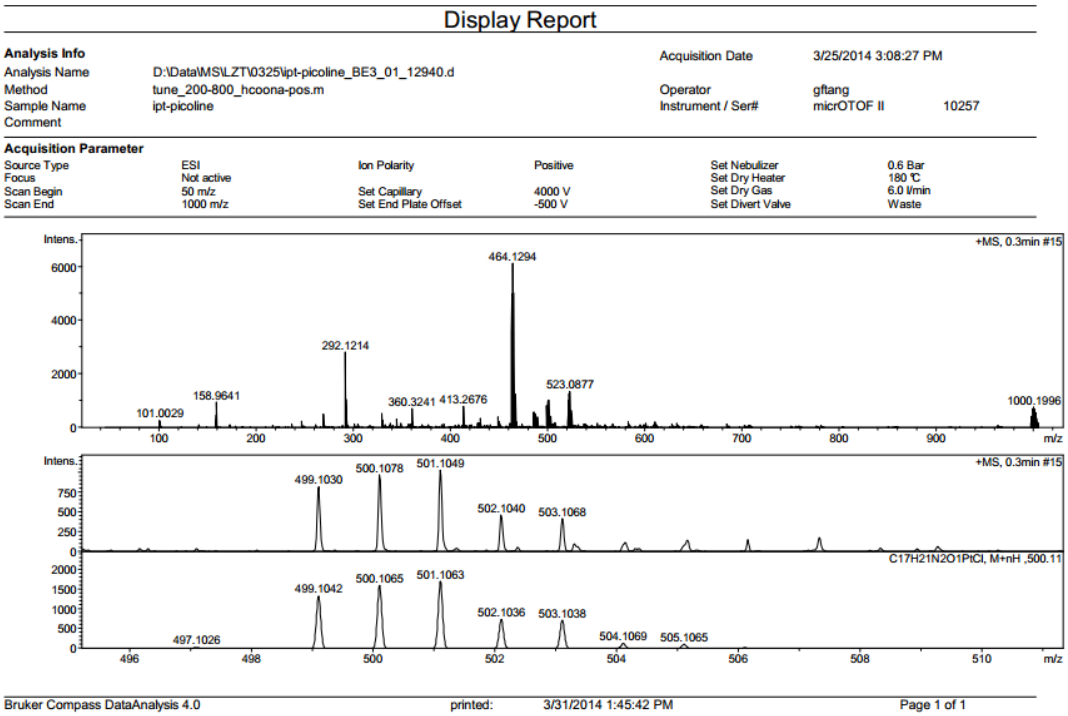

Figure S10. ESI-MS Spectrum of **C-2**, $[M + H]^+$ peaks showing isotopic abundance experimental (top) and calculated (bottom) peaks

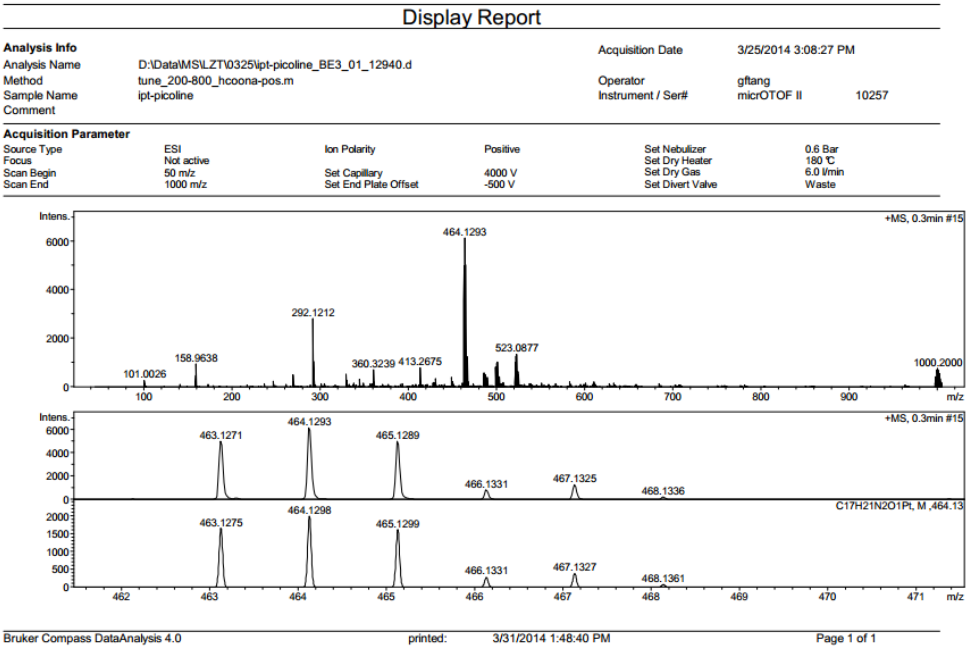

Figure S11. ESI-MS Spectrum of **C-2**, showing $[M - Cl]^+$ peaks showing isotopic abundance, top experimental, down calculated

