

(Supporting Information)

Tuning Anticancer Properties of Pt(II) Complexes via Structurally Flexible N-(2-Picolylamine)salicylimine Ligands

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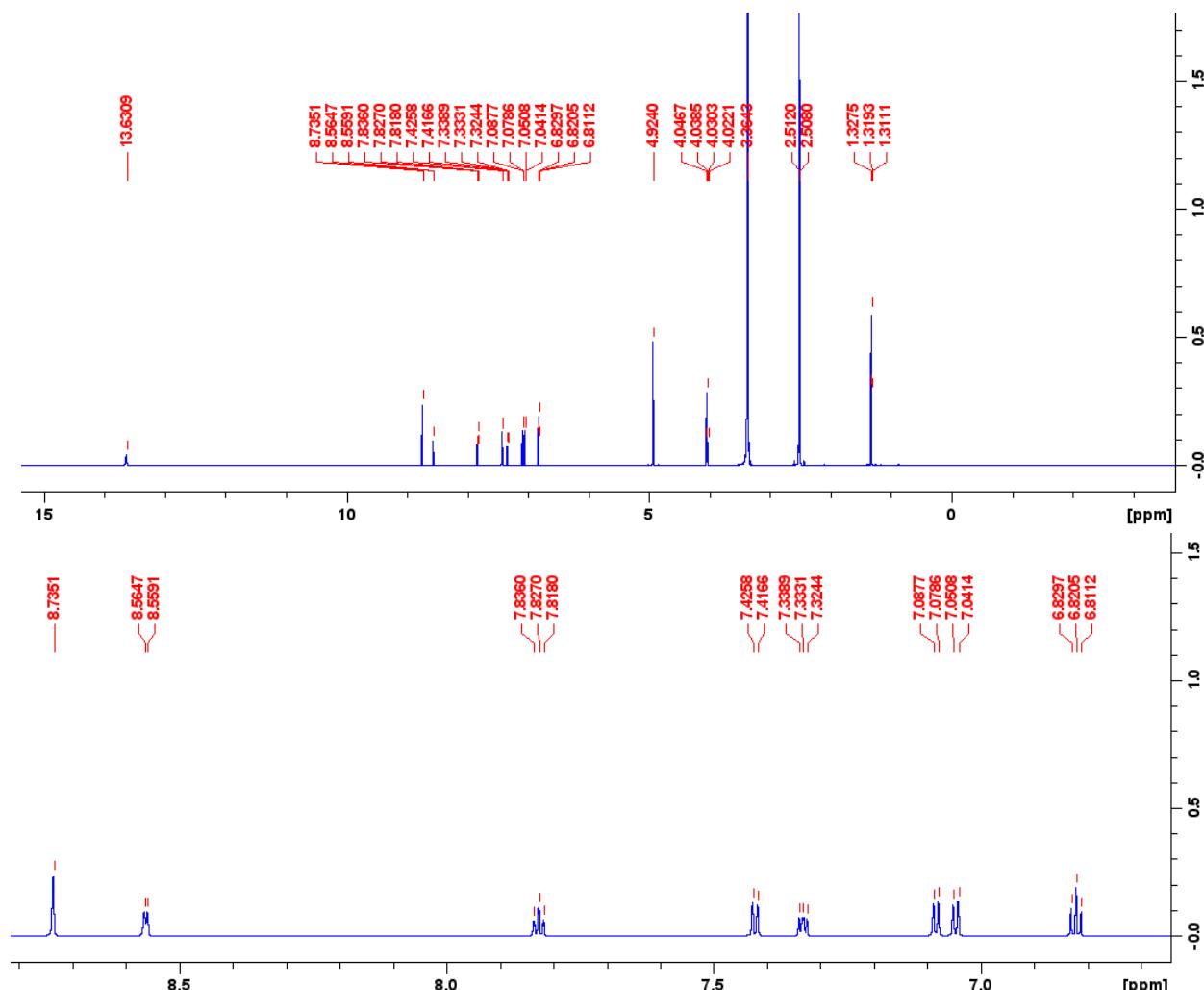


Figure S1. ¹H NMR of ligand L-OEt.

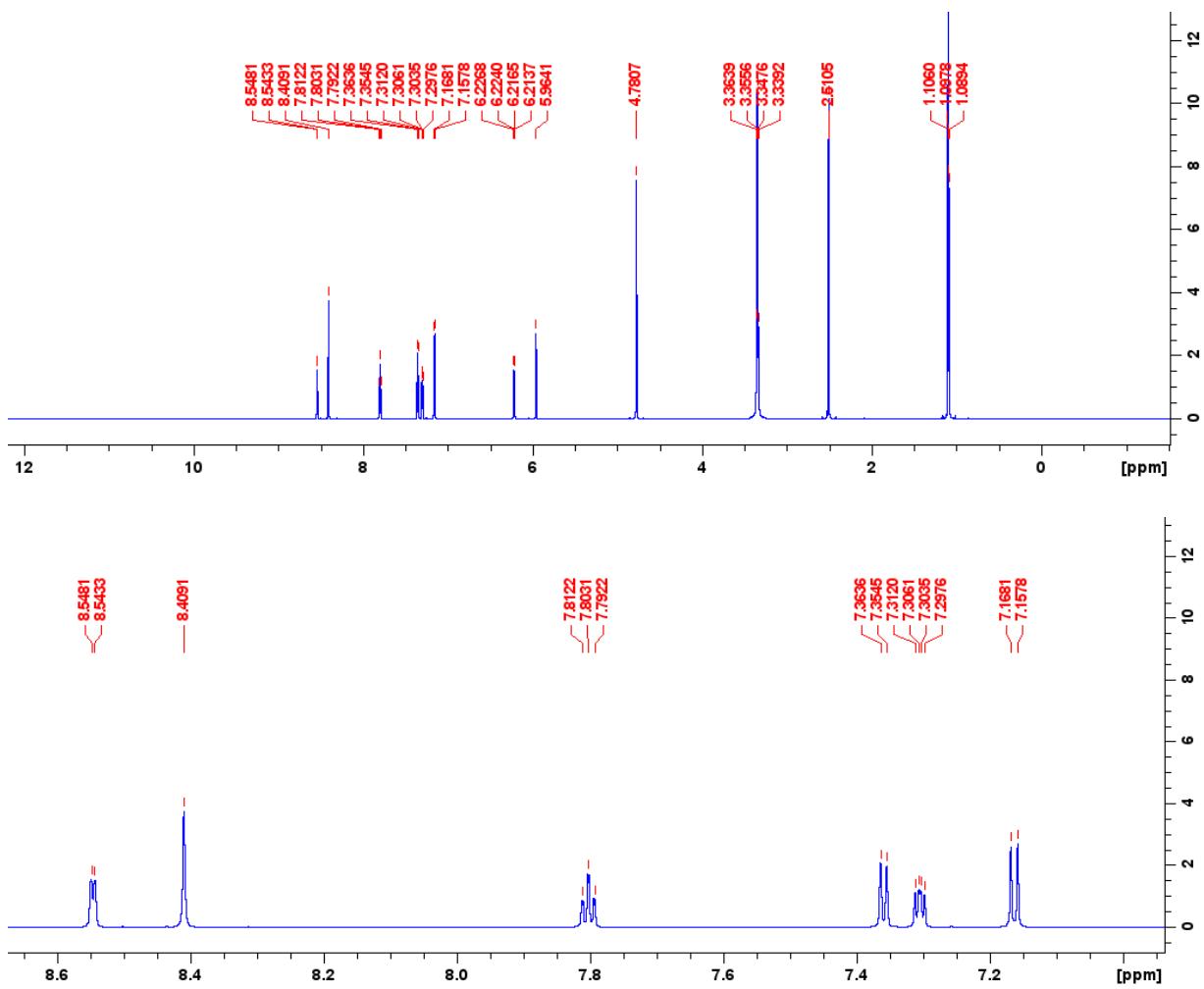


Figure S2. ¹H NMR of L-NEt₂.

KR-L3 in DCCl₃
22 December 2021
300 MHz

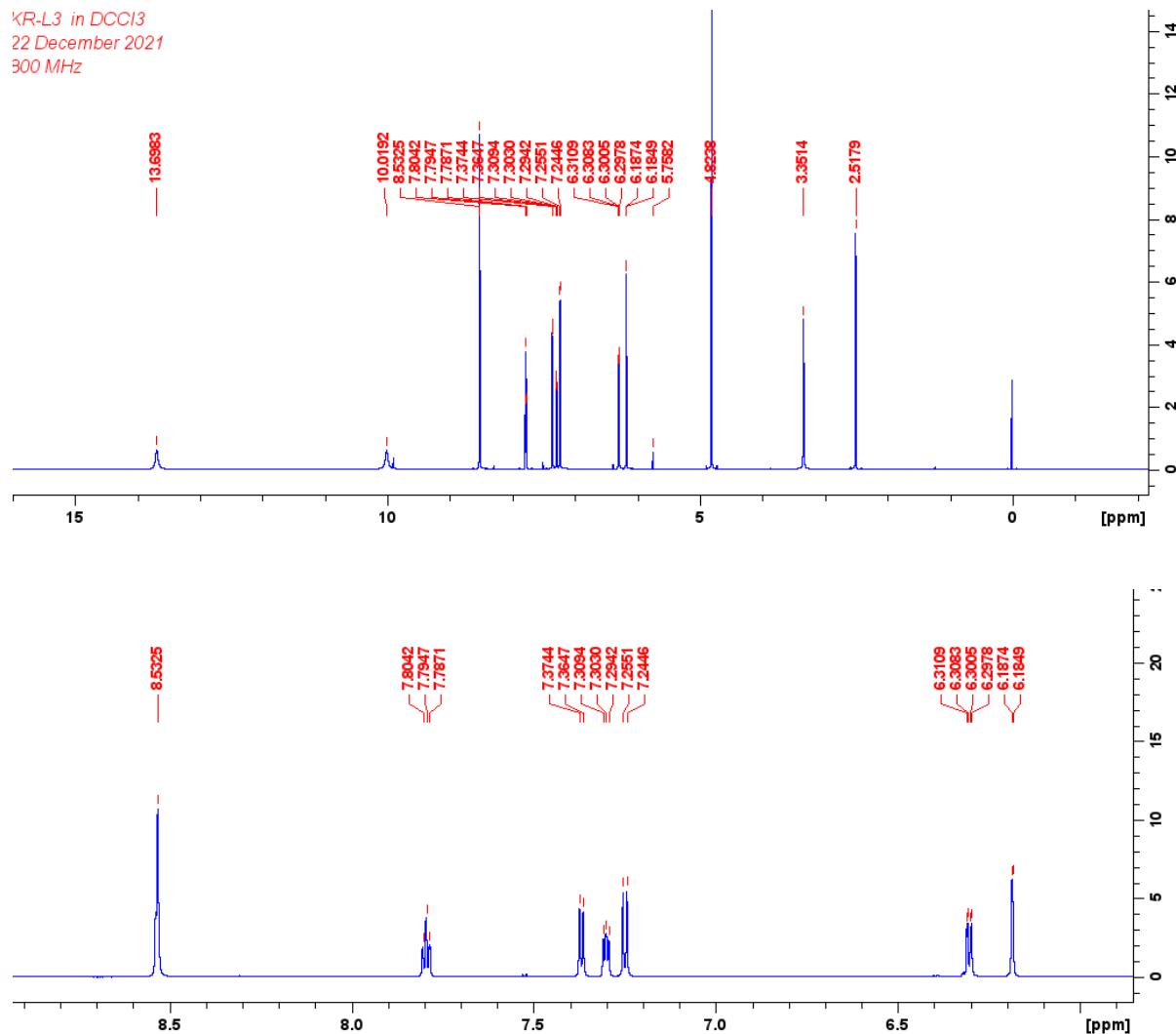


Figure S3. ¹H NMR of ligand L-OH.