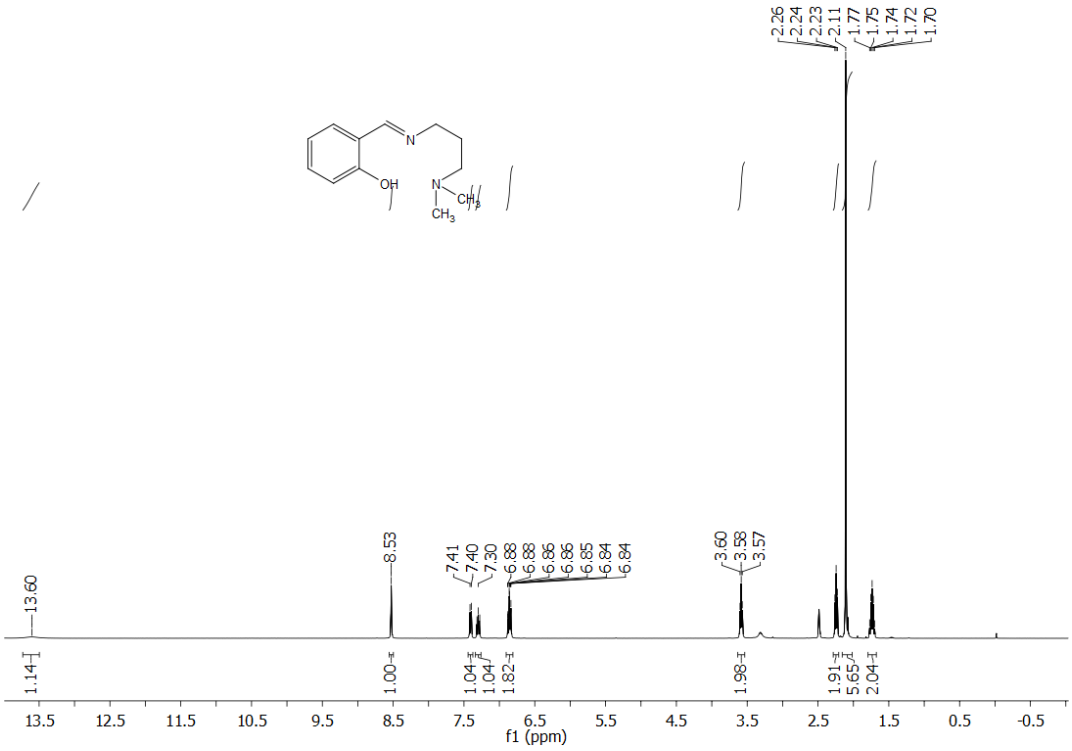

Figure S12. ^{1}H NMR spectrum of $\mathbf{L_2}$ in DMSO-D_6 at 25 °C

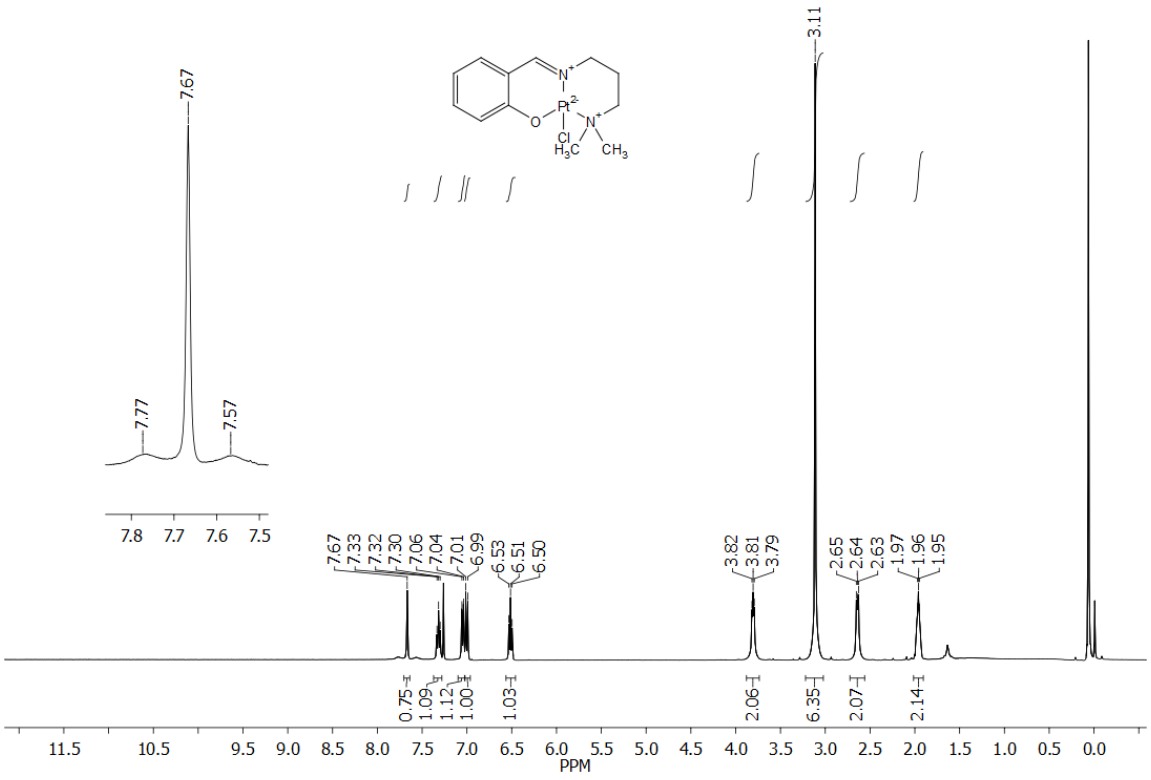

Figure S13. ^{1}H NMR spectrum of **C-3** in $CDCl_3$ at 25 °C

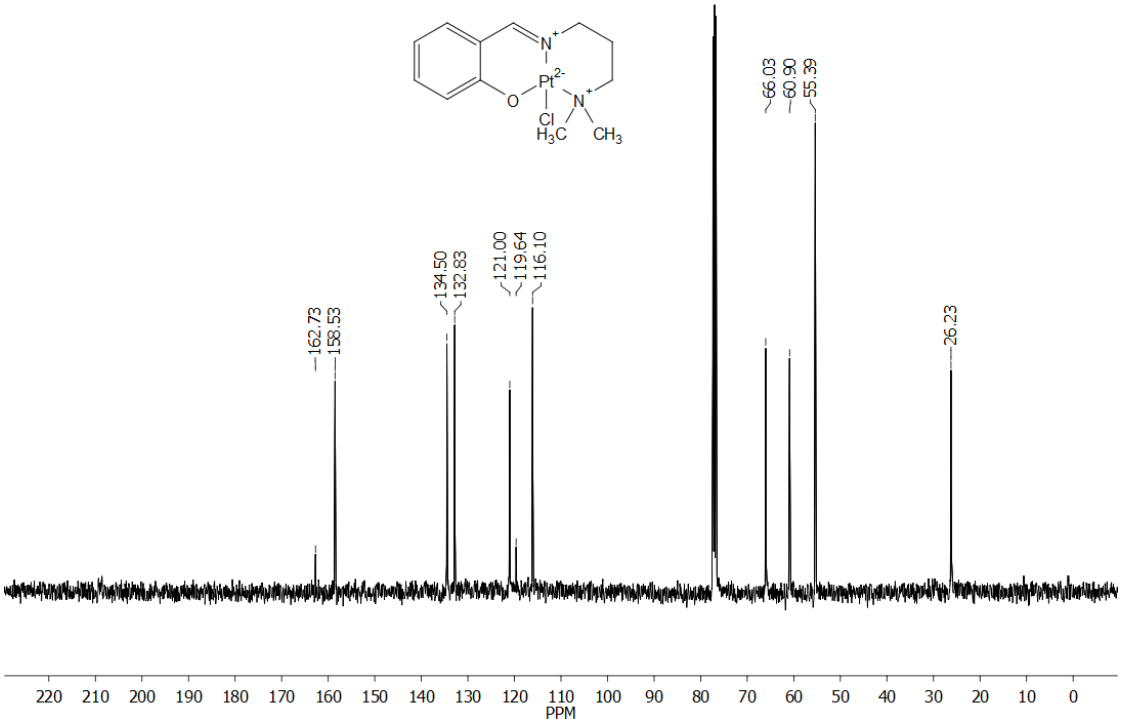

Figure S14. ^{13}C NMR spectrum of **C-3** in $CDCl_3$ at 25 °C

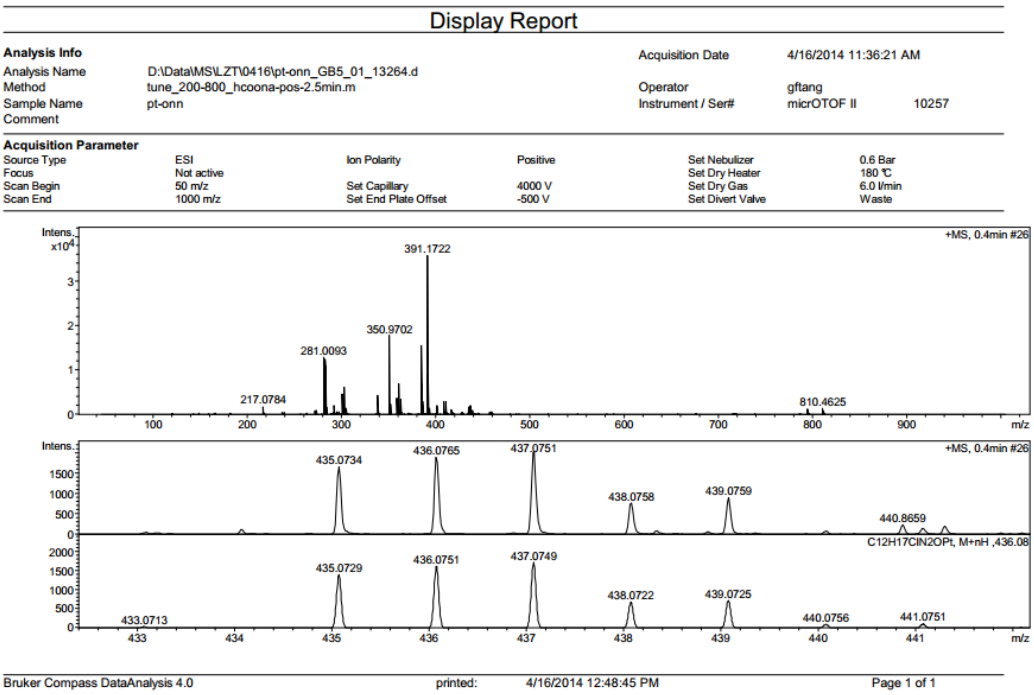

Figure S15. ESI-MS Spectrum of **C-3** experimental (top) and calculated (bottom), showing isotopic abundance