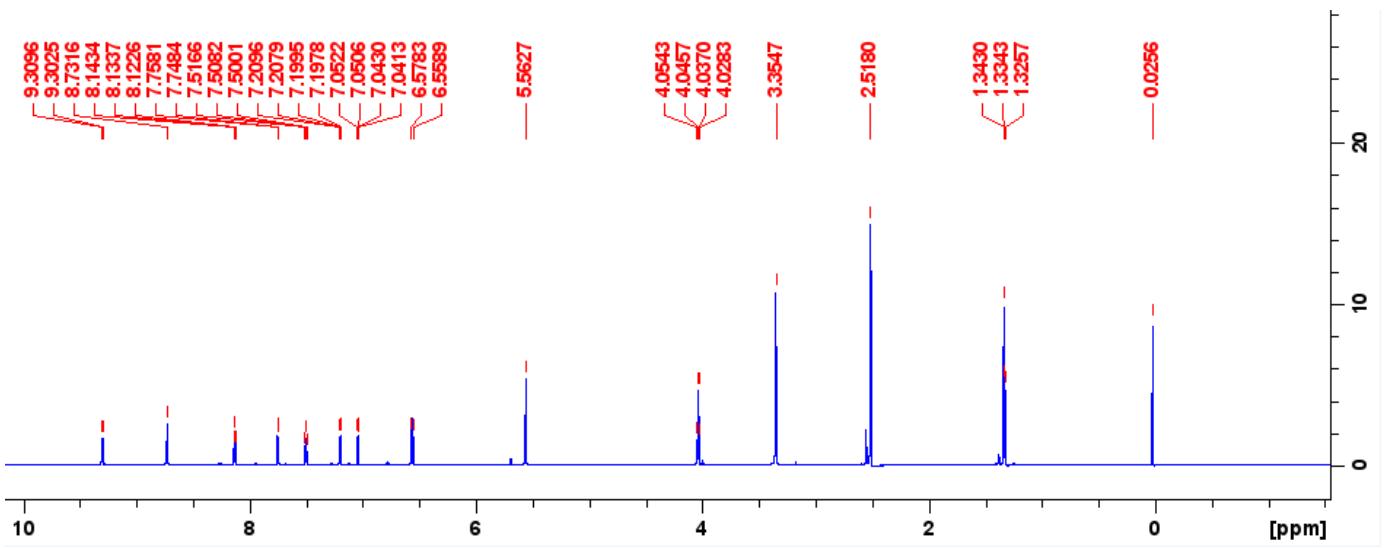


Figure S4. ¹H NMR of complex Pt-OEt.

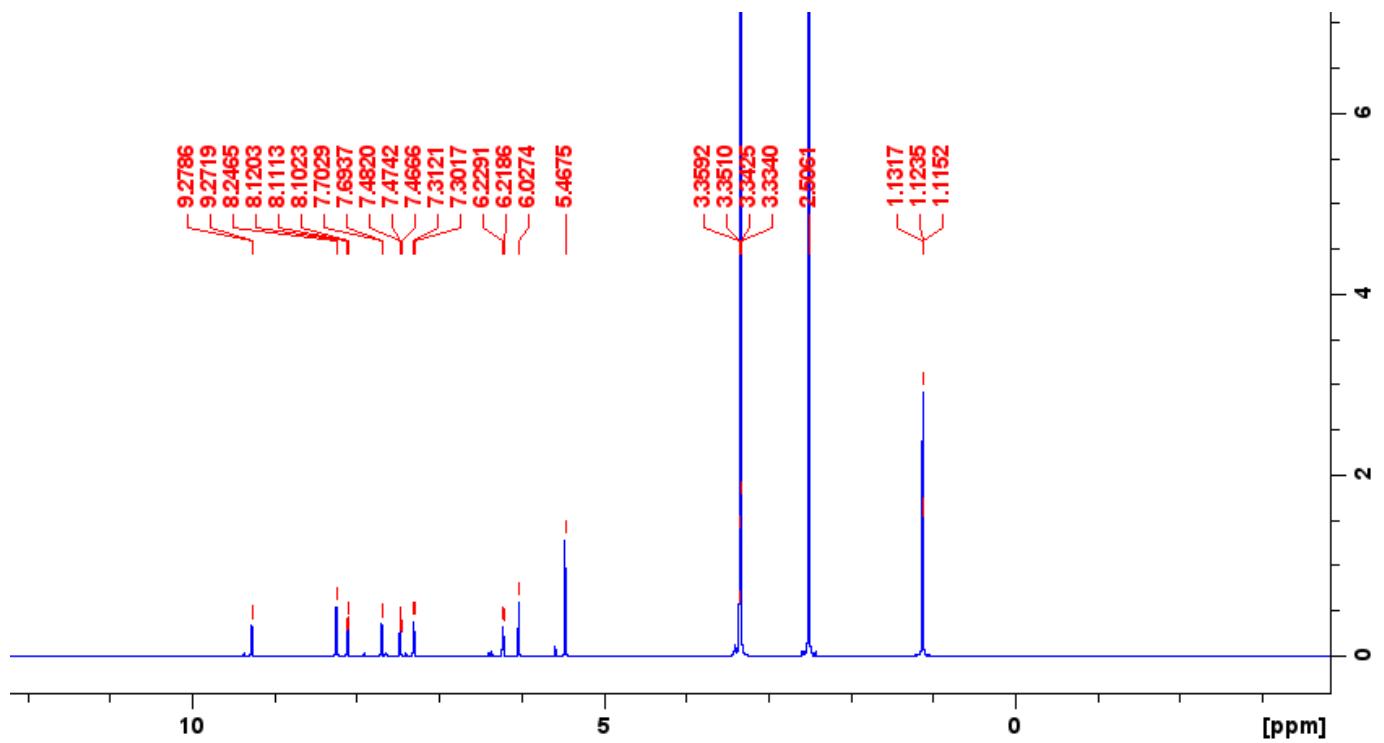


Figure S5. ¹H NMR of complex Pt-NEt₂.

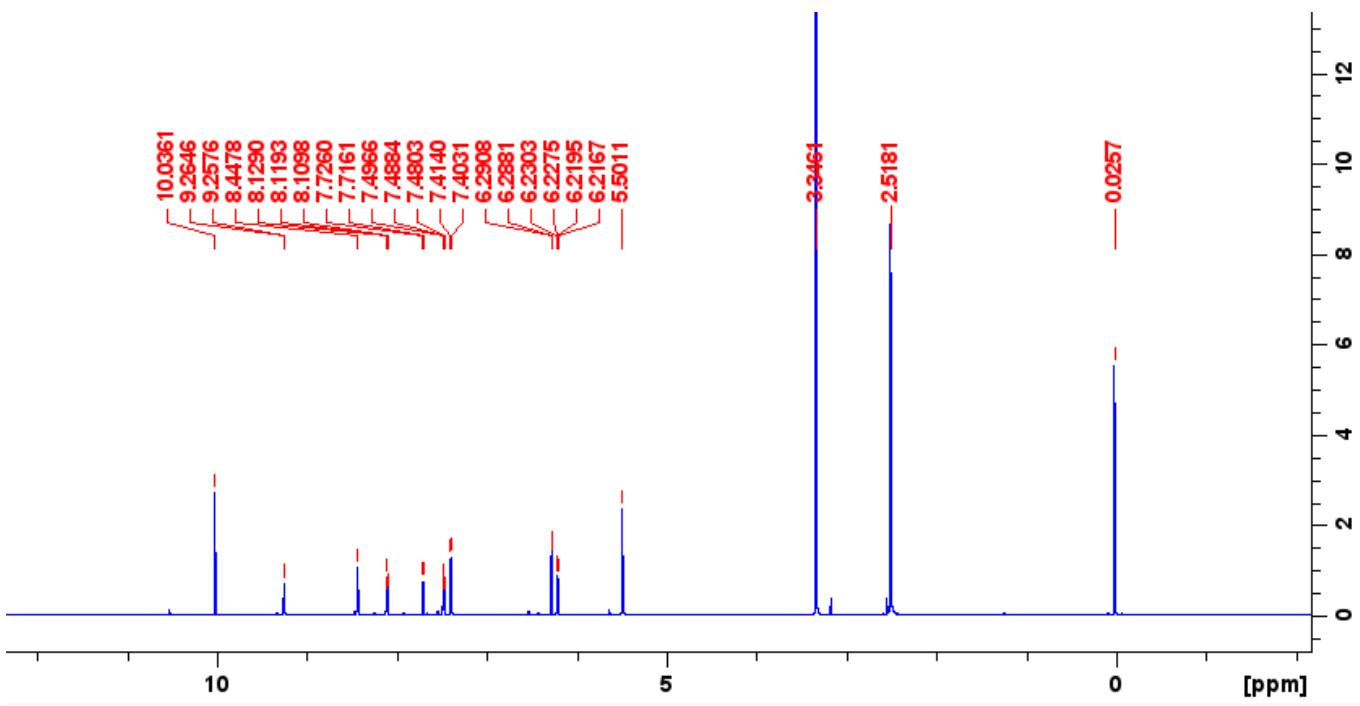


Figure S6. ¹H NMR of complex Pt-OH.

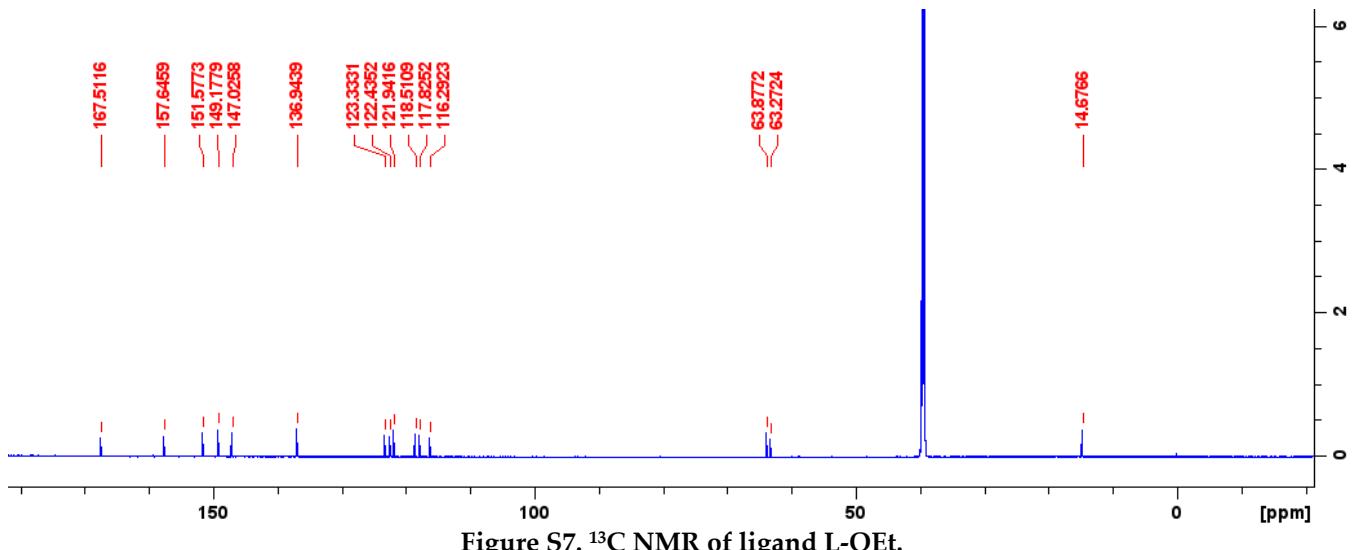


Figure S7. ¹³C NMR of ligand L-OEt.