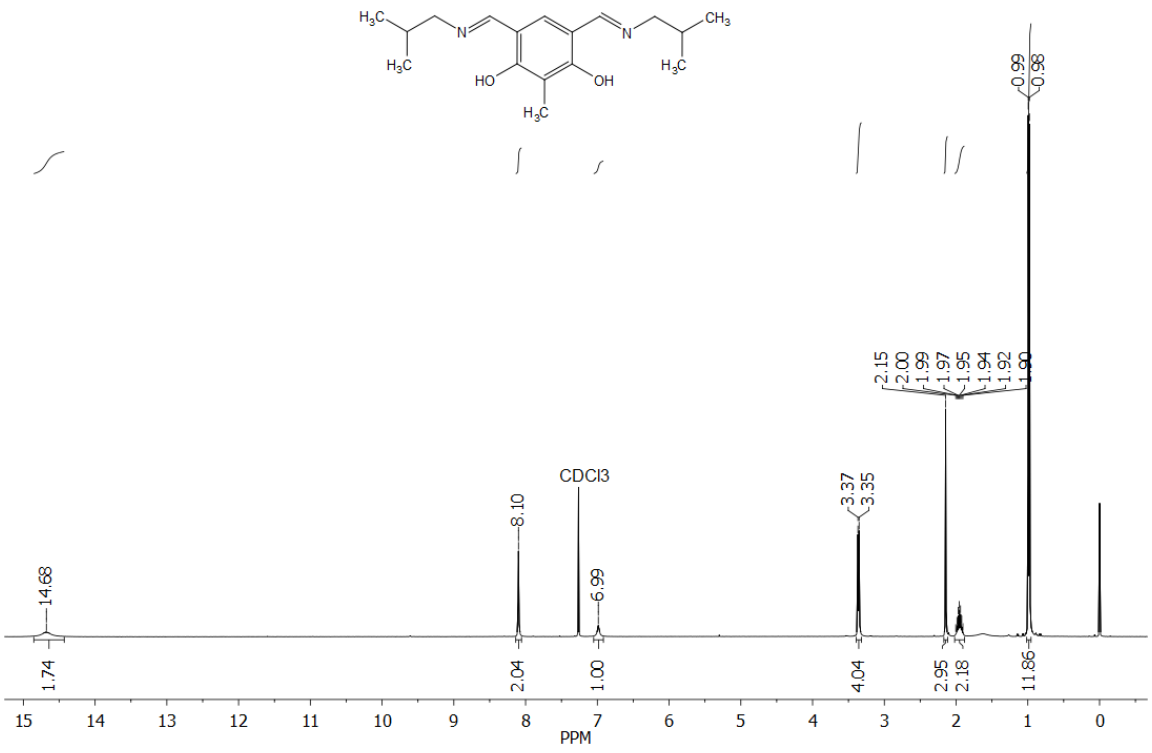

Figure S16. ^{1}H NMR spectrum of $\mathbf{L_3}$ in $CDCl_3$ at 25 °C

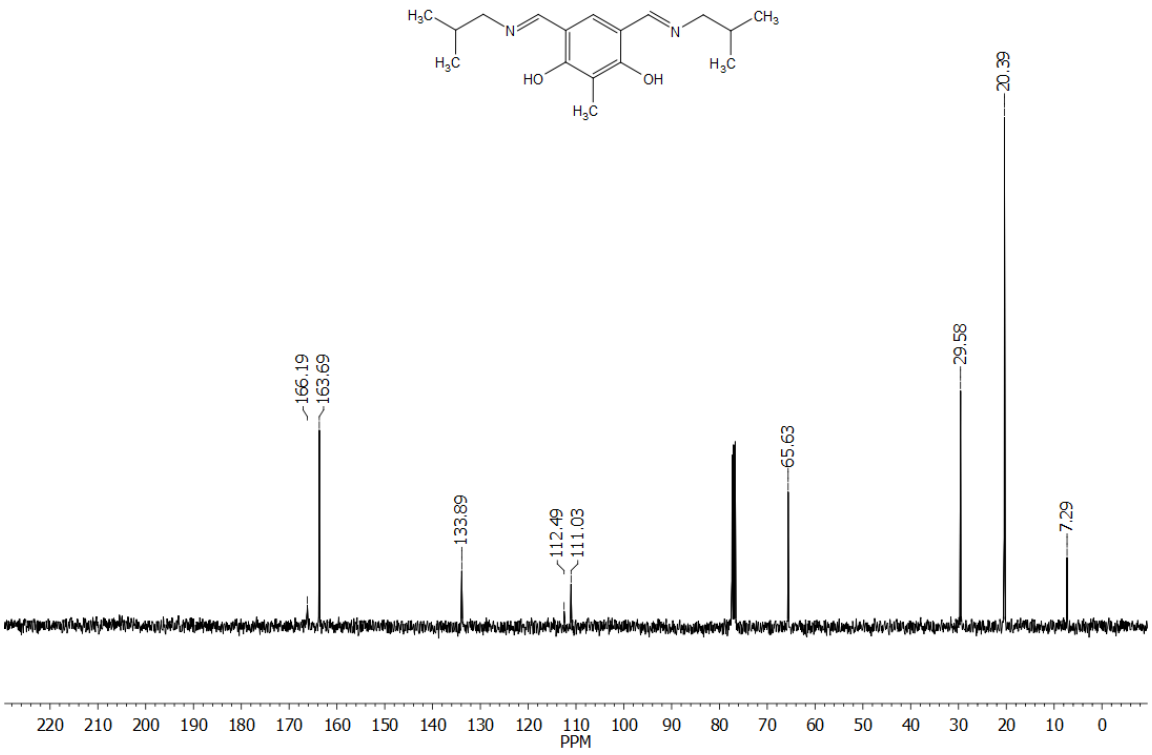

Figure S17. ^{13}C NMR spectrum of $\mathbf{L_3}$ in $CDCl_3$ at 25 °C

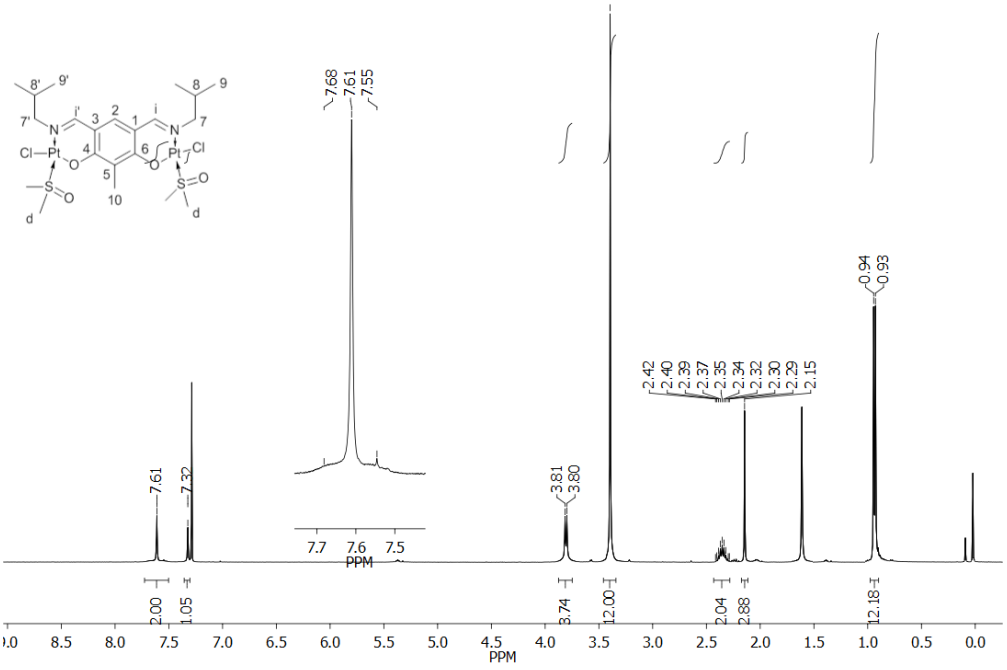

Figure S18. ^{1}H NMR spectrum of **C-4-*trans*** in $CDCl_3$ at 25 °C

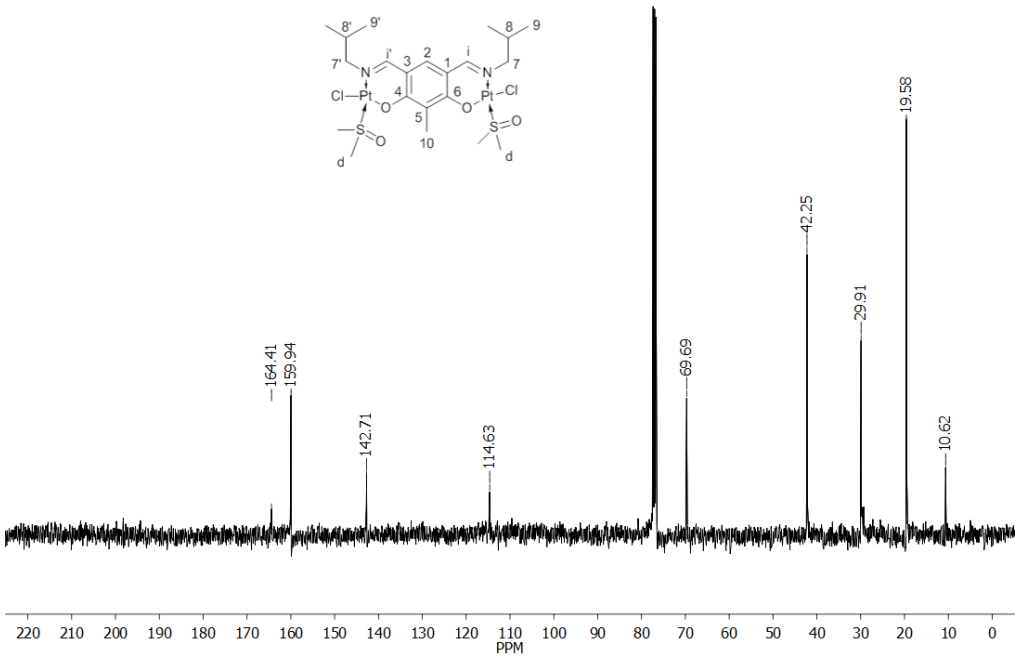

Figure S19. ^{13}C NMR spectrum of **C-4-***trans* in $CDCl_3$ at 25 °C

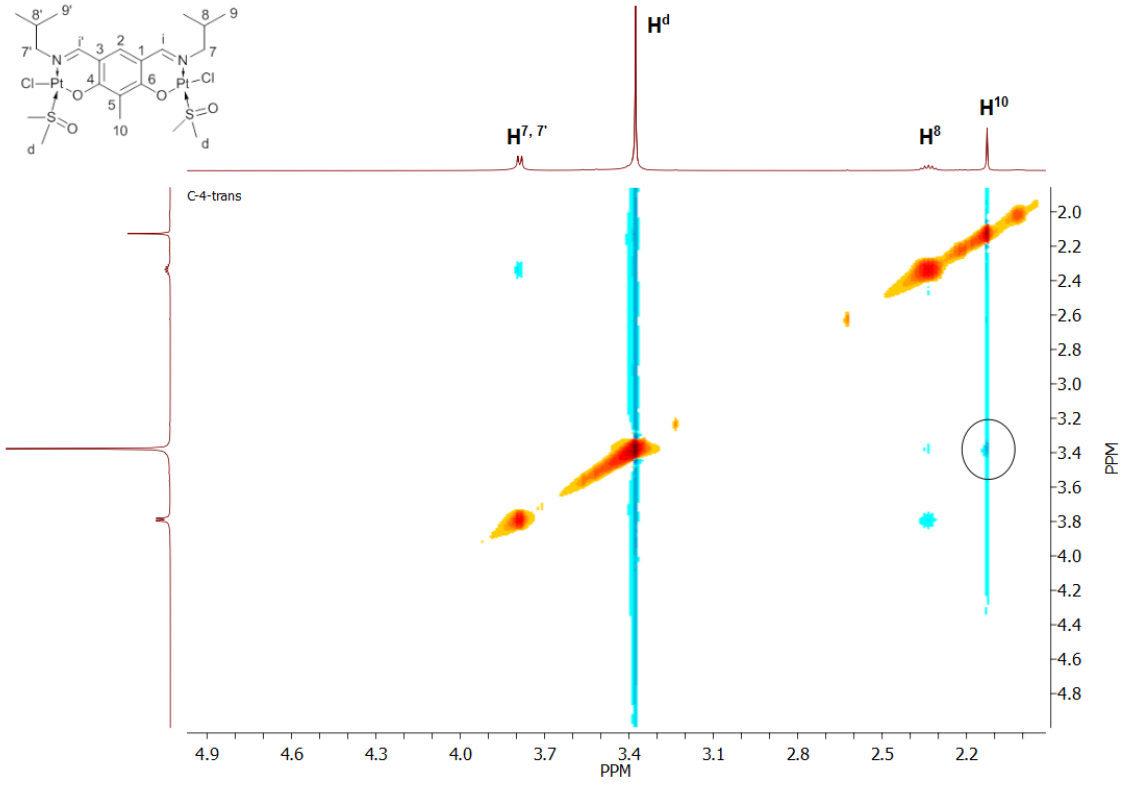

Figure S20. NOESY Spectrum of **C-4-***trans*

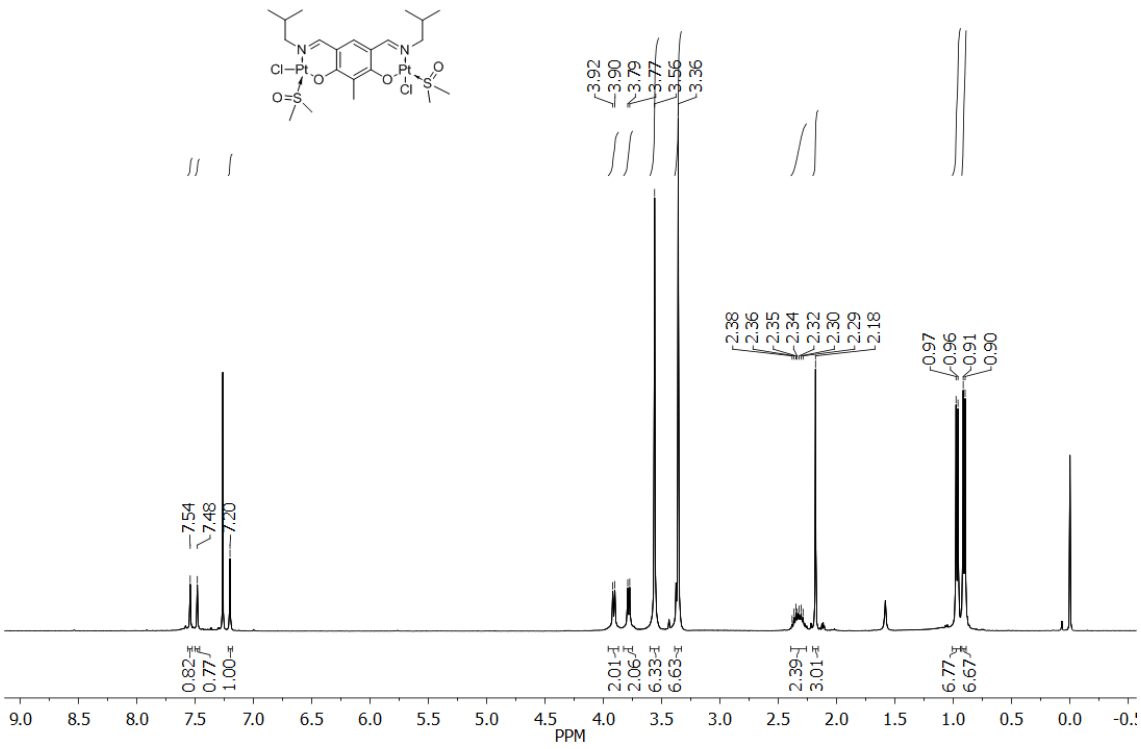

Figure S21. ^{1}H NMR spectrum of **C-4**-*cis/trans* in $CDCl_3$ at 25 °C

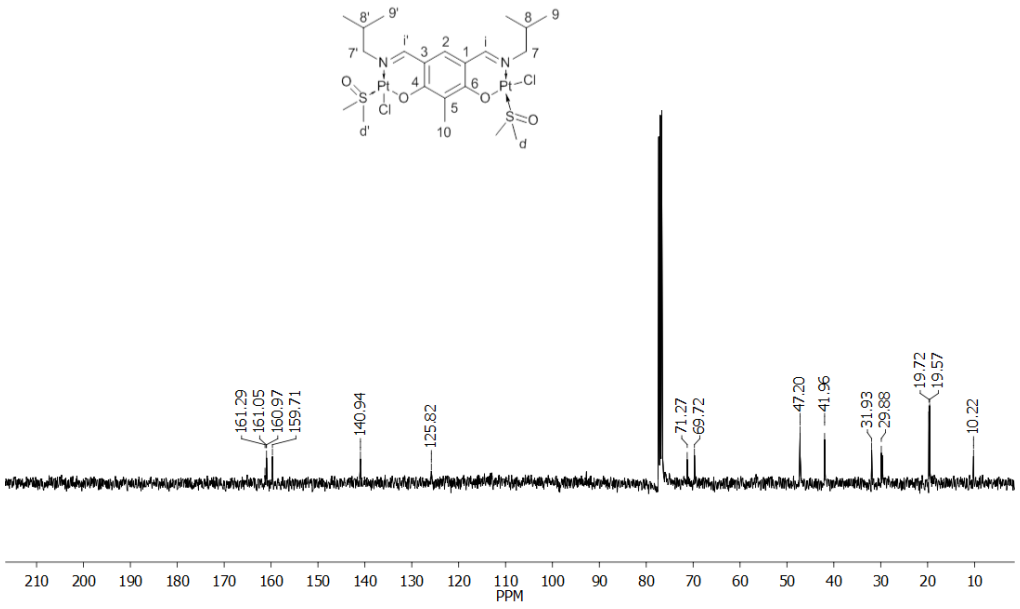

Figure S22. ^{13}C NMR spectrum of **C-4**-*cis/trans* in $CDCl_3$ at 25 °C

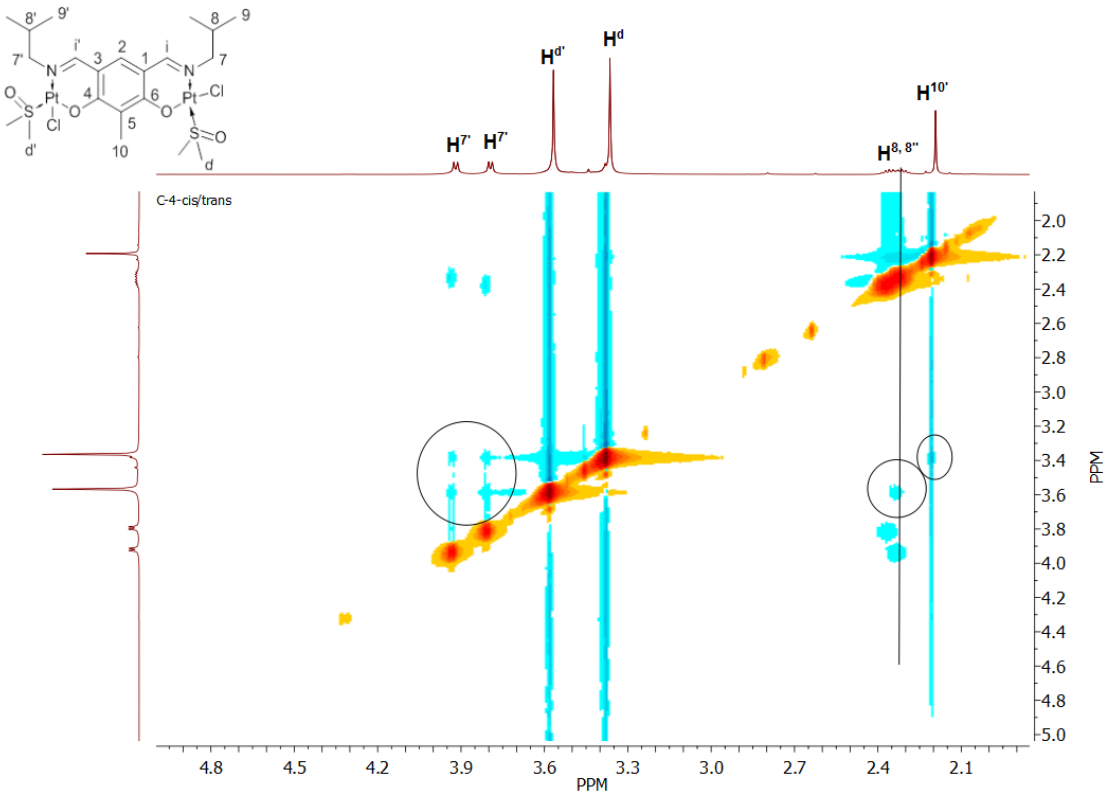

Figure S23. NOESY Spectrum of **C-4**-*cis/trans*

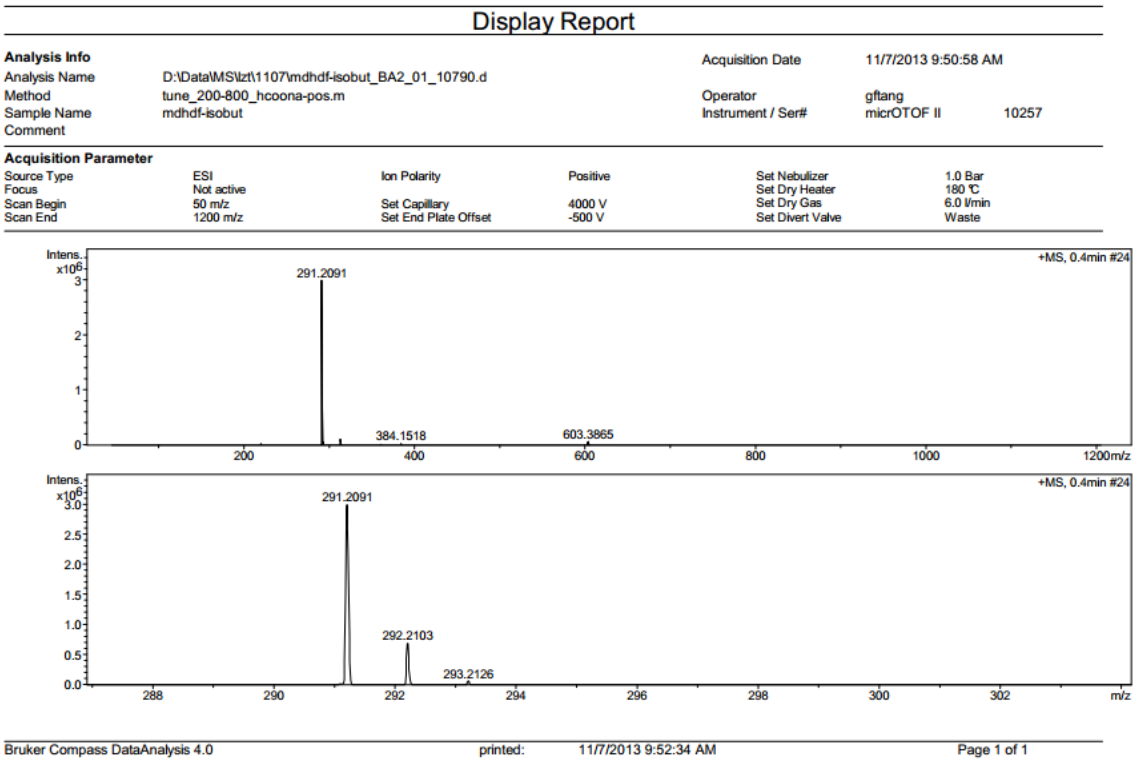

Figure S24. ESI-MS Spectrum of $\mathbf{L_3}$

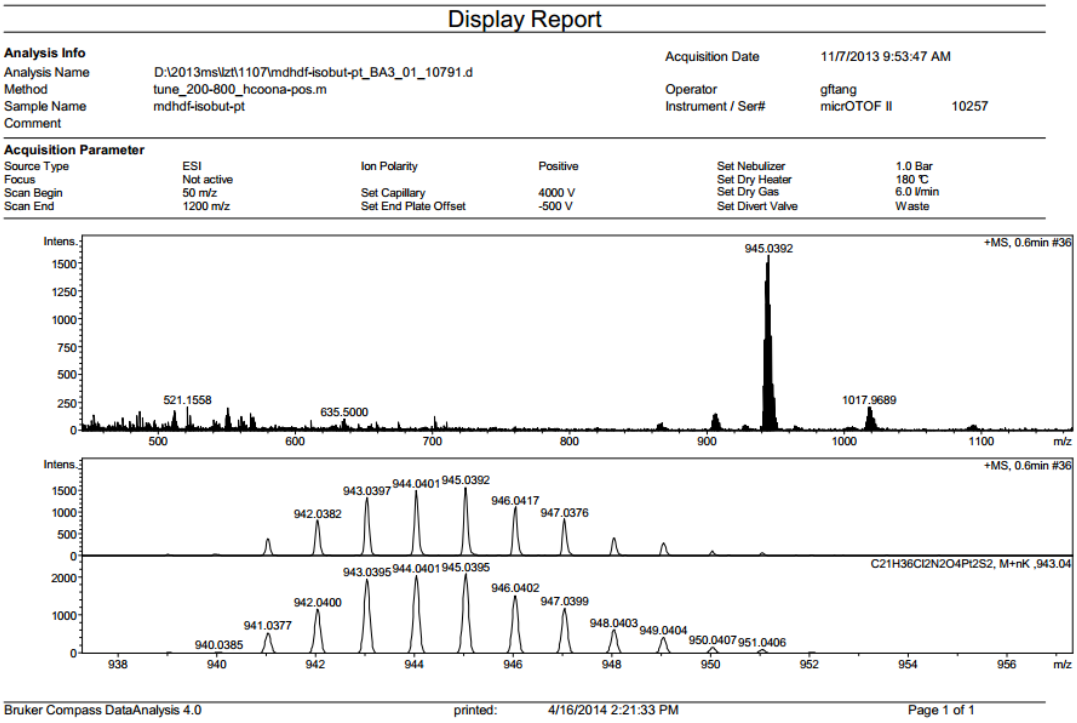