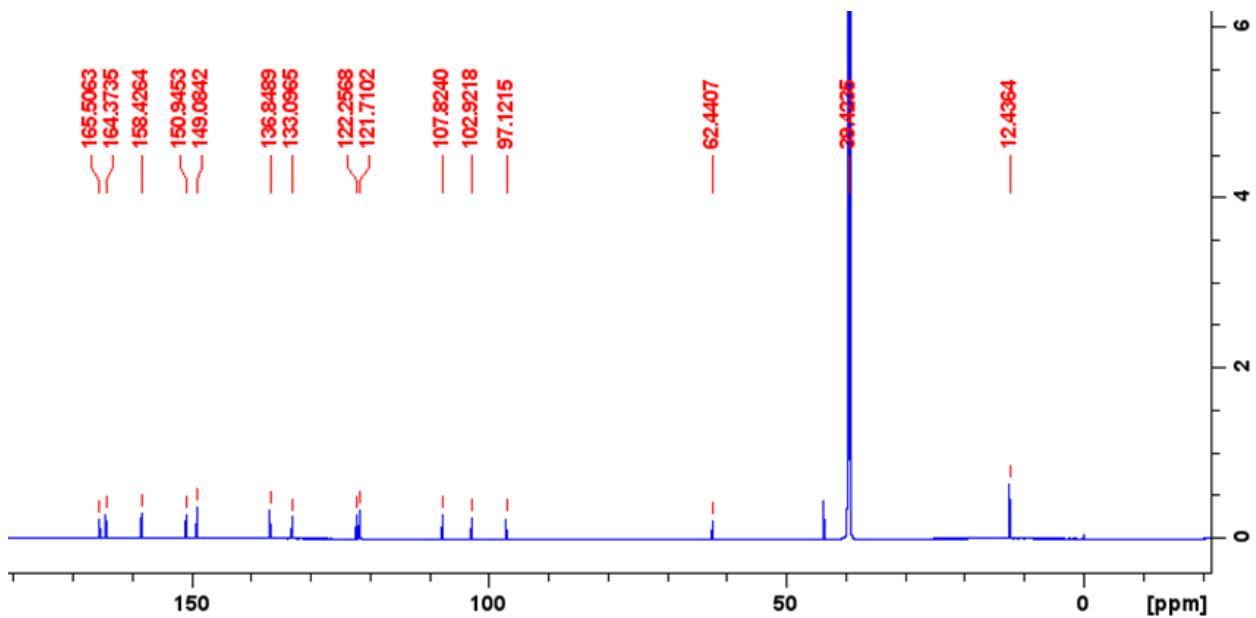


Figure S8. ¹³C NMR of ligand L-NEt₂.

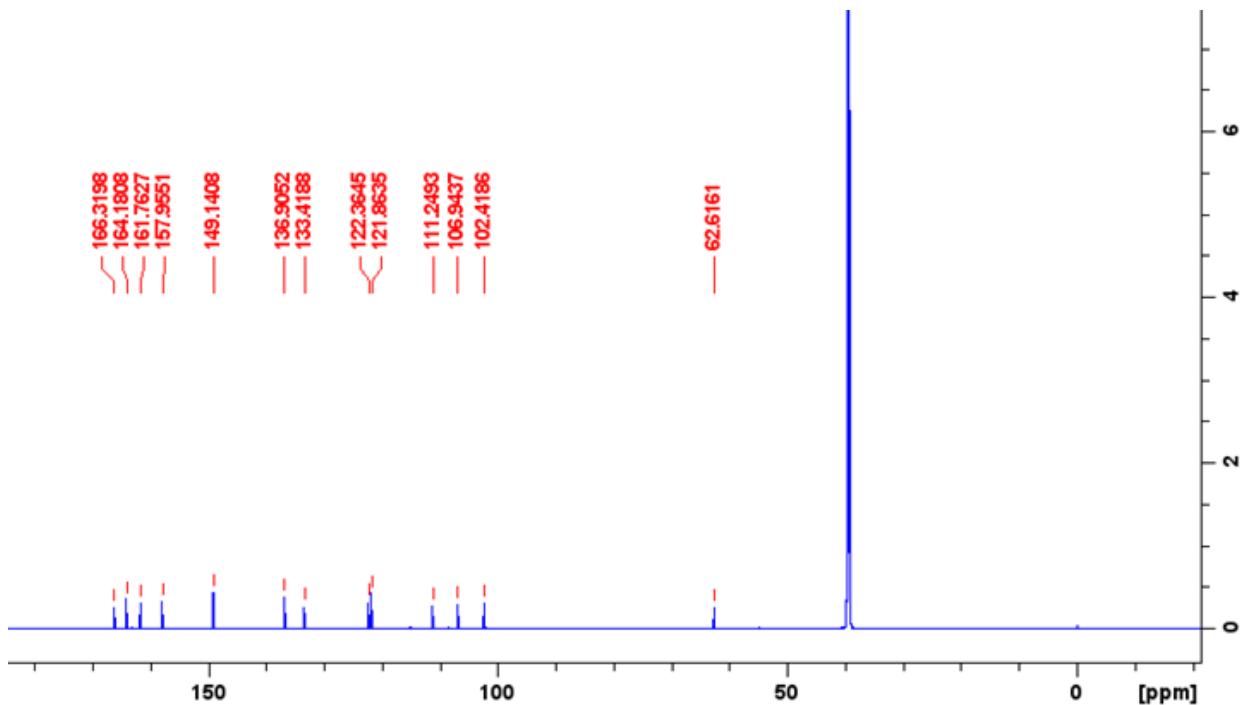


Figure S9. ¹³C NMR of ligand L-OH.

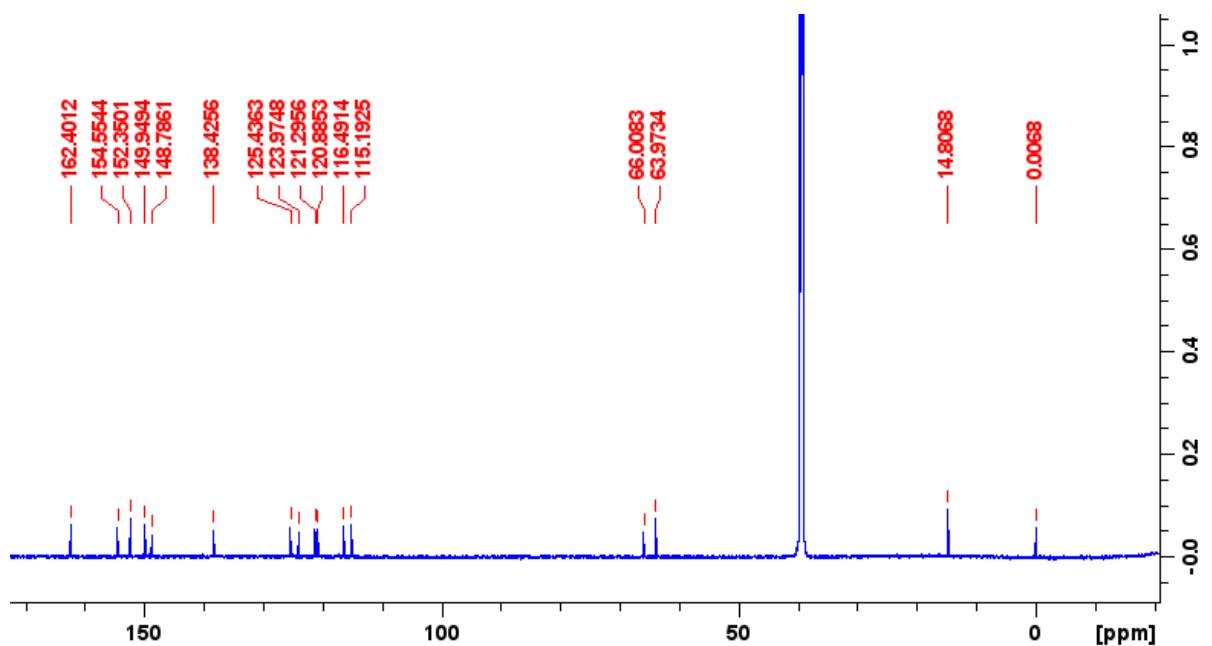


Figure S10. ^{13}C NMR of complex Pt-OEt.

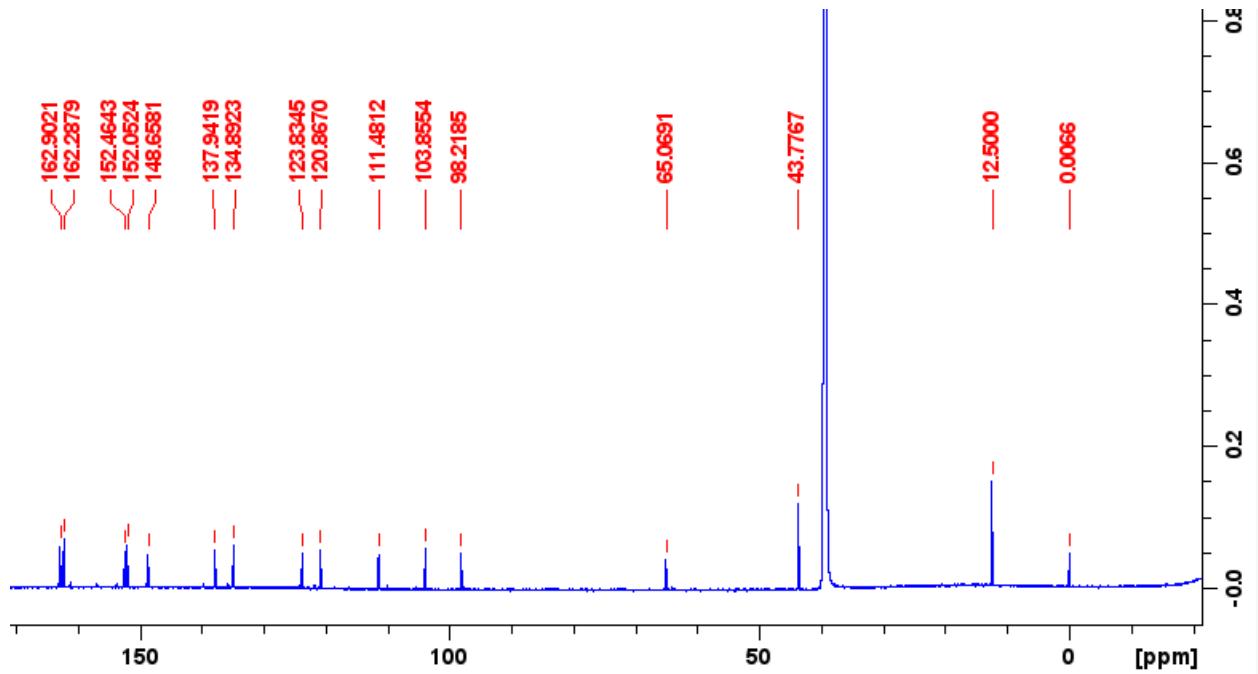


Figure S11. ^{13}C NMR of complex Pt-NEt₂.

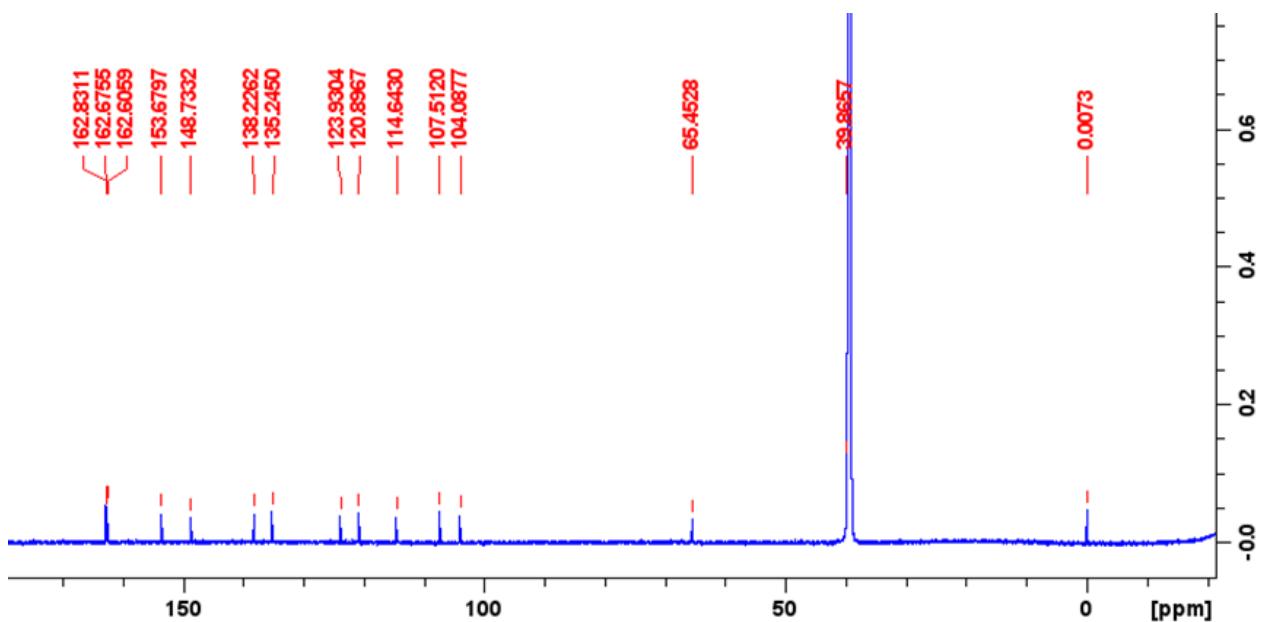


Figure S12. ^{13}C NMR of complex Pt-OH.

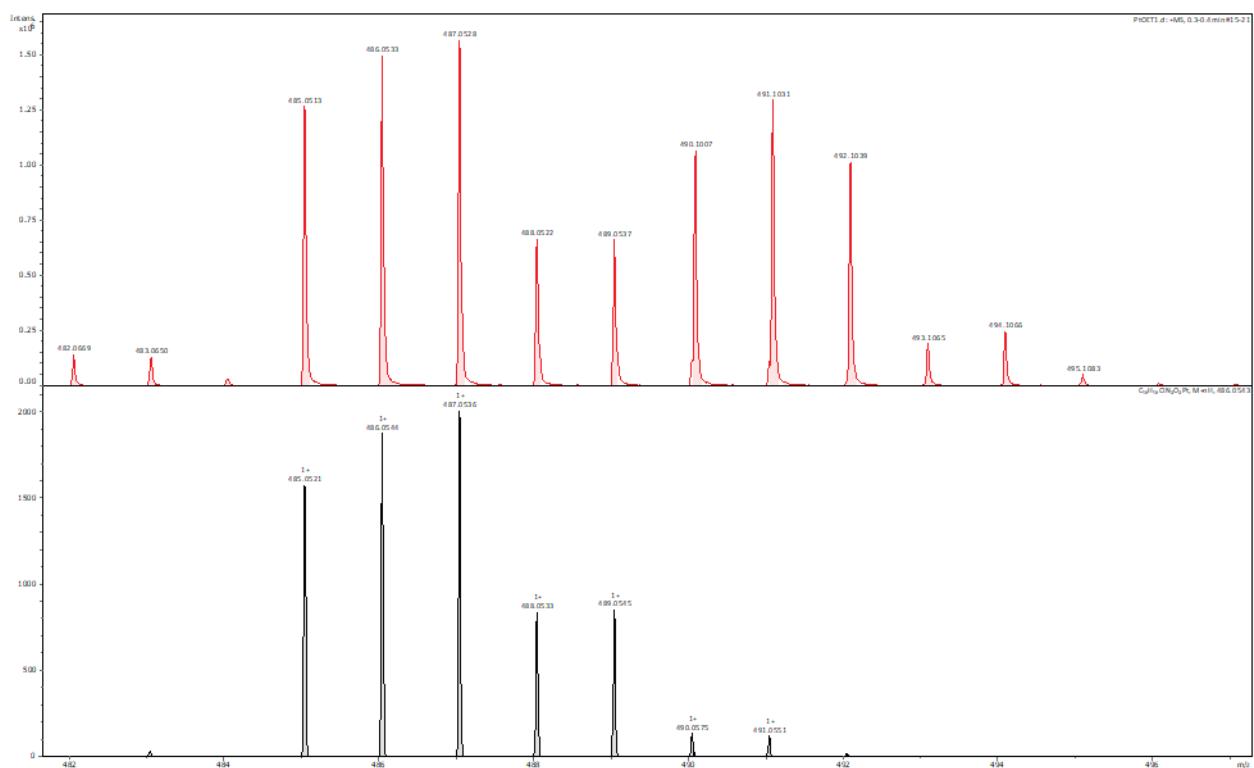


Figure S13. High-resolution mass spectrum of complex Pt-OEt.

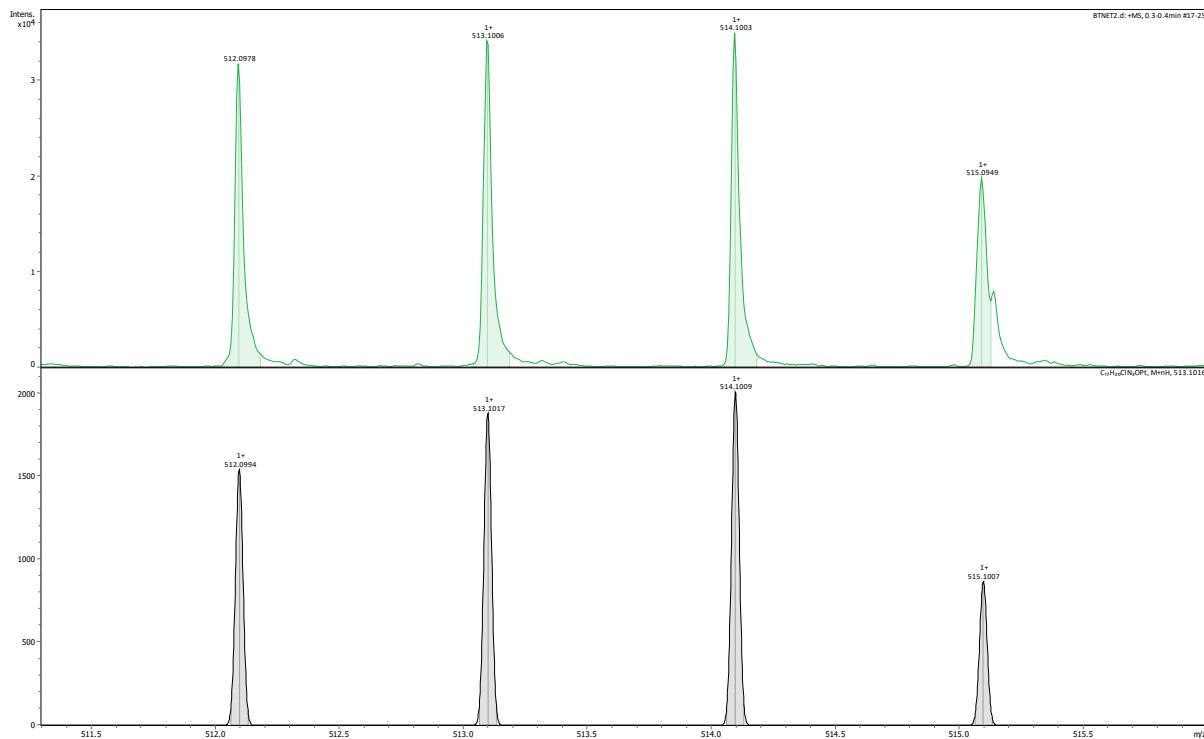


Figure S14. High-resolution mass spectrum of complex Pt-NEt₂.

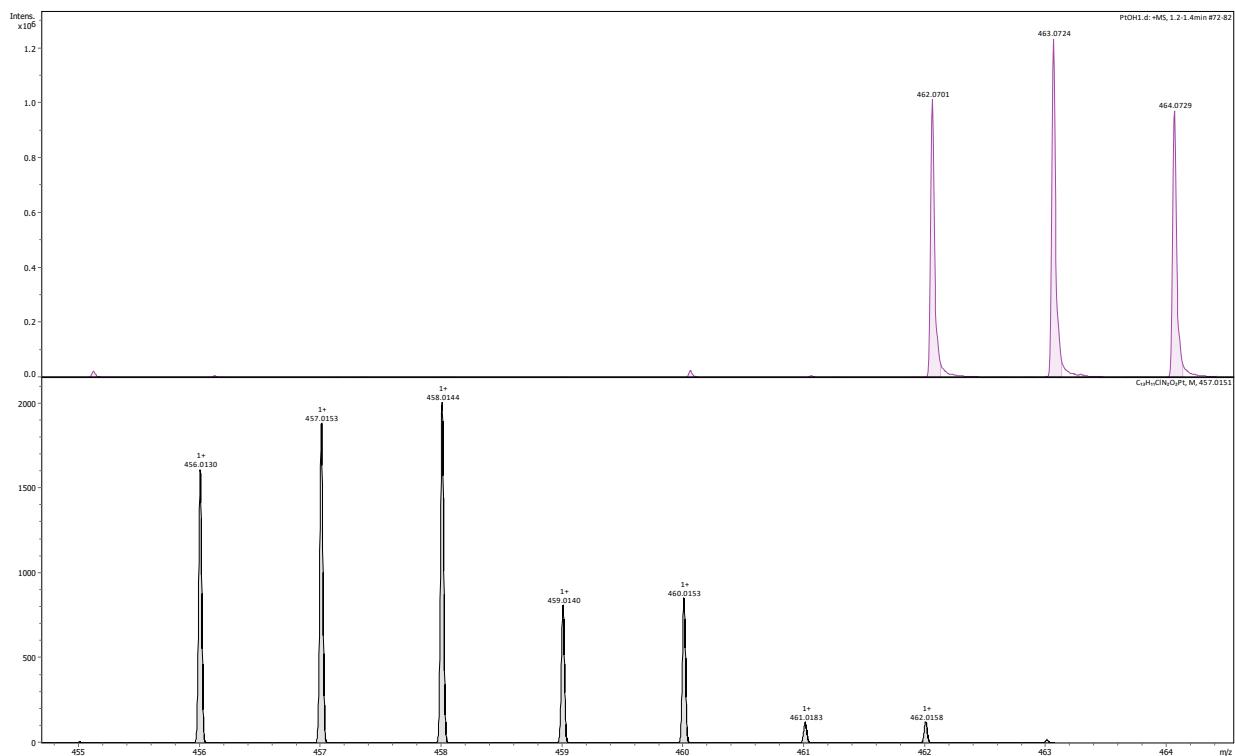


Figure S15. High-resolution mass spectrum of complex [(Pt-OH)-Cl+MeCN].

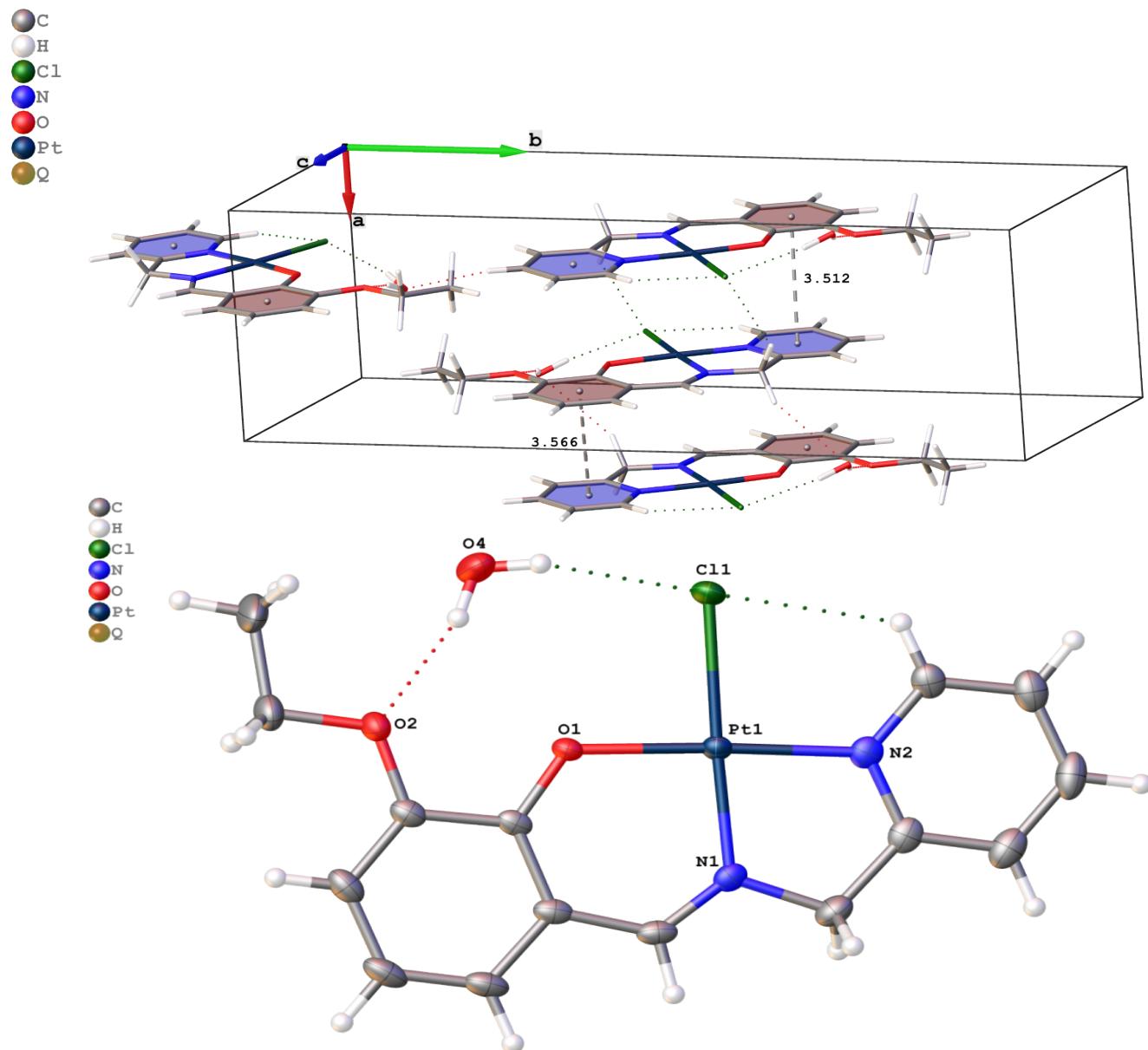


Figure S16. Crystal structure of Pt-OEt.