Figure S25. ESI-MS Spectrum of **C-4**-*cis/trans* mixture, showing isotopic abundances, experimental (top) and calculated (bottom)

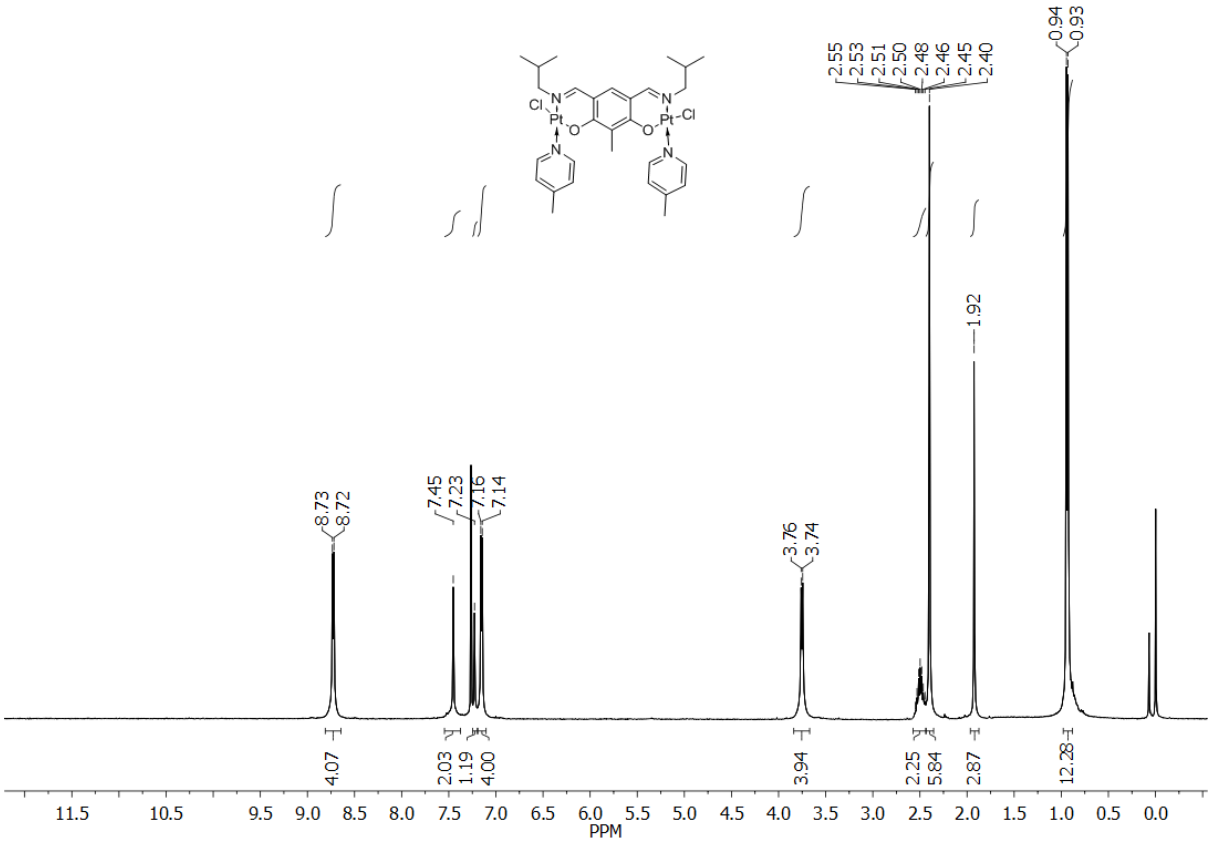

Figure S26. ^{1}H NMR spectrum of **C-5** in $CDCl_3$ at 25 °C

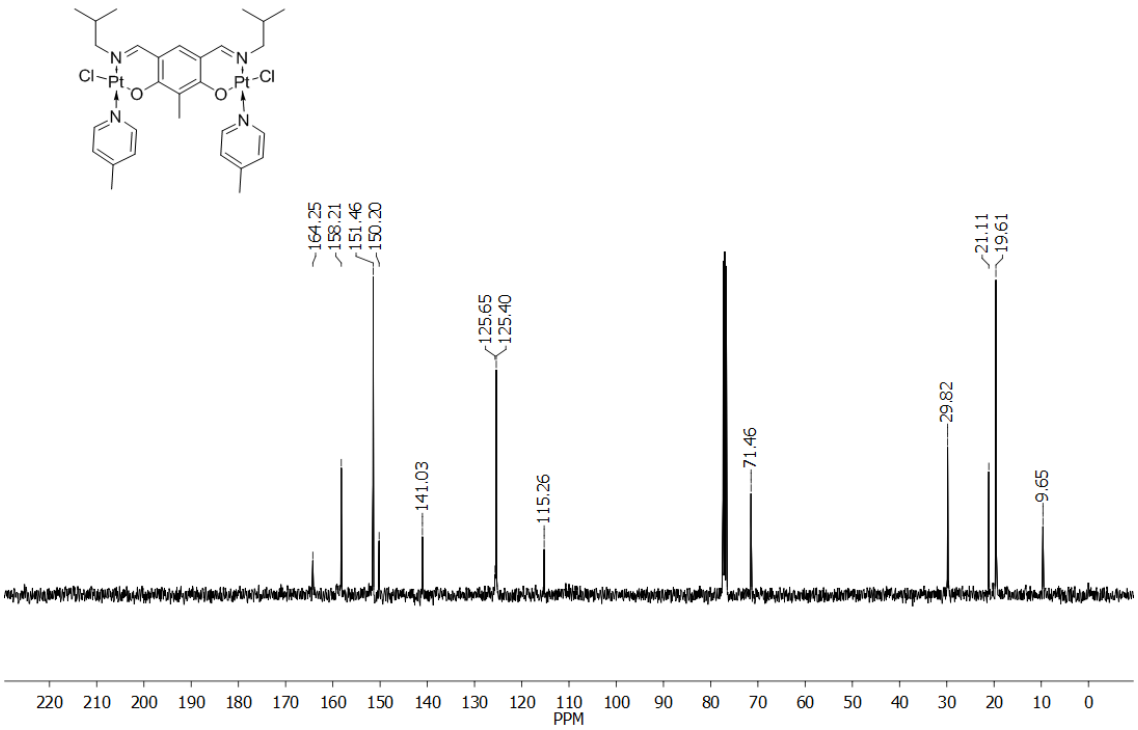

Figure S27. ^{13}C NMR spectrum of **C-5** in $CDCl_3$ at 25 °C

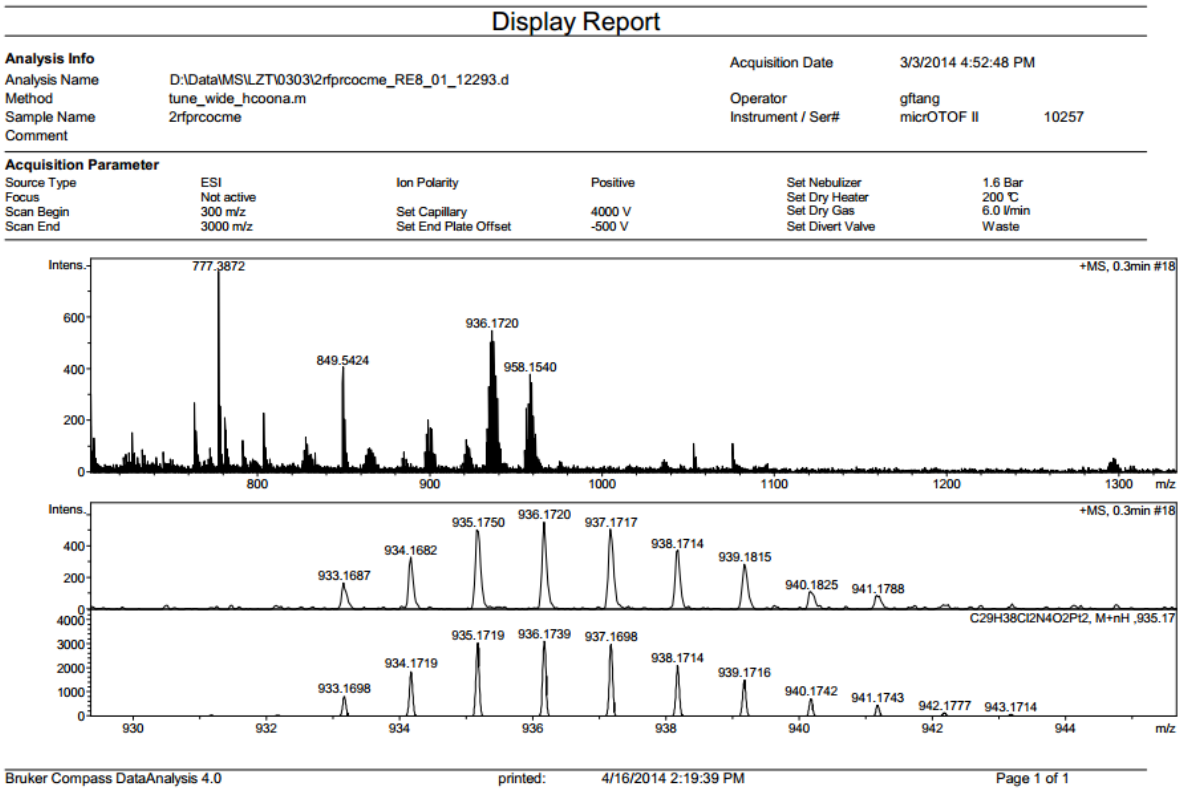

Figure S28. ESI-MS Spectrum of **C-5**, showing isotopic abundances, experimental (top) and calculated (bottom)

II. Stablility analysis of C-1-*trans* and C-2

C-1-*trans* was dissolved in 40 % and **C-2** was dissolved in 20 % D_2O/DMSO-d_6 mixture and analysed a) freshly prepared b) after 20 c) 44 and d) 70 hours under room temperature and light. During this time we did not observe any changes in the proton chemical shifts in the ^{1}H NMR spectra of these two complexes. The only changes observed in case of **C-1**-*trans* was the diplacement of DMSO in the complex by DMSO-d_6. After 20 hours the exchange observed was 50 % which is further improved to 83 % at 44 hours and about 90 % after 70 hours.