Table 1 Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Pt-OEt. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
Pt1	7354.8(2)	4780.7(2)	4523.3(2)	15.33(5)
C11	6857.4(10)	4124.8(3)	2811.7(6)	23.26(13)
O4	8442(4)	2928.7(9)	4186(2)	40.8(6)
O2	7668(3)	3039.5(8)	6807.0(17)	22.4(4)
O1	7504(3)	4060.4(8)	5648.4(16)	17.6(3)
N2	7252(3)	5525.8(10)	3465(2)	19.2(4)
C1	7898(4)	5218.9(12)	7095(3)	20.9(5)
C10	7649(4)	5992.7(12)	5531(3)	24.7(6)
C11	7443(4)	6043.3(12)	4128(3)	22.6(5)
C3	7737(3)	4094.6(12)	6888(2)	17.0(5)
C2	7919(4)	4630.5(12)	7621(2)	19.7(5)
C8	7784(5)	2465.5(13)	7433(3)	31.9(7)
C6	8170(4)	4055.3(14)	9571(3)	28.4(6)
C5	8022(4)	3523.9(14)	8868(2)	24.9(6)
C4	7814(4)	3538.3(12)	7563(2)	19.7(5)
C7	8123(4)	4594.9(14)	8960(3)	25.1(6)
C12	7415(4)	6592.4(13)	3519(3)	28.8(6)
C9	7697(7)	1997.2(15)	6409(3)	52.3(10)
C15	7026(4)	5545.1(13)	2183(3)	22.6(5)
C14	6970(4)	6082.1(13)	1542(3)	28.4(6)
C13	7175(4)	6612.9(13)	2216(3)	31.4(7)
N1	7709(3)	5358.1(9)	5914(2)	17.7(4)

Table 2 Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Pt-OEt. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + 2hka^{*}b^{*}U_{12} + \dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Pt1	14.37(6)	17.14(6)	14.96(6)	-1.75(3)	3.77(3)	0.10(3)
C11	32.7(3)	23.0(3)	14.5(3)	-3.1(2)	4.5(2)	2.3(2)
O4	72.8(18)	21.4(11)	29.9(11)	-4.1(9)	13.0(12)	1.7(11)
O2	28.4(10)	20.7(9)	17.9(9)	2.5(7)	1.7(7)	-2.5(7)
O1	20.8(9)	18.7(9)	13.1(8)	-2.2(7)	1.6(7)	-0.2(7)

Table 3 Bond Lengths for Pt-OEt.

Atom	Atom	Length/ \AA	Atom	Atom	Length/ \AA

Table 3 Bond Lengths for Pt-OEt.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Pt1	C11	2.3279(6)	C10	N1	1.471(3)
Pt1	O1	1.9982(17)	C11	C12	1.384(4)
Pt1	N2	2.003(2)	C3	C2	1.424(4)
Pt1	N1	1.954(2)	C3	C4	1.431(4)
O2	C8	1.440(3)	C2	C7	1.419(4)
O2	C4	1.369(3)	C8	C9	1.506(5)
O1	C3	1.312(3)	C6	C5	1.398(4)
N2	C11	1.350(3)	C6	C7	1.366(4)
N2	C15	1.357(3)	C5	C4	1.380(4)
C1	C2	1.425(4)	C12	C13	1.378(5)
C1	N1	1.286(3)	C15	C14	1.376(4)
C10	C11	1.488(4)	C14	C13	1.382(4)

Table 4 Bond Angles for Pt-OEt.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Pt1	C11	87.55(5)	C2	C3	C4	117.1(2)
O1	Pt1	N2	177.35(8)	C3	C2	C1	124.1(2)
N2	Pt1	C11	95.05(7)	C7	C2	C1	116.2(2)
N1	Pt1	C11	177.50(6)	C7	C2	C3	119.7(2)
N1	Pt1	O1	94.69(8)	O2	C8	C9	106.5(2)
N1	Pt1	N2	82.73(9)	C7	C6	C5	119.6(2)
C4	O2	C8	116.9(2)	C4	C5	C6	120.8(3)
C3	O1	Pt1	123.21(16)	O2	C4	C3	114.3(2)
C11	N2	Pt1	114.79(18)	O2	C4	C5	124.4(2)
C11	N2	C15	119.4(2)	C5	C4	C3	121.3(2)
C15	N2	Pt1	125.80(18)	C6	C7	C2	121.5(3)
N1	C1	C2	126.9(2)	C13	C12	C11	119.7(3)
N1	C10	C11	110.3(2)	N2	C15	C14	121.3(3)
N2	C11	C10	116.8(2)	C15	C14	C13	119.5(3)
N2	C11	C12	121.0(3)	C12	C13	C14	119.1(3)
C12	C11	C10	122.2(3)	C1	N1	Pt1	124.78(18)
O1	C3	C2	126.3(2)	C1	N1	C10	119.9(2)
O1	C3	C4	116.6(2)	C10	N1	Pt1	115.23(17)

Table 5 Hydrogen Atom Coordinates ($\text{\AA} \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for Pt-OEt.

Atom	x	y	z	U(eq)
H4A	8078.98	3027.97	4914.11	61
H4B	7965.99	3214.29	3675.92	61
H1	8038.76	5542.94	7678.84	25
H10A	8905.48	6195.53	5905.53	30
H10B	6490.79	6194.11	5851.43	30
H8A	6637.75	2415.26	7930.98	38
H8B	9063.02	2431.06	8012.21	38
H6	8302.79	4041.12	10468.93	34
H5	8066.1	3148.48	9293.46	30
H7	8229.56	4954.44	9443.22	30
H12	7559.9	6953.31	3996.43	35
H9A	6403.46	2027.5	5861.96	78
H9B	7822.37	1597.32	6793.85	78
H9C	8809.45	2062.01	5904.63	78
H15	6904.57	5180.47	1717.52	27
H14	6791.48	6087.85	643.69	34
H13	7151.45	6987.02	1787.39	38

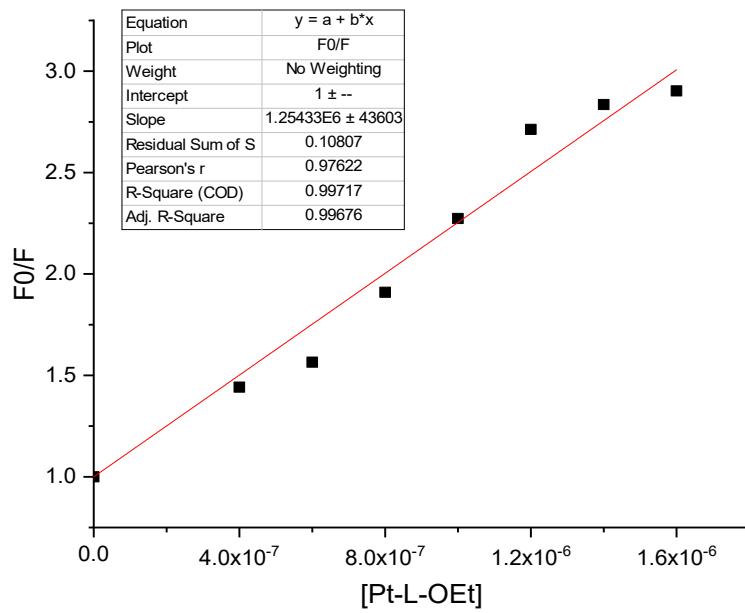
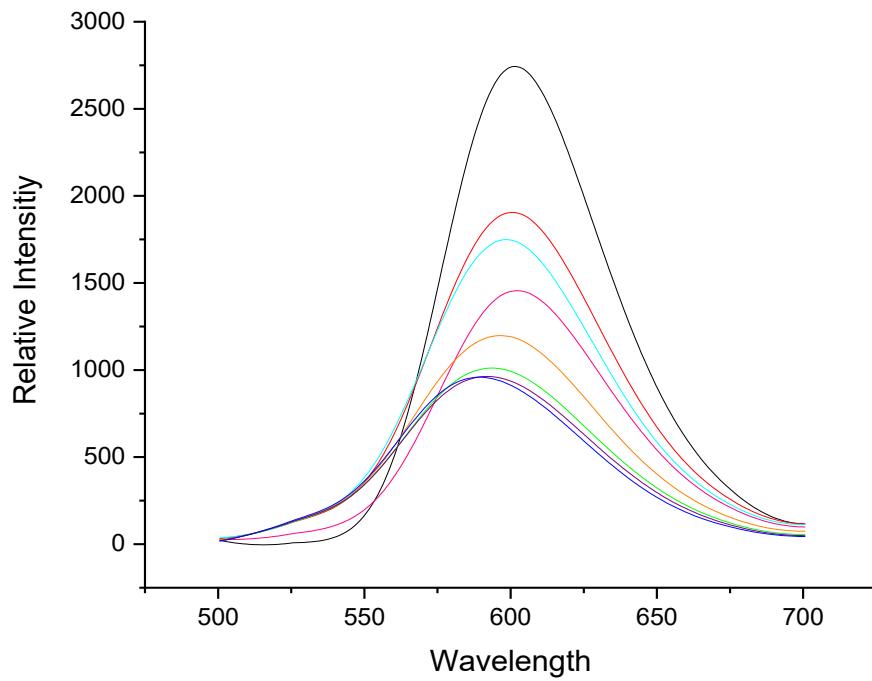


Figure S17. Changes in the emission spectra of EB-DNA adduct upon addition of Pt-OEt.