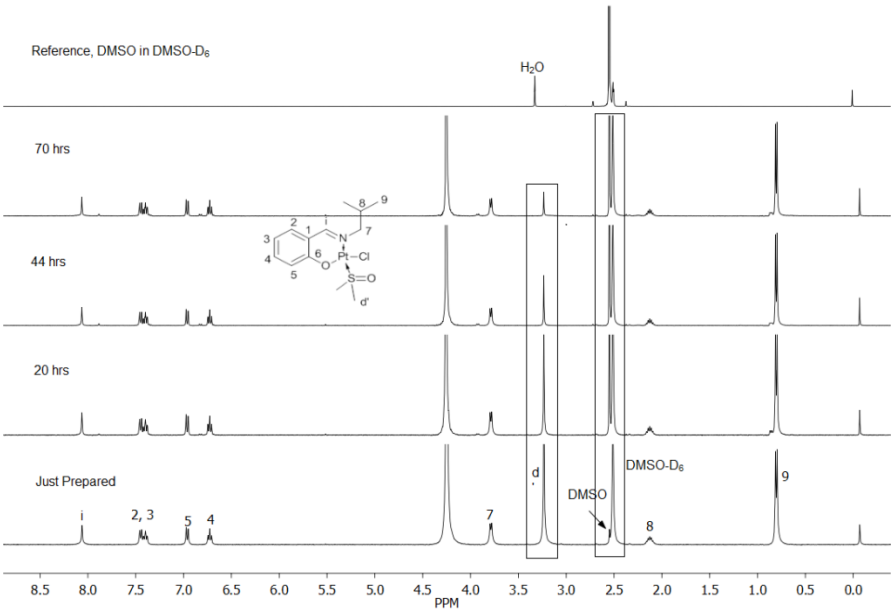

Figure S29. Comparative ^{1}H NMR spectra of **C-1-***trans* 40 % water/DMSO-d_6 at 25 °C. From bottom i) freshly prepared, ii) after 20 hrs, iii) after 44 hrs, iv) after 70 hrs, v) DMSO in DMSO-d_6; the peaks in the reactangle shows the slow displacement of the DMSO of **C-1**-*trans* by DMSO-d_6 of the solvent, this exchange was about 90% after 70 hours. The sample was stored under room temperature and room light during analysis. No changes were observed in the chemical shifts in the spectra so it is deduced that **C-1**-*trans* is quite stable under these conditions.

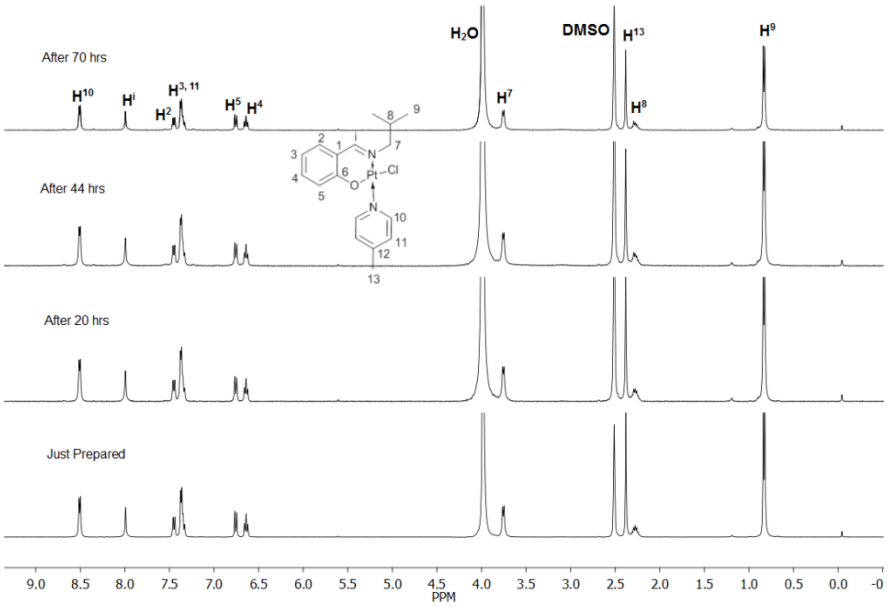

Figure S30. Comparative ^{1}H NMR spectra of **C-2** in 20 % water/DMSO-d_6 at 25 °C. From bottom i) freshly prepared, ii) after 20 hrs, iii) after 44 hrs, iv) after 70 hrs. The sample was stored under room temperature and room light during analysis. No changes were observed in the chemical shifts in the spectra which implies the high stability of **C-2**.

III. Crystallographic Data

Crystallographic Studies. X-ray diffraction intensity data for each compound were measured on a graphite-monochromated Bruker SMART APEX CCD-based diffractometer system (Mo K_α radiation, $\lambda = 0.71073$ Å). All the structures were solved by Direct Method of SHELXS-97 and refined by full-matrix leastsquares techniques using the SHELXL-97 program within WING.[1] Non-hydrogen atoms of the crystallized compounds were refined with anisotropic temperature parameters. The hydrogen atoms attached to carbons were generated geometrically.

Reference:

1. G. M. Sheldrick, *SHELXS-97, Programs for X-ray Crystal Structure Solution*; University of Göttingen: Göttingen, Germany, 1997; L. J. Farrugia, *WINGX, A Windows Program for Crystal Structure Analysis*; University of Glasgow, Glasgow, UK, 1988.

Table S1. Data and structure refinement of the complex

	C-1-*cis*	**C-1**-*trans*	**C-3**
CCDC	1016359	1026340	1016409
Empirical formula	$C_{13}H_{20}ClNO_2PtS$	$C_{13}H_{20}ClNO_2PtS$	$C_{12}H_{17}ClN_2OPt$
Temperature (K)	293(2)	223(2)	293(2)
Crystal system	Monoclinic	Triclinic	Orthorhombic
Space group	P 21/n	P -1	P b c a
Unit cell dimensions			
a (Å)	13.403(5)	10.0909(18)	10.719(4)
b (Å)	11.272(4)	11.667(2)	12.484(5)
c (Å)	21.371(8)	15.142(3)	19.494(8)
α (°)	90	71.177(3)	90
β (°)	100.987(5)	72.413(3)	90
γ (°)	90	79.211(3)	90
Volume (Å^3)	3169(2)	1600.5(5)	2608.5(17)
Z	8	4	8
Density (calculated) (mg/m^3)	2.032	2.012	2.219
Absorption coefficient (mm^{-1})	9.151	9.061	10.948
F(000)	1856	928	1648
Crystal size (mm^3)	0.200 × 0.200 × 0.050	0.270 × 0.220 × 0.120	0.400 × 0.400 × 0.050
θ range for data collection (°)	1.663 to 26.000	1.471 to 27.479	2.089 to 25.002
Index ranges	-16≤ h ≤16, -13≤ k ≤13, -24≤ l ≤26	-13≤ h ≤13, -15≤ k ≤15, -14≤ l ≤19	-11≤ h ≤12, -14≤ k ≤13, -16≤ l ≤22
Reflections collected	14237	11457	10020
Independent reflections	6193 [R(int) = 0.0504]	7141 [R(int) = 0.0409]	2300 [R(int) = 0.1137]
Completeness to theta = 25.242°	99.4 %	98.2%	97.1 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	1.000 and 0.592	0.746 and 0.317	1.000 and 0.374
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	6193 / 0 / 351	7141 / 0 / 351	2300 / 0 / 157
Goodness-of-fit on F2	0.826	1.061	1.066
Final R indices [I>2σ(I)]	R1[a] = 0.0282, wR2[b] = 0.0593	R1 = 0.0408, wR2 = 0.1222	R1[a] = 0.0807, wR2[b] = 0.2390
R indices (all data)	R1[a] = 0.0539, wR2[b] = 0.0621	R1 = 0.0522, wR2 = 0.1323	R1[a] = 0.0948, wR2[b] = 0.2653
Extinction coefficient	n/a	n/a	0.0014(4)
Largest diff. peak and hole[c]	0.829 and -0.980 e.Å^{-3}	2.143 and -2.248 e.Å^{-3}	4.859 and -6.080 e.Å^{-3}

[a] $R1 = \Sigma_{\text{all reflections}} |F_0 - F_c| / \Sigma_{\text{all reflections}} |F_0|$, [b] $wR2 = [\Sigma w(F_0^2 - F_c^2)^2 / \Sigma (w(F_0^2)^2)]^{1/2}$, [c] Because of the heavy metal atom Pt in the structure, there may exist tail effect for the structure.

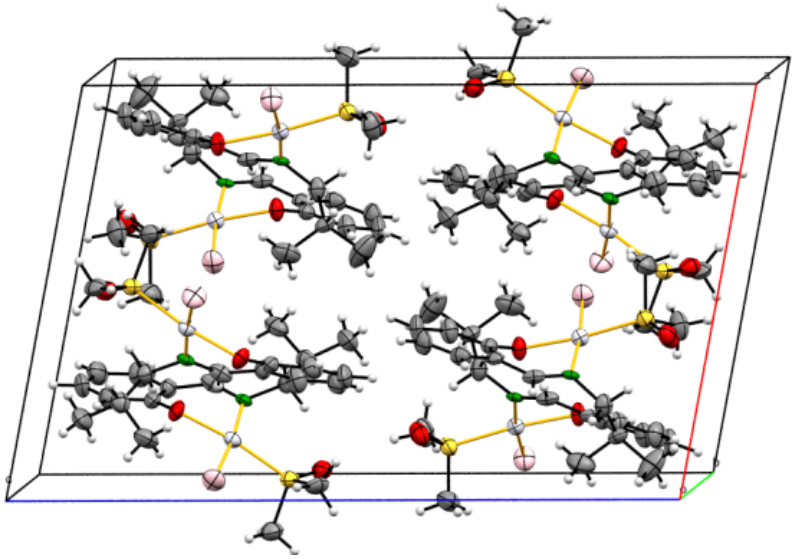

Figure S31. ORTEP plot of **C-1**-*cis* showing zigzag arrangement of molecules

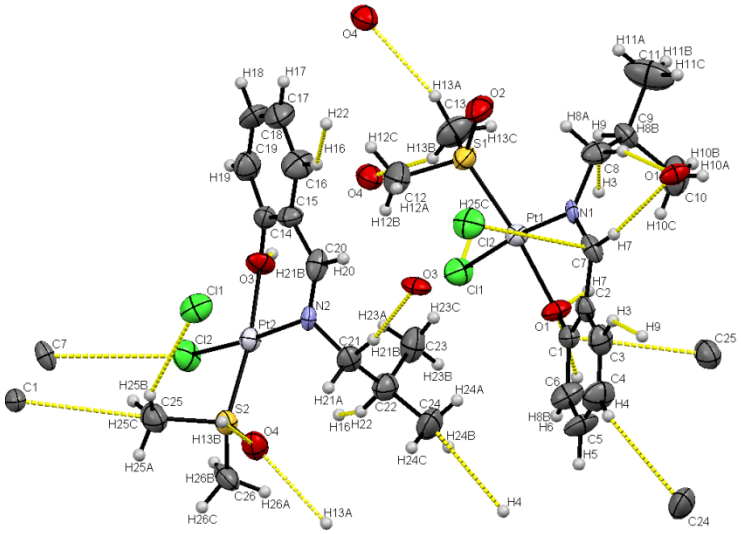

Figure S32. ORTEP plot of **C-1**-*cis*, showing single molecule short contacts with other molecules

The molecules of **C-1**-*cis* arrange in zigzag pattern (Fig. S31) in the unit cell in which one molecule is bonded to other molecules by strong electrostatic interaction (Fig. S32), strong interactions and short contacts are observed between the aromatic carbon of one molecule and methyl carbon of the DMSO of the other molecule (C(1)…C(25)), oxygen atom attached to aromatic ring of one molecule and imine and methylene hydrogen or the other (O(1)…H(7), H(8B), O(3)…H(21B)), chlorine atom of one molecule and methyl hydrogen of the DMSO of the other (Cl(1)…H(25C)), second chlorine and carbon of next molecule (Cl(2)…C(7)) and oxygen of DMSO of one molecule was strongly attached to the hydrogen of methyl attached to DMSO of the other molecule (O(4)…H(13AB)).

Table S2. Selected bond length (Å), angles (°) and torsion angles (°) of **C-1**-*cis*, **C-1**-*trans*, and **C-3**

Entry	Bond/Angle	**C-1**-*cis*		**C-1**-*trans*		**C-3**
		Conf-1	Conf-2	Conf-1	Conf-2	
1	Pt-N_1	2.015(5)	2.018	2.039(6)	2.036	1.983(13)
2	Pt-O	2.018(5)	2.010	1.963(6)	2.002	1.970(12)
3	Pt-S/N_2	2.2035(18)	2.203	2.2399(19)	2.231	2.088(15)
4	Pt-Cl	2.3018(18)	2.301	2.294(2)	2.303	2.315(4)
5	$\angle N_1PtO$	87.9(2)	88.81	92.7(3)	93.08	92.1(5)
6	$\angle A_cPtA_t$[a)]	88.81(7)	88.17	89.87(8)	87.14	88.2(5)
7	$\angle OPtA_t$	85.47(13)	85.05	83.96(18)	86.22	82.6(4)
8	$\angle N_1PtA_c$	97.76(16)	98.04	93.5(2)	93.57	97.1(6)
9	$\angle N_1PtA_t$	173.42(16)	173.73	176.61(19)	179.28	174.7(4)
10	$\angle OPtA_c$	173.54(14)	171.98	173.39(19)	173.09	170.7(6)
11[b)]	$\angle C_1OPtA_c$	–106.18	106.97	156.04	166.48	172.65
12[b)]	$\angle C_1OPtA_t$	–133.92	139.44	177.17	–177.50	166.24
13[b)]	$\angle OPtN_1C_8$	141.48	–144.53	179.66	177.83	–171.30

[a)] A_c represents the atom *cis* to N_1 and A_t represents the atom *trans* to N_1; [b)] Dihedral angle.