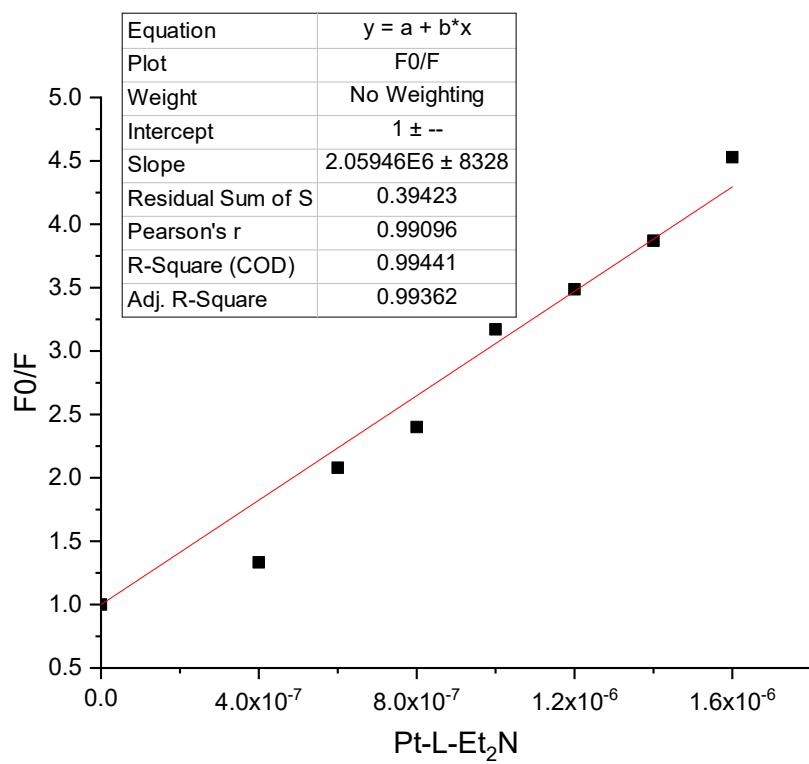
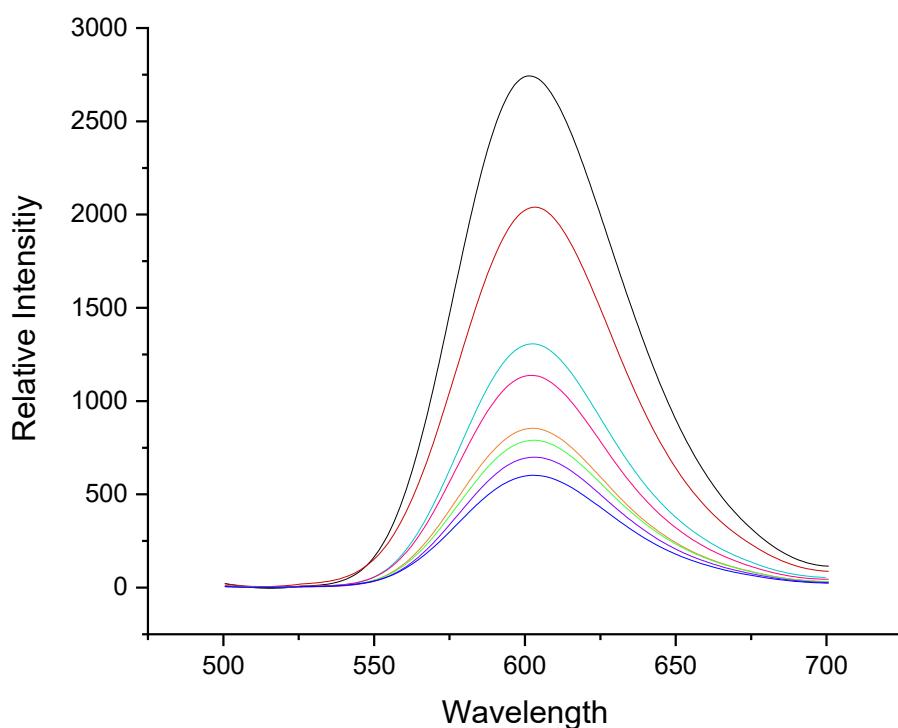


Figure S18. Changes in the emission spectra of EB-DNA adduct upon addition of Pt-NEt₂.

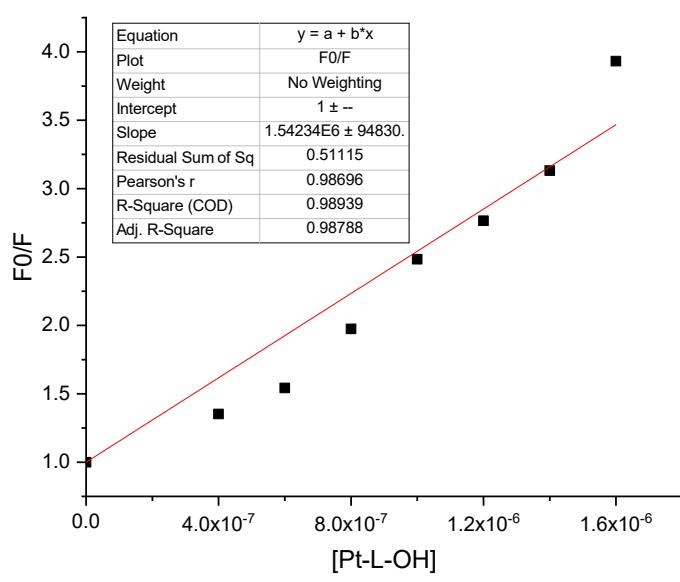
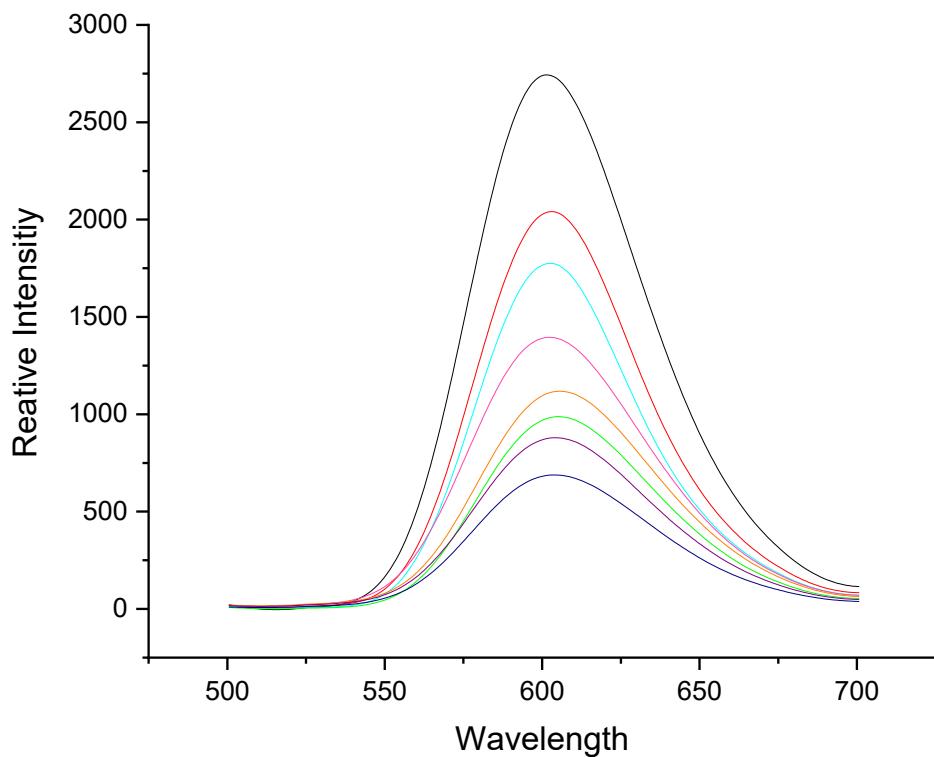


Figure S19. Changes in the emission spectra of EB-DNA adduct upon addition of Pt-OH.

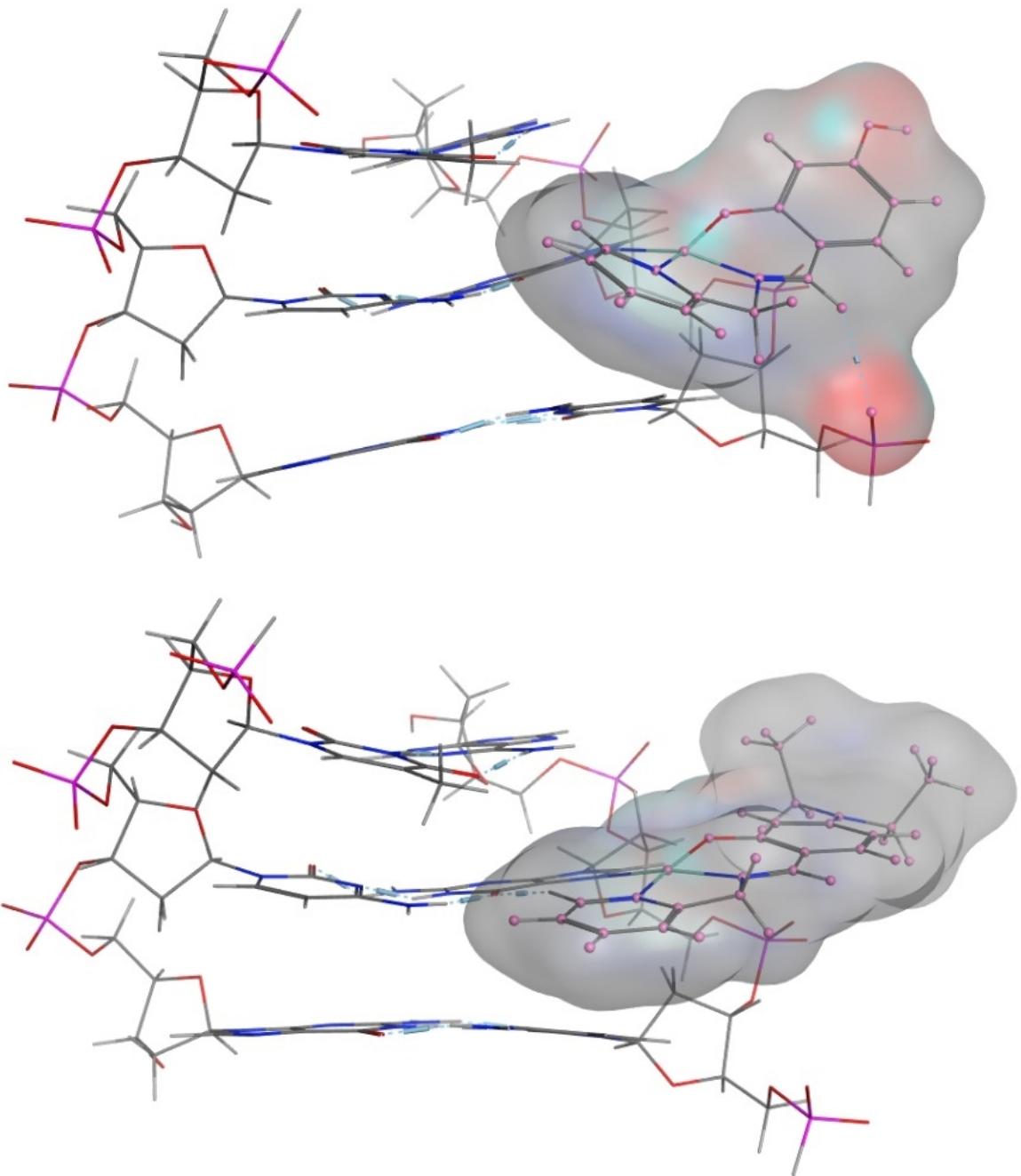


Figure S20. Optimized structures of the DNA trimer adducts with **Pt-NEt₂** (top) and **Pt-OH** (bottom)

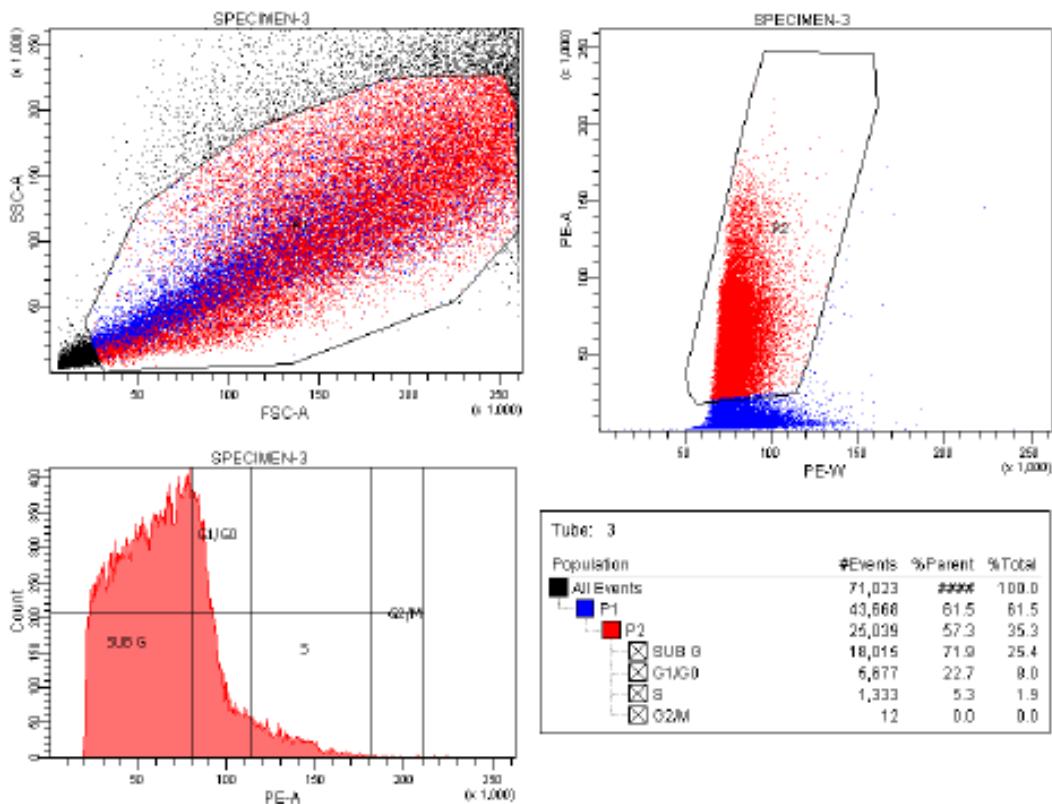


Figure S21. Cell cycle assay of HepG2 upon treatment with Cisplatin.