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for C-1-*cis*. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	3730(1)	2644(1)	2038(1)	28(1)
Cl(1)	4614(2)	4404(2)	2183(1)	47(1)
S(1)	4190(1)	2456(2)	1106(1)	37(1)
N(1)	2925(4)	1129(4)	2012(3)	24(1)
O(1)	3453(4)	2923(4)	2922(2)	37(1)
O(2)	3825(4)	1464(4)	678(3)	53(2)
C(1)	3572(5)	2048(6)	3336(4)	34(2)
C(2)	3358(5)	852(6)	3173(4)	31(2)
C(3)	3453(6)	-9(6)	3642(4)	43(2)
C(4)	3791(7)	247(7)	4256(4)	56(2)
C(5)	4039(7)	1417(7)	4431(4)	55(2)
C(6)	3923(6)	2294(6)	3983(4)	48(2)
C(7)	2923(5)	539(5)	2525(4)	32(2)
C(8)	2218(6)	699(6)	1418(4)	42(2)
C(9)	1424(5)	1578(6)	1162(4)	36(2)
C(10)	757(6)	1917(7)	1650(5)	66(3)

C(11)	750(8)	1045(8)	555(5)	88(3)
C(12)	5503(6)	2389(8)	1257(4)	67(3)
C(13)	3937(7)	3769(6)	646(4)	63(3)
Pt(2)	9006(1)	2635(1)	2885(1)	30(1)
Cl(2)	9865(2)	4374(2)	2791(1)	51(1)
S(2)	9983(1)	2389(2)	3830(1)	35(1)
N(2)	8149(4)	1163(4)	2880(3)	27(1)
O(3)	8285(4)	2971(4)	1989(2)	38(1)
O(4)	9827(4)	1398(4)	4242(3)	45(1)
C(14)	8083(5)	2122(6)	1564(3)	34(2)
C(15)	7878(5)	944(6)	1717(4)	35(2)
C(16)	7584(6)	120(6)	1226(4)	55(2)
C(17)	7543(6)	390(7)	606(4)	58(2)
C(18)	7762(6)	1556(8)	457(4)	55(2)
C(19)	8019(6)	2394(7)	921(4)	49(2)
C(20)	7785(6)	611(6)	2347(4)	40(2)
C(21)	7785(5)	732(6)	3448(4)	38(2)
C(22)	7152(6)	1648(6)	3713(4)	43(2)
C(23)	6316(6)	2148(7)	3211(4)	55(2)
C(24)	6722(6)	1086(8)	4258(4)	67(3)
C(25)	11241(5)	2235(7)	3698(4)	53(2)
C(26)	10056(6)	3691(6)	4311(4)	46(2)

Table S4. Bond lengths [Å] and angles [°] for C-1-*cis*.

Pt(1)-N(1)	2.015(5)
Pt(1)-O(1)	2.018(5)
Pt(1)-S(1)	2.2035(18)
Pt(1)-Cl(1)	2.3018(18)
S(1)-O(2)	1.469(5)
S(1)-C(12)	1.729(8)
S(1)-C(13)	1.773(7)
N(1)-C(7)	1.281(8)
N(1)-C(8)	1.513(9)
O(1)-C(1)	1.314(8)
C(1)-C(6)	1.401(10)
C(1)-C(2)	1.408(9)
C(2)-C(3)	1.383(9)
C(2)-C(7)	1.441(10)
C(3)-C(4)	1.336(11)
C(4)-C(5)	1.393(10)
C(5)-C(6)	1.364(10)
C(8)-C(9)	1.481(9)
C(9)-C(10)	1.546(10)
C(9)-C(11)	1.553(11)
Pt(2)-O(3)	2.010(5)
Pt(2)-N(2)	2.018(5)
Pt(2)-S(2)	2.203(2)
Pt(2)-Cl(2)	2.3009(18)
S(2)-O(4)	1.463(5)
S(2)-C(25)	1.771(7)
S(2)-C(26)	1.784(7)
N(2)-C(20)	1.308(9)
N(2)-C(21)	1.473(8)
O(3)-C(14)	1.312(8)
C(14)-C(19)	1.395(10)
C(14)-C(15)	1.407(9)
C(15)-C(16)	1.401(10)
C(15)-C(20)	1.425(10)
C(16)-C(17)	1.350(11)
C(17)-C(18)	1.397(10)

C(18)-C(19)	1.365(10)
C(21)-C(22)	1.513(9)
C(22)-C(23)	1.505(10)
C(22)-C(24)	1.532(9)

N(1)-Pt(1)-O(1)	87.9(2)
N(1)-Pt(1)-S(1)	97.76(16)
O(1)-Pt(1)-S(1)	173.54(14)
N(1)-Pt(1)-Cl(1)	173.42(16)
O(1)-Pt(1)-Cl(1)	85.47(13)
S(1)-Pt(1)-Cl(1)	88.81(7)
O(2)-S(1)-C(12)	106.8(3)
O(2)-S(1)-C(13)	106.5(4)
C(12)-S(1)-C(13)	102.7(4)
O(2)-S(1)-Pt(1)	121.3(2)
C(12)-S(1)-Pt(1)	106.6(3)
C(13)-S(1)-Pt(1)	111.4(3)
C(7)-N(1)-C(8)	116.6(5)
C(7)-N(1)-Pt(1)	120.3(5)
C(8)-N(1)-Pt(1)	122.7(4)
C(1)-O(1)-Pt(1)	119.6(4)
O(1)-C(1)-C(6)	119.4(6)
O(1)-C(1)-C(2)	124.0(7)
C(6)-C(1)-C(2)	116.6(7)
C(3)-C(2)-C(1)	120.4(7)
C(3)-C(2)-C(7)	119.3(6)
C(1)-C(2)-C(7)	119.9(6)
C(4)-C(3)-C(2)	121.8(7)
C(3)-C(4)-C(5)	119.1(8)
C(6)-C(5)-C(4)	120.6(8)
C(5)-C(6)-C(1)	121.4(7)
N(1)-C(7)-C(2)	128.9(6)
C(9)-C(8)-N(1)	112.7(5)
C(8)-C(9)-C(10)	112.6(6)
C(8)-C(9)-C(11)	108.2(6)
C(10)-C(9)-C(11)	109.8(7)
O(3)-Pt(2)-N(2)	88.8(2)
O(3)-Pt(2)-S(2)	171.98(14)

N(2)-Pt(2)-S(2)	98.04(17)
O(3)-Pt(2)-Cl(2)	85.05(14)
N(2)-Pt(2)-Cl(2)	173.73(17)
S(2)-Pt(2)-Cl(2)	88.18(7)
O(4)-S(2)-C(25)	105.7(3)
O(4)-S(2)-C(26)	106.2(3)
C(25)-S(2)-C(26)	102.9(3)
O(4)-S(2)-Pt(2)	121.3(2)
C(25)-S(2)-Pt(2)	106.5(3)
C(26)-S(2)-Pt(2)	112.5(3)
C(20)-N(2)-C(21)	115.7(5)
C(20)-N(2)-Pt(2)	120.9(5)
C(21)-N(2)-Pt(2)	122.9(5)
C(14)-O(3)-Pt(2)	121.4(4)
O(3)-C(14)-C(19)	119.2(6)
O(3)-C(14)-C(15)	123.5(6)
C(19)-C(14)-C(15)	117.3(7)
C(16)-C(15)-C(14)	119.4(7)
C(16)-C(15)-C(20)	118.0(6)
C(14)-C(15)-C(20)	121.6(6)
C(17)-C(16)-C(15)	122.6(7)
C(16)-C(17)-C(18)	117.7(8)
C(19)-C(18)-C(17)	121.3(8)
C(18)-C(19)-C(14)	121.5(7)
N(2)-C(20)-C(15)	127.7(6)
N(2)-C(21)-C(22)	112.4(5)
C(23)-C(22)-C(21)	112.5(7)
C(23)-C(22)-C(24)	111.1(7)
C(21)-C(22)-C(24)	108.7(6)

Symmetry transformations used to generate equivalent atoms:

Table S5. Anisotropic displacement parameters (Å^{2}x 10^3) for C-1-*cis*. The anisotropic displacement factor exponent takes the form: -2π^2[h^2 a*^{2}U^{11} + ... + 2 h k a* b* U^{12}]

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	30(1)	24(1)	30(1)	-1(1)	6(1)	0(1)
Cl(1)	61(1)	35(1)	47(1)	-3(1)	13(1)	-14(1)
S(1)	38(1)	40(1)	35(1)	-3(1)	13(1)	-2(1)
N(1)	9(3)	30(3)	34(4)	-1(3)	6(3)	0(2)
O(1)	58(3)	30(2)	25(3)	-4(2)	12(3)	-2(2)
O(2)	60(4)	56(3)	49(4)	-19(3)	25(3)	-12(3)
C(1)	25(4)	45(4)	32(5)	-5(4)	6(3)	-1(3)
C(2)	18(4)	36(4)	38(5)	8(3)	1(3)	4(3)
C(3)	41(5)	39(4)	52(6)	8(4)	11(4)	-7(4)
C(4)	72(7)	55(5)	44(6)	17(4)	17(5)	-5(5)
C(5)	77(7)	65(5)	25(5)	3(4)	19(5)	0(5)
C(6)	66(6)	41(4)	39(5)	1(4)	18(4)	6(4)
C(7)	20(4)	23(3)	52(5)	-3(4)	0(4)	0(3)
C(8)	58(6)	33(4)	35(5)	-6(4)	11(4)	-3(4)
C(9)	27(4)	36(4)	39(5)	2(3)	-3(4)	-4(3)
C(10)	50(6)	60(5)	93(8)	3(5)	23(6)	10(4)
C(11)	110(9)	68(6)	67(8)	-4(6)	-29(6)	21(6)
C(12)	45(5)	91(6)	67(6)	-13(6)	20(5)	2(5)
C(13)	89(8)	57(5)	49(7)	14(4)	25(6)	7(5)
Pt(2)	30(1)	27(1)	34(1)	1(1)	8(1)	-2(1)
Cl(2)	54(1)	40(1)	58(2)	6(1)	10(1)	-17(1)
S(2)	28(1)	39(1)	36(1)	-2(1)	5(1)	1(1)
N(2)	17(3)	32(3)	34(4)	2(3)	11(3)	-1(2)
O(3)	46(3)	36(3)	26(3)	12(2)	-4(2)	0(2)
O(4)	39(3)	51(3)	45(4)	12(3)	4(3)	-1(2)
C(14)	29(4)	42(4)	29(4)	4(3)	4(3)	1(3)
C(15)	40(5)	37(4)	28(5)	-6(3)	7(4)	1(3)
C(16)	71(7)	39(4)	56(7)	-7(4)	18(5)	-5(4)
C(17)	59(6)	70(6)	49(7)	-17(5)	19(5)	-5(5)
C(18)	60(6)	80(6)	28(5)	4(5)	17(4)	-5(5)
C(19)	48(5)	51(5)	49(5)	9(4)	13(4)	-4(4)
C(20)	38(5)	24(3)	61(6)	0(4)	23(4)	-2(3)

C(21)	38(5)	39(4)	36(5)	13(4)	6(4)	-2(3)
C(22)	46(5)	43(4)	43(6)	1(4)	13(4)	-7(4)
C(23)	42(5)	59(5)	70(6)	12(5)	24(5)	9(4)
C(24)	50(6)	105(7)	50(7)	12(5)	22(5)	-4(5)
C(25)	36(5)	63(5)	56(6)	-7(5)	3(4)	4(4)
C(26)	31(5)	52(4)	52(6)	-14(4)	-3(4)	-6(4)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C-1-*cis*.

	x	y	z	U(eq)
H(3)	3276	-788	3526	52
H(4)	3861	-348	4563	67
H(5)	4285	1601	4856	66
H(6)	4081	3072	4110	57
H(7)	2597	-192	2471	39
H(8A)	2614	521	1094	50
H(8B)	1894	-30	1515	50
H(9)	1754	2296	1042	43
H(10A)	414	1223	1762	100
H(10B)	264	2498	1466	100
H(10C)	1178	2240	2025	100
H(11A)	1170	817	259	132
H(11B)	265	1627	362	132
H(11C)	398	361	670	132
H(12A)	5720	1645	1456	100
H(12B)	5773	3028	1535	100
H(12C)	5744	2456	863	100
H(13A)	4082	3635	229	95
H(13B)	4357	4401	850	95
H(13C)	3234	3981	609	95
H(16)	7411	-644	1331	66
H(17)	7375	-181	290	70
H(18)	7731	1766	33	66
H(19)	8156	3164	806	59
H(20)	7423	-81	2383	48
H(21A)	8365	521	3774	45
H(21B)	7381	22	3337	45
H(22)	7601	2302	3889	52
H(23A)	6608	2588	2906	83
H(23B)	5897	2665	3408	83
H(23C)	5910	1512	3000	83
H(24A)	6216	509	4088	100

H(24B)	6421	1690	4478	100
H(24C)	7261	705	4549	100
H(25A)	11711	2314	4095	79
H(25B)	11375	2840	3408	79
H(25C)	11320	1468	3518	79
H(26A)	9487	3712	4525	70
H(26B)	10043	4381	4046	70
H(26C)	10676	3681	4622	70