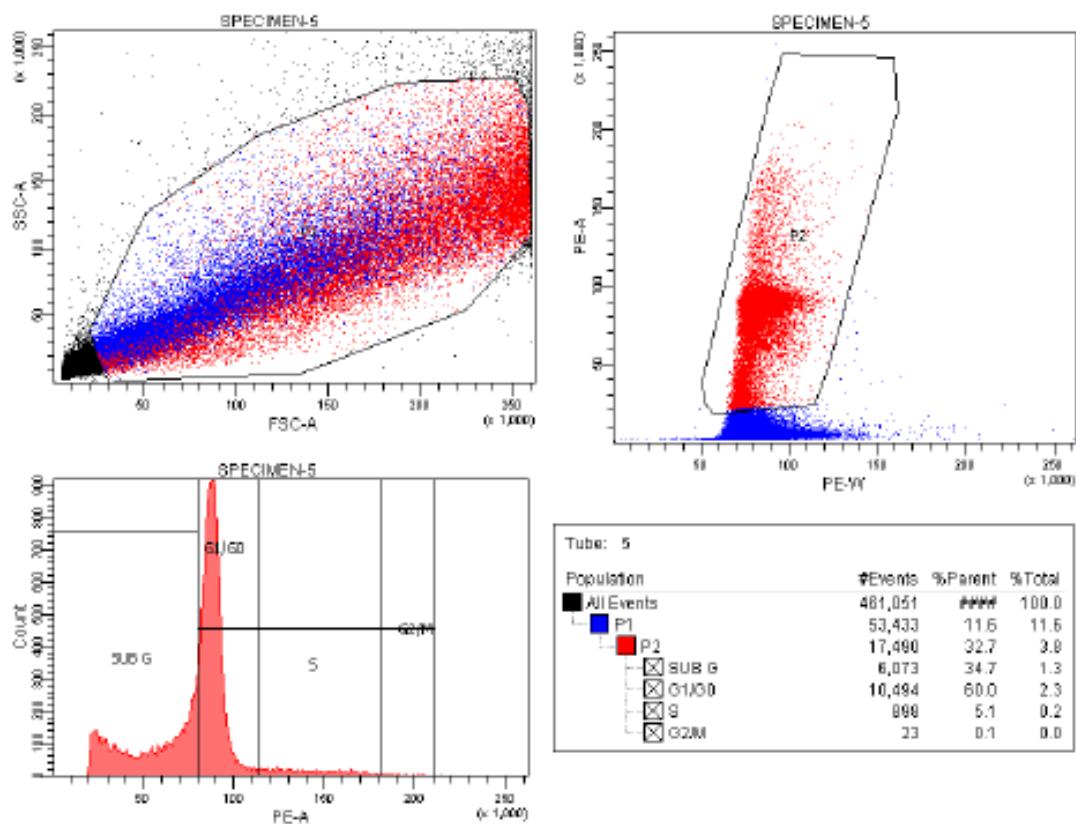


Figure S22. Cell cycle assay of HepG2 upon treatment with Pt-OEt.

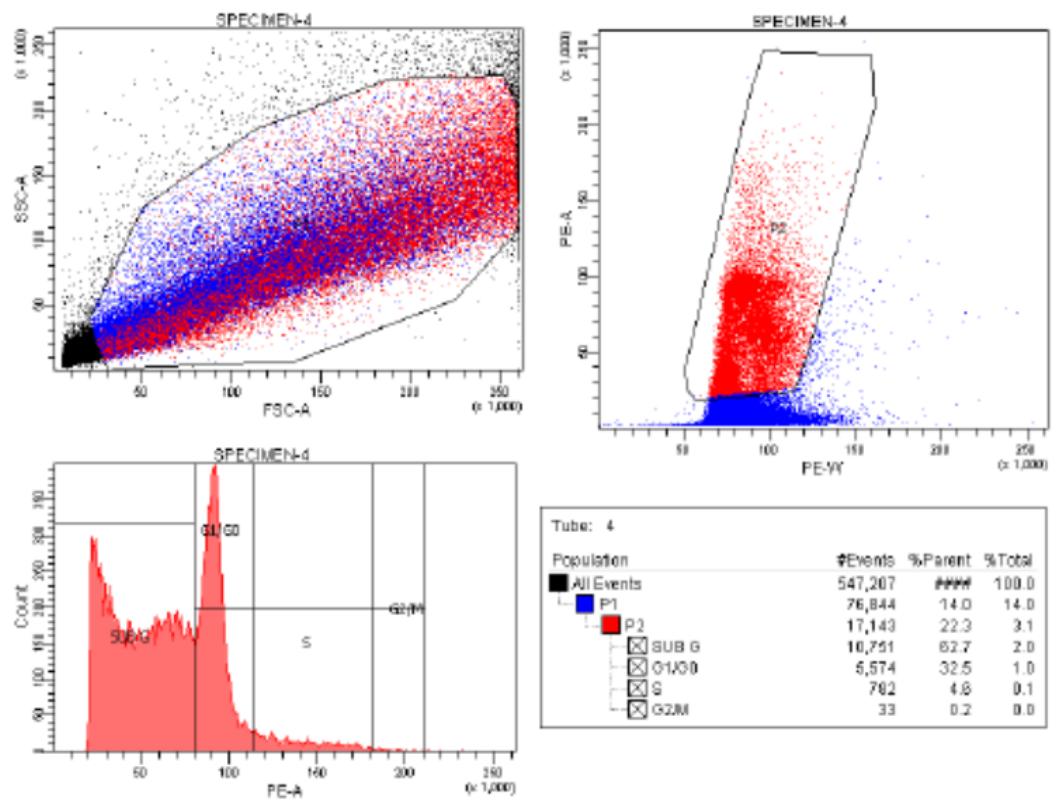


Figure S23. Cell cycle assay of HepG2 upon treatment with Pt-NEt₂.

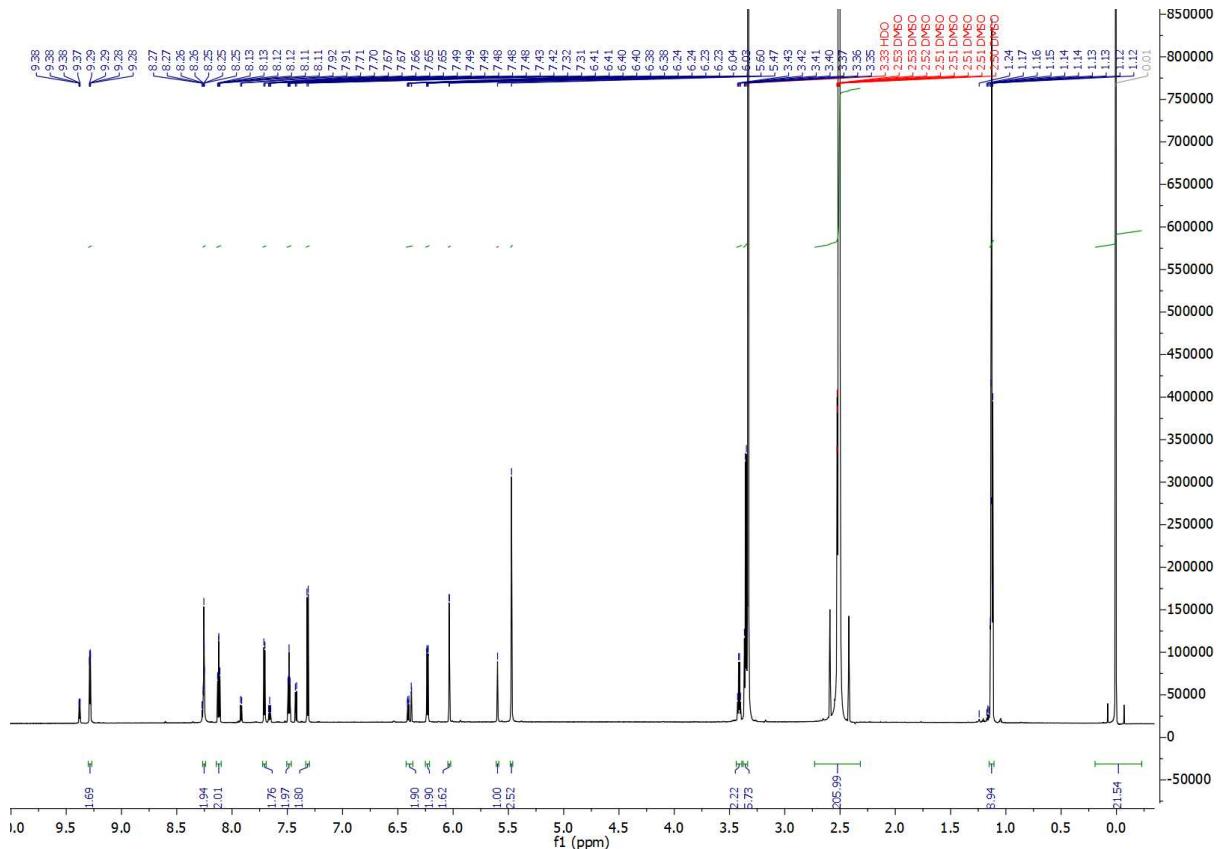


Figure S24. ¹H NMR of Pt-Net₂ in DMSO after 24 h.