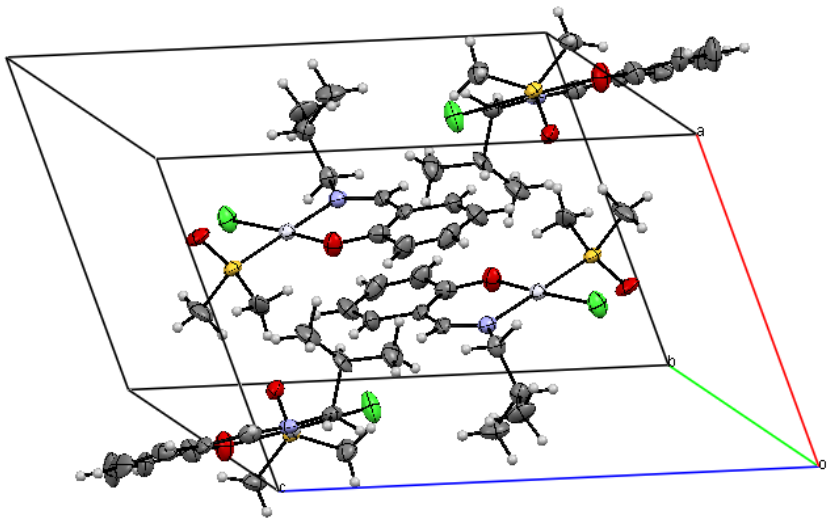

Figure S33. ORTEP plot of **C-1**-*trans***,** showing unit cell

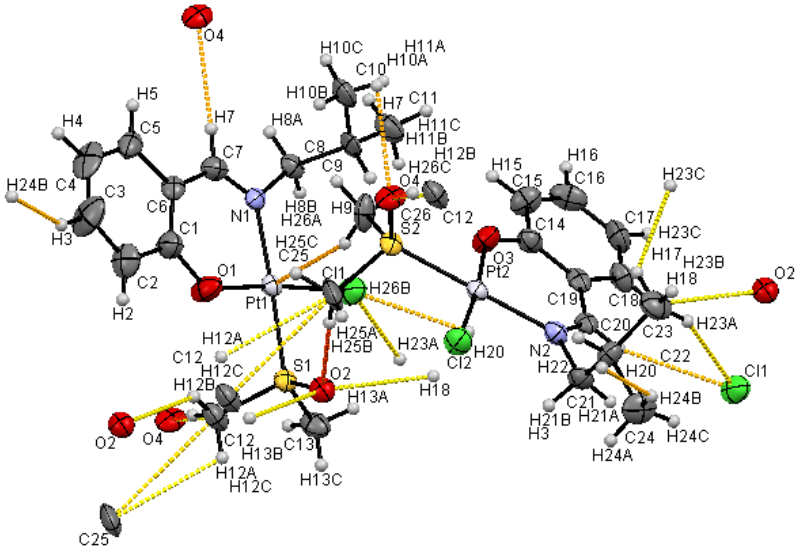

Figure S34. ORTEP plot of **C-1**-*trans***,** showing single molecule short contacts with other molecules

The molecules of **C-1**-*trans* also arrange in zigzag pattern (Fig. S33) in the unit cell in which one molecule is bonded to other molecules by strong electrostatic interaction. Short contacts are observed between Pt(1)….H(26), C(l1)….H(20) and H(23A), O(2)….H(18), H(25B) and H(12C), O(4)….C(12), H(7) and H(12B), H(12A)….C(25).

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **C-1**-*trans*. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	8892(1)	7823(1)	1104(1)	24(1)
Cl(1)	8358(3)	7741(2)	2705(2)	52(1)
N(1)	8214(6)	9627(6)	690(5)	27(1)
O(1)	9339(8)	7689(6)	-217(4)	48(2)
O(2)	8592(6)	5015(5)	1640(4)	34(1)
S(1)	9649(2)	5839(2)	1468(1)	27(1)
C(1)	9151(10)	8548(8)	-1030(7)	42(2)
C(2)	9604(11)	8202(10)	-1889(6)	48(2)
C(3)	9426(15)	9089(11)	-2703(7)	69(3)
C(4)	8954(11)	10274(12)	-2755(7)	64(3)
C(5)	8491(9)	10597(9)	-1944(7)	45(2)
C(6)	8626(8)	9759(8)	-1012(6)	31(2)
C(7)	8193(8)	10208(7)	-184(6)	35(2)
C(8)	7679(8)	10338(7)	1412(6)	30(2)
C(9)	6193(9)	10167(8)	1989(6)	36(2)
C(10)	5162(10)	10796(9)	1415(7)	49(2)
C(11)	5923(10)	10647(9)	2847(7)	49(2)
C(12)	11125(8)	5538(8)	533(7)	40(2)
C(13)	10384(10)	5332(9)	2466(7)	43(2)
Pt(2)	3888(1)	5169(1)	2886(1)	25(1)
Cl(2)	3916(3)	3677(2)	2187(2)	43(1)
N(2)	3343(7)	4049(6)	4257(5)	30(1)
O(3)	3860(7)	6609(5)	3339(4)	39(1)
O(4)	3378(6)	6855(5)	873(4)	39(1)
S(2)	4491(2)	6414(2)	1392(1)	28(1)
C(14)	3608(8)	6630(7)	4245(6)	34(2)
C(15)	3663(10)	7756(8)	4378(7)	43(2)
C(16)	3365(10)	7880(9)	5248(8)	48(2)
C(17)	3087(10)	6885(9)	6099(7)	48(2)
C(18)	3077(9)	5760(8)	5986(6)	38(2)
C(19)	3306(7)	5613(8)	5061(6)	30(2)
C(20)	3249(7)	4424(7)	4999(5)	27(2)
C(21)	3109(9)	2765(7)	4498(6)	32(2)

C(22)	1737(9)	2581(7)	4432(6)	33(2)
C(23)	477(9)	3263(10)	4988(8)	54(3)
C(24)	1616(11)	1174(8)	4817(8)	51(3)
C(25)	5941(10)	5743(10)	650(7)	56(3)
C(26)	5225(10)	7659(9)	1368(6)	46(2)

Table S8. Bond lengths [Å] and angles [°] for **C-1**-*trans*.

Pt(1)-O(1)	1.963(6)
Pt(1)-N(1)	2.039(6)
Pt(1)-S(1)	2.2399(19)
Pt(1)-Cl(1)	2.294(2)
N(1)-C(7)	1.282(10)
N(1)-C(8)	1.495(10)
O(1)-C(1)	1.353(10)
O(2)-S(1)	1.478(6)
S(1)-C(13)	1.765(9)
S(1)-C(12)	1.788(8)
C(1)-C(2)	1.406(13)
C(1)-C(6)	1.419(12)
C(2)-C(3)	1.365(14)
C(3)-C(4)	1.361(18)
C(4)-C(5)	1.325(16)
C(5)-C(6)	1.463(11)
C(6)-C(7)	1.429(12)
C(8)-C(9)	1.504(11)
C(9)-C(10)	1.492(14)
C(9)-C(11)	1.508(12)
Pt(2)-O(3)	2.002(6)
Pt(2)-N(2)	2.037(7)
Pt(2)-S(2)	2.2311(19)
Pt(2)-Cl(2)	2.303(2)
N(2)-C(20)	1.303(10)
N(2)-C(21)	1.471(10)
O(3)-C(14)	1.325(10)
O(4)-S(2)	1.483(6)
S(2)-C(26)	1.736(9)
S(2)-C(25)	1.778(9)
C(14)-C(15)	1.406(11)
C(14)-C(19)	1.410(11)
C(15)-C(16)	1.308(13)
C(16)-C(17)	1.424(14)
C(17)-C(18)	1.379(13)
C(18)-C(19)	1.412(11)

C(19)-C(20)	1.433(11)
C(21)-C(22)	1.478(12)
C(22)-C(23)	1.538(13)
C(22)-C(24)	1.569(12)

O(1)-Pt(1)-N(1)	92.7(3)
O(1)-Pt(1)-S(1)	83.96(18)
N(1)-Pt(1)-S(1)	176.61(19)
O(1)-Pt(1)-Cl(1)	173.39(19)
N(1)-Pt(1)-Cl(1)	93.5(2)
S(1)-Pt(1)-Cl(1)	89.87(8)
C(7)-N(1)-C(8)	116.4(7)
C(7)-N(1)-Pt(1)	122.8(6)
C(8)-N(1)-Pt(1)	120.8(5)
C(1)-O(1)-Pt(1)	129.0(6)
O(2)-S(1)-C(13)	107.7(4)
O(2)-S(1)-C(12)	108.4(4)
C(13)-S(1)-C(12)	100.5(5)
O(2)-S(1)-Pt(1)	114.9(2)
C(13)-S(1)-Pt(1)	113.9(3)
C(12)-S(1)-Pt(1)	110.3(3)
O(1)-C(1)-C(2)	116.7(8)
O(1)-C(1)-C(6)	120.5(8)
C(2)-C(1)-C(6)	122.5(8)
C(3)-C(2)-C(1)	115.6(10)
C(4)-C(3)-C(2)	125.6(10)
C(5)-C(4)-C(3)	118.7(9)
C(4)-C(5)-C(6)	122.1(9)
C(1)-C(6)-C(7)	126.6(7)
C(1)-C(6)-C(5)	114.8(8)
C(7)-C(6)-C(5)	118.5(8)
N(1)-C(7)-C(6)	128.3(8)
N(1)-C(8)-C(9)	113.9(7)
C(10)-C(9)-C(8)	112.8(7)
C(10)-C(9)-C(11)	110.0(7)
C(8)-C(9)-C(11)	107.9(8)
O(3)-Pt(2)-N(2)	93.1(2)
O(3)-Pt(2)-S(2)	86.21(17)

N(2)-Pt(2)-S(2)	179.27(19)
O(3)-Pt(2)-Cl(2)	173.08(17)
N(2)-Pt(2)-Cl(2)	93.58(19)
S(2)-Pt(2)-Cl(2)	87.14(8)
C(20)-N(2)-C(21)	114.6(7)
C(20)-N(2)-Pt(2)	120.9(5)
C(21)-N(2)-Pt(2)	124.4(5)
C(14)-O(3)-Pt(2)	126.9(5)
O(4)-S(2)-C(26)	108.8(4)
O(4)-S(2)-C(25)	107.9(5)
C(26)-S(2)-C(25)	99.5(5)
O(4)-S(2)-Pt(2)	116.5(2)
C(26)-S(2)-Pt(2)	111.5(3)
C(25)-S(2)-Pt(2)	111.3(4)
O(3)-C(14)-C(15)	116.2(7)
O(3)-C(14)-C(19)	124.6(7)
C(15)-C(14)-C(19)	119.2(8)
C(16)-C(15)-C(14)	120.6(9)
C(15)-C(16)-C(17)	122.9(9)
C(18)-C(17)-C(16)	117.5(9)
C(17)-C(18)-C(19)	121.0(9)
C(14)-C(19)-C(18)	118.7(8)
C(14)-C(19)-C(20)	123.3(7)
C(18)-C(19)-C(20)	118.0(7)
N(2)-C(20)-C(19)	130.7(7)
N(2)-C(21)-C(22)	114.1(6)
C(21)-C(22)-C(23)	114.8(7)
C(21)-C(22)-C(24)	106.7(7)
C(23)-C(22)-C(24)	110.4(7)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **C-1**-*trans*. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	20(1)	29(1)	24(1)	-9(1)	-6(1)	-2(1)
Cl(1)	77(2)	46(1)	28(1)	-13(1)	-12(1)	10(1)
N(1)	18(3)	29(3)	31(3)	-4(3)	-7(3)	-4(2)
O(1)	73(5)	38(3)	34(3)	-7(3)	-23(3)	3(3)
O(2)	32(3)	42(3)	32(3)	-13(2)	-13(2)	-2(2)
S(1)	22(1)	32(1)	29(1)	-8(1)	-10(1)	-2(1)
C(1)	48(5)	41(5)	34(5)	-10(4)	-9(4)	0(4)
C(2)	55(6)	66(6)	32(5)	-17(4)	-16(4)	-12(5)
C(3)	114(11)	70(7)	28(5)	-7(5)	-25(6)	-22(7)
C(4)	48(6)	98(9)	36(6)	17(5)	-31(5)	-14(6)
C(5)	28(4)	53(5)	41(5)	6(4)	-11(4)	-3(4)
C(6)	22(4)	43(4)	28(4)	-6(3)	-13(3)	-2(3)
C(7)	31(4)	30(4)	46(5)	-12(3)	-12(4)	-1(3)
C(8)	21(4)	33(4)	40(4)	-14(3)	-6(3)	-6(3)
C(9)	38(5)	35(4)	29(4)	-19(3)	8(3)	4(3)
C(10)	39(5)	53(5)	46(6)	-25(4)	9(4)	3(4)
C(11)	48(6)	59(6)	44(5)	-31(5)	-7(4)	11(5)
C(12)	26(4)	46(5)	50(5)	-25(4)	2(4)	-4(4)
C(13)	38(5)	51(5)	43(5)	-18(4)	-19(4)	9(4)
Pt(2)	21(1)	27(1)	28(1)	-10(1)	-8(1)	0(1)
Cl(2)	60(1)	34(1)	37(1)	-19(1)	-7(1)	-2(1)
N(2)	25(3)	33(3)	35(4)	-14(3)	-7(3)	-3(3)
O(3)	56(4)	31(3)	31(3)	-5(2)	-14(3)	-9(3)
O(4)	29(3)	41(3)	50(4)	-3(3)	-25(3)	-5(2)
S(2)	19(1)	36(1)	31(1)	-7(1)	-10(1)	-5(1)
C(14)	31(4)	30(4)	44(5)	-15(3)	-5(4)	-4(3)
C(15)	53(6)	37(4)	49(5)	-11(4)	-21(5)	-12(4)
C(16)	50(6)	44(5)	71(7)	-37(5)	-30(5)	6(4)
C(17)	40(5)	64(6)	37(5)	-25(5)	4(4)	-2(4)
C(18)	34(4)	50(5)	34(4)	-24(4)	-3(4)	-6(4)
C(19)	18(3)	48(5)	28(4)	-15(3)	-12(3)	3(3)
C(20)	21(3)	35(4)	26(4)	-9(3)	-11(3)	3(3)
C(21)	40(4)	26(4)	33(4)	-15(3)	-8(3)	2(3)