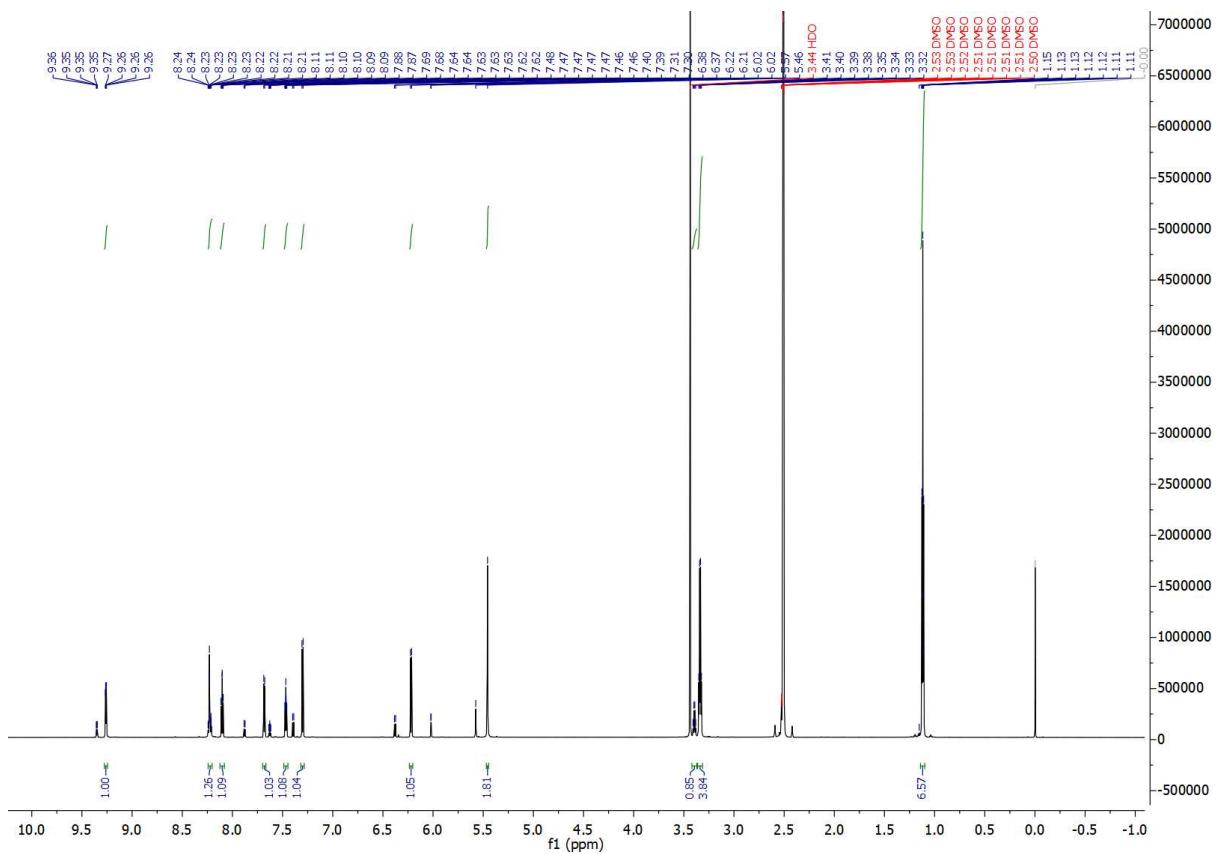


Figure S25. ^1H NMR of Pt- NEt_2 in DMSO/ D_2O after 24 h.

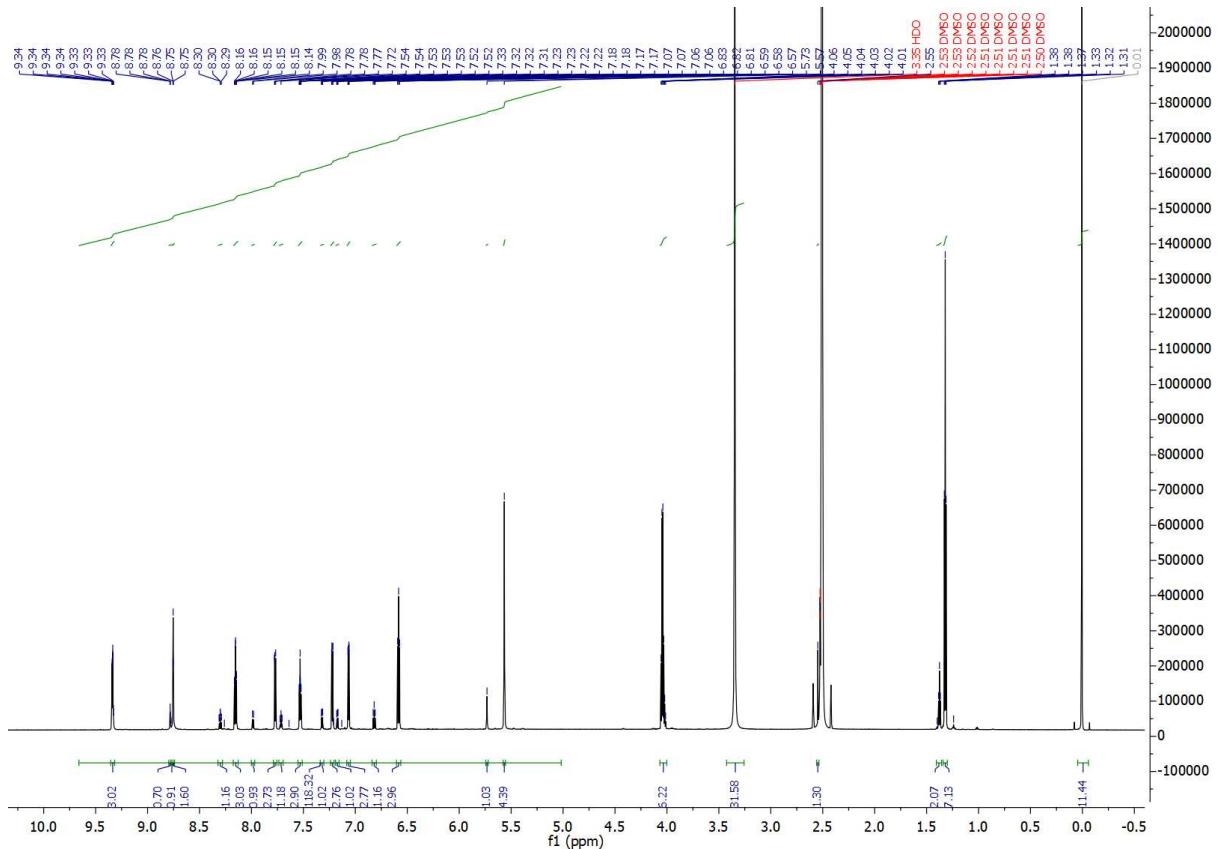


Figure S26. ^1H NMR of Pt-OEt in DMSO after 24 h.

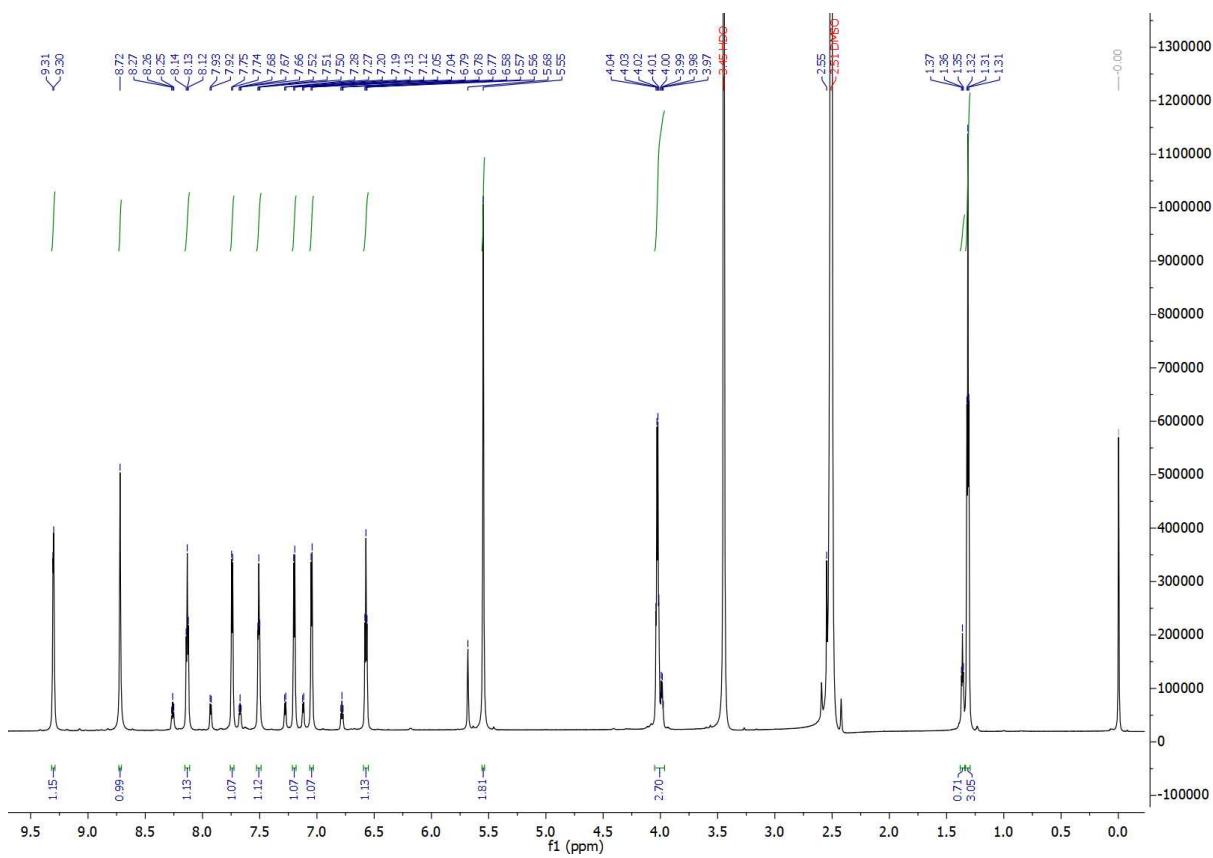


Figure S27. ^1H NMR of Pt-OEt in DMSO/D₂O after 30 min.

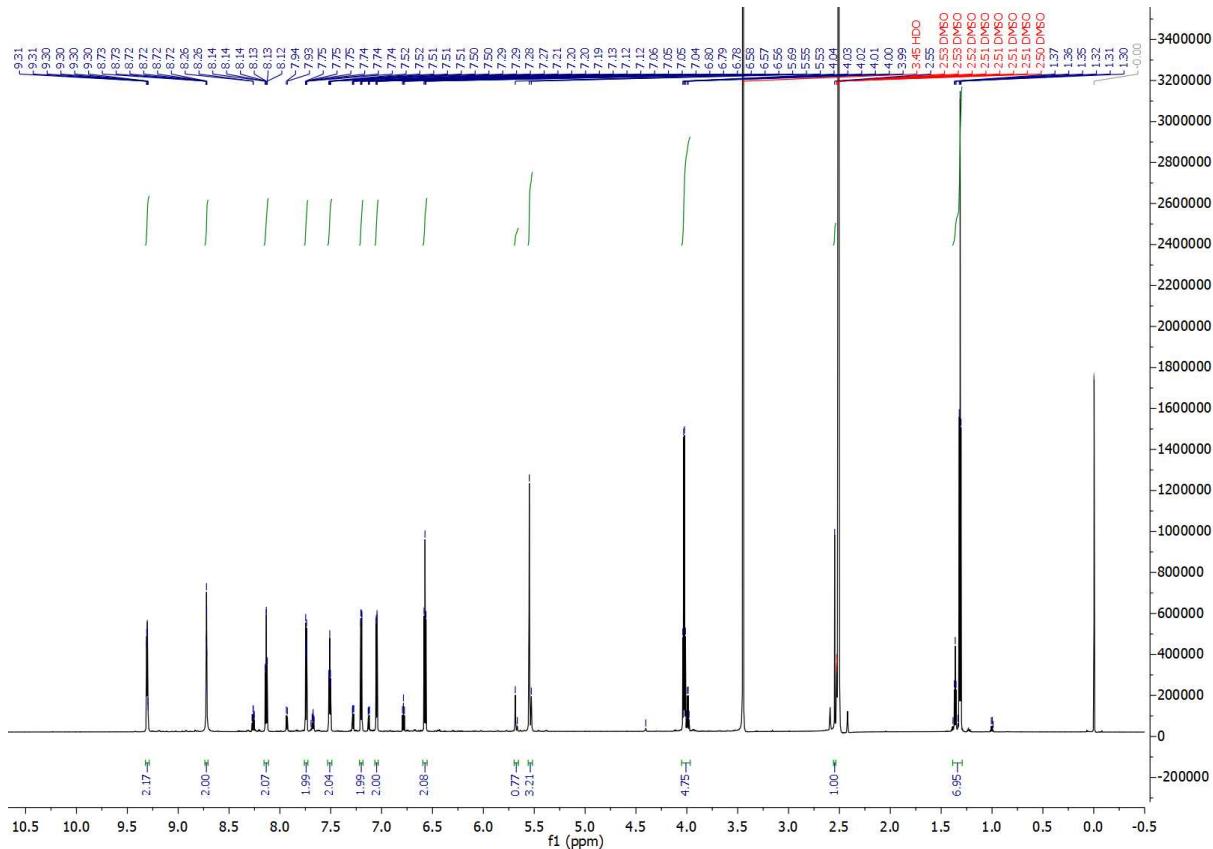


Figure S28. ^1H NMR of Pt-OEt in DMSO/D₂O after 24 h.