C(22)	41(5)	28(4)	31(4)	-5(3)	-12(4)	-7(3)
C(23)	28(5)	56(6)	74(7)	-18(5)	-12(5)	-2(4)
C(24)	46(5)	40(5)	74(7)	-14(5)	-22(5)	-18(4)
C(25)	31(5)	79(7)	40(5)	-18(5)	12(4)	4(5)
C(26)	48(5)	58(6)	33(5)	-14(4)	4(4)	-32(4)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **C-1**-*trans*.

	x	y	z	U(eq)
H(2)	10004	7410	-1903	58
H(3)	9650	8862	-3276	83
H(4)	8955	10852	-3354	77
H(5)	8063	11391	-1968	54
H(7)	7850	11034	-294	42
H(8A)	7749	11204	1072	37
H(8B)	8279	10097	1858	37
H(9)	6080	9286	2226	44
H(10A)	4224	10655	1818	74
H(10B)	5339	10480	866	74
H(10C)	5253	11663	1186	74
H(11A)	6152	11481	2626	74
H(11B)	6498	10151	3270	74
H(11C)	4945	10618	3198	74
H(12A)	11441	4676	699	60
H(12B)	11873	6001	465	60
H(12C)	10862	5774	-71	60
H(13A)	9699	5495	3029	64
H(13B)	11196	5759	2321	64
H(13C)	10662	4464	2595	64
H(15)	3917	8427	3837	52
H(16)	3333	8660	5313	58
H(17)	2916	6990	6715	58
H(18)	2915	5081	6534	45
H(20)	3123	3812	5592	32
H(21A)	3192	2352	5157	39
H(21B)	3845	2381	4061	39
H(22)	1732	2854	3742	39
H(23A)	443	2982	5671	80
H(23B)	-376	3107	4896	80
H(23C)	570	4129	4748	80
H(24A)	2466	749	4514	76

H(24B)	826	994	4662	76
H(24C)	1481	909	5512	76
H(25A)	5688	5012	593	84
H(25B)	6723	5535	938	84
H(25C)	6201	6315	13	84
H(26A)	5157	8313	789	68
H(26B)	6200	7429	1369	68
H(26C)	4728	7931	1934	68

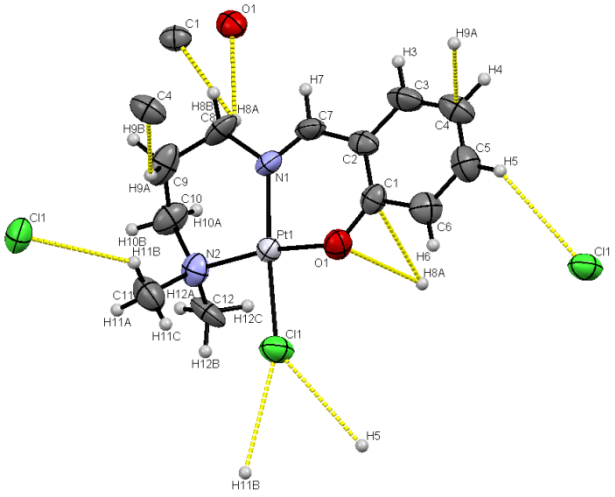

Figure S35. ORTEP plot of **C-3** showing short contacts

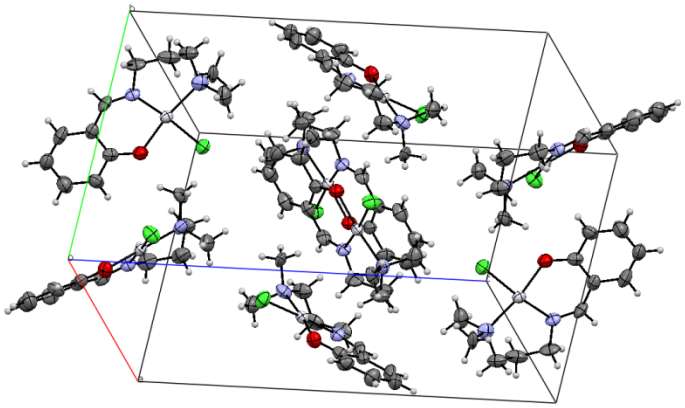

Figure S36. ORTEP plot of **C-3** unit cell showing zigzag arrangement of the molecules

In packing pattern each molecule bonded through short interactions with other molecule around it. Important inter-molecular interactions observed in the crystal packing of **C-3** were, interaction of C(1)O(1)…H(8A), C(4)…H(9A) and Cl(1)…H(5, 11B) (Fig. S35).

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C-3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	7147(1)	6877(1)	4014(1)	33(1)
Cl(1)	8992(4)	6632(4)	3417(2)	54(1)
O(1)	7815(9)	5700(9)	4578(7)	48(3)
N(1)	5621(11)	6983(9)	4585(7)	38(3)
N(2)	6686(16)	8079(10)	3314(9)	48(4)
C(1)	7422(16)	5384(12)	5183(9)	41(3)
C(2)	6328(14)	5764(11)	5497(8)	41(3)
C(3)	6025(19)	5379(15)	6143(10)	56(5)
C(4)	6770(20)	4670(14)	6493(10)	55(4)
C(5)	7832(19)	4306(17)	6184(14)	63(6)
C(6)	8163(19)	4650(13)	5545(10)	52(4)
C(7)	5490(14)	6487(13)	5153(8)	45(3)
C(8)	4505(15)	7653(14)	4415(10)	54(4)
C(9)	4460(20)	7985(13)	3666(13)	63(6)
C(10)	5515(16)	8687(13)	3479(11)	56(4)
C(11)	6560(20)	7557(17)	2628(10)	64(5)
C(12)	7610(20)	8899(14)	3280(9)	54(4)

Table S12. Bond lengths [Å] and angles [°] for C-3.

Pt(1)-O(1)	1.970(12)
Pt(1)-N(1)	1.983(13)
Pt(1)-N(2)	2.088(15)
Pt(1)-Cl(1)	2.315(4)
O(1)-C(1)	1.31(2)
N(1)-C(7)	1.28(2)
N(1)-C(8)	1.498(18)
N(2)-C(12)	1.43(2)
N(2)-C(11)	1.49(2)
N(2)-C(10)	1.50(2)
C(1)-C(6)	1.40(2)
C(1)-C(2)	1.41(2)
C(2)-C(3)	1.39(2)
C(2)-C(7)	1.44(2)
C(3)-C(4)	1.37(3)
C(4)-C(5)	1.36(3)
C(5)-C(6)	1.36(3)
C(8)-C(9)	1.52(3)
C(9)-C(10)	1.48(3)
O(1)-Pt(1)-N(1)	92.1(5)
O(1)-Pt(1)-N(2)	170.7(6)
N(1)-Pt(1)-N(2)	97.1(6)
O(1)-Pt(1)-Cl(1)	82.6(4)
N(1)-Pt(1)-Cl(1)	174.7(4)
N(2)-Pt(1)-Cl(1)	88.2(5)
C(1)-O(1)-Pt(1)	127.5(10)
C(7)-N(1)-C(8)	112.0(13)
C(7)-N(1)-Pt(1)	123.1(10)
C(8)-N(1)-Pt(1)	124.9(11)
C(12)-N(2)-C(11)	109.7(16)
C(12)-N(2)-C(10)	103.3(13)
C(11)-N(2)-C(10)	109.6(15)
C(12)-N(2)-Pt(1)	112.3(12)
C(11)-N(2)-Pt(1)	107.1(10)
C(10)-N(2)-Pt(1)	114.8(13)

O(1)-C(1)-C(6)	117.8(16)
O(1)-C(1)-C(2)	123.8(14)
C(6)-C(1)-C(2)	118.4(17)
C(3)-C(2)-C(1)	118.3(16)
C(3)-C(2)-C(7)	119.6(15)
C(1)-C(2)-C(7)	122.0(15)
C(4)-C(3)-C(2)	122.5(17)
C(5)-C(4)-C(3)	118.7(19)
C(6)-C(5)-C(4)	121(2)
C(5)-C(6)-C(1)	121.2(18)
N(1)-C(7)-C(2)	129.7(13)
N(1)-C(8)-C(9)	113.0(15)
C(10)-C(9)-C(8)	112.1(17)
C(9)-C(10)-N(2)	113.2(13)

Symmetry transformations used to generate equivalent atoms:

Table S13. Anisotropic displacement parameters ($Å^2 x 10^3$) C-3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	33(1)	34(1)	33(1)	-4(1)	-1(1)	2(1)
Cl(1)	51(2)	57(2)	55(3)	7(2)	17(2)	10(2)
O(1)	48(7)	48(7)	46(8)	-2(5)	-2(5)	11(4)
N(1)	24(6)	44(7)	47(8)	-3(5)	-1(6)	2(4)
N(2)	51(9)	46(8)	48(10)	-10(5)	-11(8)	-3(6)
C(1)	40(8)	37(7)	47(10)	-5(7)	-8(8)	2(6)
C(2)	43(8)	41(8)	40(9)	-6(6)	7(7)	-10(6)
C(3)	54(10)	69(12)	46(10)	-12(8)	21(9)	-8(9)
C(4)	71(11)	50(10)	44(10)	-4(8)	16(10)	-6(9)
C(5)	72(15)	63(14)	52(13)	11(10)	-5(9)	2(9)
C(6)	58(9)	36(8)	62(12)	9(8)	4(9)	2(7)
C(7)	28(7)	63(9)	43(9)	-11(8)	10(7)	1(7)
C(8)	27(7)	55(10)	80(13)	-9(9)	-5(8)	16(7)
C(9)	58(11)	41(9)	92(17)	-10(9)	-26(11)	14(8)
C(10)	47(9)	40(8)	81(13)	-3(8)	0(9)	9(7)
C(11)	81(14)	71(12)	41(10)	3(8)	0(10)	-14(10)
C(12)	83(12)	51(10)	28(9)	2(7)	20(9)	-13(9)

Table S14. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for C-3.

	x	y	z	U(eq)
H(3)	5288	5610	6347	68
H(4)	6556	4441	6931	66
H(5)	8338	3818	6413	75
H(6)	8892	4393	5346	62
H(7)	4738	6610	5378	54
H(8A)	4512	8291	4699	65
H(8B)	3755	7253	4524	65
H(9A)	4479	7349	3380	76
H(9B)	3683	8358	3577	76
H(10A)	5681	9172	3857	67
H(10B)	5280	9116	3085	67
H(11A)	6492	8097	2280	96
H(11B)	5819	7120	2624	96
H(11C)	7274	7117	2541	96
H(12A)	7242	9551	3118	81
H(12B)	8265	8683	2971	81
H(12C)	7960	9014	3728	81

Table S15. Torsion angles [°] for C-3.

Pt(1)-O(1)-C(1)-C(6)	-169.3(12)
Pt(1)-O(1)-C(1)-C(2)	9(2)
O(1)-C(1)-C(2)-C(3)	-179.0(16)
C(6)-C(1)-C(2)-C(3)	-1(2)
O(1)-C(1)-C(2)-C(7)	5(2)
C(6)-C(1)-C(2)-C(7)	-177.6(15)
C(1)-C(2)-C(3)-C(4)	2(3)
C(7)-C(2)-C(3)-C(4)	178.5(17)
C(2)-C(3)-C(4)-C(5)	-2(3)
C(3)-C(4)-C(5)-C(6)	1(3)
C(4)-C(5)-C(6)-C(1)	0(3)
O(1)-C(1)-C(6)-C(5)	178.3(18)
C(2)-C(1)-C(6)-C(5)	0(3)
C(8)-N(1)-C(7)-C(2)	179.6(15)
Pt(1)-N(1)-C(7)-C(2)	-1(2)
C(3)-C(2)-C(7)-N(1)	175.0(17)
C(1)-C(2)-C(7)-N(1)	-9(3)
C(7)-N(1)-C(8)-C(9)	-163.1(14)
Pt(1)-N(1)-C(8)-C(9)	17.7(19)
N(1)-C(8)-C(9)-C(10)	-64.2(19)
C(8)-C(9)-C(10)-N(2)	83(2)
C(12)-N(2)-C(10)-C(9)	-169.4(17)
C(11)-N(2)-C(10)-C(9)	74(2)
Pt(1)-N(2)-C(10)-C(9)	-47(2)

Symmetry transformations used to generate equivalent atoms: