

Cytotoxic platinum(II) intercalators that incorporate 1*R*,2*R*- diaminocyclopentane

Supplementary material

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Table S1: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **1**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
C1	2826(3)	6580(20)	9546(3)	20.3(8)
C2	3000(3)	6606(18)	8413(3)	19.9(8)
C3	4108(3)	6575(19)	8097(3)	20.0(8)
C4	5075(3)	6620(20)	8937(3)	17.3(7)
C5	4840(3)	6580(20)	10060(3)	16.1(7)
C6	5768(3)	6605(18)	10950(3)	16.8(7)
C7	6944(3)	6630(20)	10720(3)	18.3(8)
C8	7818(3)	6540(20)	11648(3)	21.9(8)
C9	7485(3)	6630(20)	12703(3)	22.9(9)
C10	6295(3)	6560(30)	12875(3)	20.9(8)
C11	6286(3)	6610(18)	8721(3)	19.5(8)
C12	7173(3)	6581(19)	9570(3)	20.1(7)
C13	2579(4)	6891(18)	14057(3)	28(2)
C14	1779(4)	5674(9)	13235(4)	24.1(11)
C15	610(4)	5832(9)	13713(4)	29.7(14)
C16	987(5)	5681(14)	14977(5)	63(3)
C17	2283(4)	6220(20)	15197(4)	40(3)
Cl1	5852.1(9)	6745(5)	5768.6(8)	29.5(4)
N1	3720(2)	6581(19)	10362(2)	15.9(6)
N2	5457(2)	6623(19)	12007(2)	16.3(7)
N3	3773(3)	6620(20)	13754(2)	28.6(9)
N4	1915(2)	6540(20)	12110(2)	22.4(7)
Cl2	9798.8(11)	5511(2)	8054.8(11)	31.6(3)
Pt1	3704.58(10)	6619.1(4)	12050.04(10)	15.88(5)
O1W	10177(3)	4518(6)	10601(3)	31.8(9)
O2W	1587(7)	1210(30)	14572(7)	52(4)
C1	2826(3)	6580(20)	9546(3)	20.3(8)
C2	3000(3)	6606(18)	8413(3)	19.9(8)
C3	4108(3)	6575(19)	8097(3)	20.0(8)
C4	5075(3)	6620(20)	8937(3)	17.3(7)
C5	4840(3)	6580(20)	10060(3)	16.1(7)
C6	5768(3)	6605(18)	10950(3)	16.8(7)
C7	6944(3)	6630(20)	10720(3)	18.3(8)
C8	7818(3)	6540(20)	11648(3)	21.9(8)
C9	7485(3)	6630(20)	12703(3)	22.9(9)
C10	6295(3)	6560(30)	12875(3)	20.9(8)
C11	6286(3)	6610(18)	8721(3)	19.5(8)
C12	7173(3)	6581(19)	9570(3)	20.1(7)
C13	2579(4)	6891(18)	14057(3)	28(2)
C14	1779(4)	5674(9)	13235(4)	24.1(11)
C15	610(4)	5832(9)	13713(4)	29.7(14)
C16	987(5)	5681(14)	14977(5)	63(3)
C17	2283(4)	6220(20)	15197(4)	40(3)
Cl1	5852.1(9)	6745(5)	5768.6(8)	29.5(4)
N1	3720(2)	6581(19)	10362(2)	15.9(6)
N2	5457(2)	6623(19)	12007(2)	16.3(7)
N3	3773(3)	6620(20)	13754(2)	28.6(9)

Table S1: Continued

Atom	x	y	z	U(eq)
N4	1915(2)	6540(20)	12110(2)	22.4(7)
C13	2579(4)	6891(18)	14057(3)	28(2)
C14	1779(4)	5674(9)	13235(4)	24.1(11)
C15	610(4)	5832(9)	13713(4)	29.7(14)
C16	987(5)	5681(14)	14977(5)	63(3)
C17	2283(4)	6220(20)	15197(4)	40(3)
C11	5852.1(9)	6745(5)	5768.6(8)	29.5(4)
N1	3720(2)	6581(19)	10362(2)	15.9(6)
N2	5457(2)	6623(19)	12007(2)	16.3(7)
N3	3773(3)	6620(20)	13754(2)	28.6(9)
N4	1915(2)	6540(20)	12110(2)	22.4(7)
C13	2579(4)	6891(18)	14057(3)	28(2)
C14	1779(4)	5674(9)	13235(4)	24.1(11)

Table S2: Bond Lengths for **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.398(5)	C10	N2	1.336(4)
C1	N1	1.335(4)	C11	C12	1.356(5)
C2	C3	1.369(5)	C13	C14	1.507(9)
C3	C4	1.413(5)	C13	C17	1.517(8)
C4	C5	1.405(4)	C13	N3	1.470(6)
C4	C11	1.443(5)	C14	C15	1.522(6)
C5	C6	1.420(5)	C14	N4	1.495(7)
C5	N1	1.376(4)	C15	C16	1.534(7)
C6	C7	1.409(5)	C16	C17	1.524(8)
C6	N2	1.357(4)	N1	Pt1	2.029(3)
C7	C8	1.413(5)	N2	Pt1	2.018(3)
C7	C12	1.435(5)	N3	Pt1	2.039(3)
C8	C9	1.365(5)	N4	Pt1	2.064(3)

Table S3: Bond Angles of **1**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	C1	C2	122.1(3)	N3	C13	C17	119.8(6)
C3	C2	C1	120.6(3)	C13	C14	C15	102.3(4)
C2	C3	C4	118.9(3)	N4	C14	C13	105.3(6)
C3	C4	C11	124.5(3)	N4	C14	C15	120.1(4)
C5	C4	C3	117.6(3)	C14	C15	C16	102.0(4)
C5	C4	C11	117.9(3)	C17	C16	C15	108.4(4)
C4	C5	C6	120.8(3)	C13	C17	C16	103.2(4)
N1	C5	C4	122.8(3)	C1	N1	C5	118.0(3)
N1	C5	C6	116.4(3)	C1	N1	Pt1	129.7(2)
C7	C6	C5	120.4(3)	C5	N1	Pt1	112.2(2)
N2	C6	C5	116.7(3)	C6	N2	Pt1	113.1(2)
N2	C6	C7	122.9(3)	C10	N2	C6	119.1(3)
C6	C7	C8	117.0(3)	C10	N2	Pt1	127.7(2)
C6	C7	C12	118.2(3)	C13	N3	Pt1	108.5(3)
C8	C7	C12	124.5(3)	C14	N4	Pt1	104.4(3)
C9	C8	C7	118.8(3)	N1	Pt1	N3	177.2(2)
C8	C9	C10	121.0(3)	N1	Pt1	N4	98.99(11)
N2	C10	C9	120.7(3)	N2	Pt1	N1	81.52(11)
C12	C11	C4	121.4(3)	N2	Pt1	N3	95.80(11)
C11	C12	C7	121.2(3)	N2	Pt1	N4	178.5(6)
C14	C13	C17	104.4(7)	N3	Pt1	N4	83.68(12)
N3	C13	C14	106.6(6)				

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z

#2 -x,1/2+y,-z

Table S4: Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **1**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + \dots + 2hka \times b \times U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	20.0(16)	20(2)	21.0(17)	12(5)	1.6(14)	3(5)
C2	24.9(17)	15(2)	17.7(16)	-8(5)	-4.4(14)	2(5)
C3	29.0(19)	17(2)	14.4(15)	2(5)	2.5(14)	10(5)
C4	25.0(17)	10(2)	17.0(15)	-4(5)	4.4(13)	-3(5)
C5	20.5(16)	10.7(18)	16.6(15)	4(5)	0.5(13)	5(5)
C6	18.3(16)	14.3(19)	17.7(15)	-1(5)	1.5(13)	-3(5)
C7	21.8(16)	12(2)	21.6(16)	-2(5)	2.6(14)	3(5)
C8	19.0(16)	18(2)	27.9(18)	-4(6)	0.7(14)	-1(5)
C9	20.0(17)	27(2)	19.7(16)	2(5)	-6.1(14)	-3(5)
C10	22.8(17)	21(2)	18.2(16)	1(5)	-0.9(14)	-4(4)
C11	27.7(18)	14(2)	17.0(15)	4(5)	5.1(14)	5(5)
C12	20.5(16)	17(2)	23.9(17)	6(5)	7.1(14)	-1(5)
C13	25(2)	40(8)	18.1(18)	0(3)	2.5(16)	0(3)
C14	21(2)	34(3)	17(2)	7(2)	1.7(18)	-2(2)
C15	19(2)	45(4)	26(2)	9(2)	5.1(19)	2(2)
C16	29(3)	131(9)	30(3)	23(4)	9(2)	4(3)
C17	33(2)	67(10)	19(2)	5(3)	1.8(18)	6(3)
Cl1	30.6(5)	39.3(11)	17.3(4)	1.7(9)	-3.2(4)	-4.2(10)
N1	19.0(13)	13.4(16)	15.4(13)	7(4)	1.5(11)	1(5)
N2	14.1(13)	17.3(19)	16.8(13)	-6(4)	-1.7(11)	-1(4)
N3	18.5(15)	51(3)	15.6(14)	-6(5)	-0.4(12)	-8(5)
N4	18.3(14)	34(2)	15.0(14)	5(5)	0.9(11)	4(5)
Cl2	32.6(6)	30.9(8)	31.9(6)	-2.5(6)	7.0(5)	-3.7(6)
Pt1	15.21(7)	19.68(9)	12.47(7)	0.44(18)	0.36(5)	-0.69(18)
O1W	31.7(19)	29(2)	34.0(19)	-1.4(17)	-1.6(16)	0.0(17)
O2W	49(4)	53(13)	54(4)	0(5)	8(4)	4(5)

Table S5: Hydrogen Atom Coordinates ($\text{\AA}^2 \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **1**.

Atom	x	y	z	U(eq)
H1	2064	6554	9738	24
H2	2356	6646	7868	24
H3	4222	6528	7343	24
H8	8605	6427	11543	26
H9	8054	6734	13317	27
H10	6090	6478	13600	25
H11	6462	6625	7984	23
H12	7944	6526	9404	24
H13	2366	8305	13959	33
H14	2040	4278	13260	29
H15A	89	4746	13451	36
H15B	228	7098	13518	36
H16A	527	6594	15378	75
H16B	859	4333	15236	75
H17A	2412	7282	15745	48
H17B	2748	5063	15462	48
H3A	4070	5449	14032	34
H3B	4240	7613	14045	34
H4A	1607	7779	12043	27
H4B	1562	5766	11558	27

Table S6: Torsion Angles for **1**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C1	C2	C3	C4	-3.2(19)	C8	C9	C10	N2	-7(2)
C1	N1	Pt1	N2	-179.4(13)	C9	C10	N2	C6	5(2)
C1	N1	Pt1	N3	164(13)	C9	C10	N2	Pt1	-178.3(12)
C1	N1	Pt1	N4	2.0(13)	C10	N2	Pt1	N1	-177.0(15)
C2	C1	N1	C5	-1.0(19)	C10	N2	Pt1	N3	2.2(15)
C2	C1	N1	Pt1	178.1(10)	C10	N2	Pt1	N4	-67(11)
C2	C3	C4	C5	3(2)	C11	C4	C5	C6	2(2)
C2	C3	C4	C11	-179.4(13)	C11	C4	C5	N1	-179.8(12)
C3	C4	C5	C6	179.5(13)	C12	C7	C8	C9	179.3(12)
C3	C4	C5	N1	-2(2)	C13	C14	C15	C16	-39.4(7)
C3	C4	C11	C12	-177.7(13)	C13	C14	N4	Pt1	50.8(7)
C4	C5	C6	C7	-0.8(19)	C13	N3	Pt1	N1	-171(13)
C4	C5	C6	N2	178.3(13)	C13	N3	Pt1	N2	172.3(10)
C4	C5	N1	C1	1(2)	C13	N3	Pt1	N4	-9.1(9)
C4	C5	N1	Pt1	-178.2(11)	C14	C13	C17	C16	-31.3(9)
C4	C11	C12	C7	-2.4(19)	C14	C13	N3	Pt1	39.8(10)
C5	C4	C11	C12	0(2)	C14	C15	C16	C17	20.5(8)
C5	C6	C7	C8	-176.6(12)	C14	N4	Pt1	N1	155.9(7)
C5	C6	C7	C12	-1.8(18)	C14	N4	Pt1	N2	46(11)
C5	C6	N2	C10	177.4(14)	C14	N4	Pt1	N3	-23.3(7)
C5	C6	N2	Pt1	-0.1(14)	C15	C14	N4	Pt1	165.3(5)
C5	N1	Pt1	N2	-0.2(10)	C15	C16	C17	C13	6.3(10)
C5	N1	Pt1	N3	-16(14)	C17	C13	C14	C15	44.9(7)
C5	N1	Pt1	N4	-178.8(10)	C17	C13	C14	N4	171.2(7)
C6	C5	N1	C1	179.5(12)	C17	C13	N3	Pt1	157.8(9)
C6	C5	N1	Pt1	0.2(15)	N1	C1	C2	C3	2.1(19)
C6	C7	C8	C9	-6.3(18)	N1	C5	C6	C7	-179.2(12)
C6	C7	C12	C11	3.5(18)	N1	C5	C6	N2	-0.1(18)
C6	N2	Pt1	N1	0.2(9)	N2	C6	C7	C8	4.3(19)
C6	N2	Pt1	N3	179.4(10)	N2	C6	C7	C12	179.1(12)
C6	N2	Pt1	N4	110(10)	N3	C13	C14	C15	172.7(7)
C7	C6	N2	C10	-4(2)	N3	C13	C14	N4	-61.1(9)
C7	C6	N2	Pt1	179.0(10)	N3	C13	C17	C16	-150.4(10)
C7	C8	C9	C10	8(2)	N4	C14	C15	C16	-155.4(7)
C8	C7	C12	C11	177.8(13)					

Table S7: Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for [PHENSS]Cl₂. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor.

Atom	x	y	z	U(eq)
Pt	8748(1)	6866(1)	2240(1)	14(1)
N(1)	10450(2)	6902(13)	1946(2)	19(1)
N(2)	8597(2)	6865(13)	622(2)	18(1)
C(1)	7633(3)	6885(14)	-16(2)	22(1)
C(2)	7675(3)	6871(13)	-1133(2)	27(1)
C(3)	8707(3)	6936(14)	-1601(2)	26(1)
C(4)	9747(3)	6936(15)	-948(2)	22(1)
C(12)	9638(2)	6936(11)	160(2)	17(1)
C(11)	10641(2)	6861(13)	875(2)	19(1)
C(5)	10882(3)	6974(11)	-1348(3)	25(1)
C(6)	11845(3)	6920(18)	-661(3)	30(1)
C(7)	11748(3)	6930(15)	477(3)	24(1)
C(8)	12697(3)	6870(14)	1226(3)	30(1)
C(9)	12501(3)	6849(13)	2293(3)	31(1)
C(10)	11372(2)	6870(20)	2643(2)	26(1)
N(3)	7034(2)	6765(13)	2511(2)	18(1)
N(4)	8913(2)	6895(14)	3861(2)	22(1)
C(13)	7815(3)	6219(6)	4306(3)	22(1)
C(14)	7748(3)	6533(13)	5506(3)	30(2)
C(15)	6554(4)	5881(8)	5826(3)	40(1)
C(16)	5602(3)	6980(20)	5204(3)	38(1)
C(17)	5671(3)	6685(17)	3999(3)	28(1)
C(18)	6853(3)	7241(6)	3656(3)	21(1)
Cl(1)	11076(1)	6393(2)	5571(1)	37(1)
Cl(2)	5250(1)	9901(2)	1445(1)	29(1)
W(1)	5330(3)	4492(6)	1045(3)	43(1)

Table S8: Bonds Lengths of [PHENSS]Cl₂.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
PT	N1	2.0239(1)	C10	H10	0.9300(1)
PT	N2	2.0227(1)	N3	H3A	0.9
PT	N3	2.0330(1)	N3	H3B	0.9
PT	N4	2.0259(1)	N3	C18	1.4963(1)
N1	C11	1.3695(1)	N4	H4A	0.9
N1	C10	1.3411(1)	N4	H4B	0.9
N2	C1	1.3350(1)	N4	C13	1.4925(1)
N2	C12	1.3659(1)	C13	H13	0.9800(1)
C1	H1	0.93	C13	C14	1.5234(1)
C1	C2	1.4017(1)	C13	C18	1.5216(1)
C2	H2	0.93	C14	H14A	0.9700(1)
C2	C3	1.3587(1)	C14	H14B	0.97
C3	H3	0.9300(1)	C14	C15	1.5296(1)
C3	C4	1.4176(1)	C15	H15A	0.9700(1)
C4	C12	1.3984(1)	C15	H15B	0.9700(1)
C4	C5	1.4321(1)	C15	C16	1.5213(1)
C12	C11	1.4274(1)	C16	H16A	0.9700(1)
C11	C7	1.4007(1)	C16	H16B	0.97
C5	H5	0.9300(1)	C16	C17	1.5272(1)
C5	C6	1.3711(1)	C17	H17A	0.9700(1)
C6	H6	0.93	C17	H17B	0.97
C6	C7	1.4338(1)	C17	C18	1.5068(1)
C7	C8	1.4049(1)	C18	H18	0.9800(1)
C8	H8	0.93	W1	HW1A	0.8981(1)
C8	C9	1.3665(1)	W1	HW1B	0.759
C9	H9	0.93	W2	HW2A	0.8994
C9	C10	1.4009(1)	W2	HW2B	0.77

Table S9: Bond Angles of [PHENSS]Cl₂.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N1	Pt	N2	81.38	Pt	N3	H3B	109.68
N1	Pt	N3	178.43	Pt	N3	C18	109.91
N1	Pt	N4	98.19	H3A	N3	H3B	108.18
N2	Pt	N3	97.71	H3A	N3	C18	109.68
N2	Pt	N4	179.3	H3B	N3	C18	109.68
N3	Pt	N4	82.73	Pt	N4	H4A	109.77
Pt	N1	C11	112.87	Pt	N4	H4B	109.77
Pt	N1	C10	129.04	Pt	N4	C13	109.52
C11	N1	C10	118	H4A	N4	H4B	108.23
Pt	N2	C1	128.45	H4A	N4	C13	109.77
Pt	N2	C12	113.1	H4B	N4	C13	109.77
C1	N2	C12	118.38	N4	C13	H13	108.11
N2	C1	H1	119.25	N4	C13	C14	114.32
N2	C1	C2	121.5	N4	C13	C18	105.4
H1	C1	C2	119.25	H13	C13	C14	108.11
C1	C2	H2	119.74	H13	C13	C18	108.11
C1	C2	C3	120.51	C14	C13	C18	112.55
H2	C2	C3	119.74	C13	C14	H14A	110.09
C2	C3	H3	120.3	C13	C14	H14B	110.08
C2	C3	C4	119.41	C13	C14	C15	108.08
H3	C3	C4	120.3	H14A	C14	H14B	108.42
C3	C4	C12	116.86	H14A	C14	C15	110.08
C3	C4	C5	124.41	H14B	C14	C15	110.08
C12	C4	C5	118.71	C14	C15	H15A	109.48
N2	C12	C4	123.2	C14	C15	H15B	109.48
N2	C12	C11	116.16	C14	C15	C16	110.82
C4	C12	C11	120.47	H15A	C15	H15B	108.06
N1	C11	C12	116.26	H15A	C15	C16	109.48
N1	C11	C7	123.16	H15B	C15	C16	109.48
C12	C11	C7	120.3	C15	C16	H16A	109.37
C4	C5	H5	119.65	C15	C16	H16B	109.37
C4	C5	C6	120.71	C15	C16	C17	111.28
H5	C5	C6	119.65	H16A	C16	H16B	108
C5	C6	H6	119.43	H16A	C16	C17	109.37
C5	C6	C7	121.15	H16B	C16	C17	109.37
H6	C6	C7	119.43	C16	C17	H17A	109.64
C11	C7	C6	118.41	C16	C17	H17B	109.64
C11	C7	C8	117.34	C16	C17	C18	110.1
C6	C7	C8	124.1	H17A	C17	H17B	108.15
C7	C8	H8	120.45	H17A	C17	C18	109.64
C7	C8	C9	119.09	H17B	C17	C18	109.64
H8	C8	C9	120.45	N3	C18	C13	105.68
C8	C9	H9	119.6	N3	C18	C17	113.07
C8	C9	C10	120.8	N3	C18	H18	108.61
H9	C9	C10	119.6	C13	C18	C17	112.11
N1	C10	C9	121.39	C13	C18	H18	108.61
N1	C10	H10	119.31	C17	C18	H18	108.61
C9	C10	H10	119.31	HW1A	W1	HW1B	108.79
PT	N3	H3A	109.68	HW2A	W2	HW2B	108.34

Symmetry transformations used to generate equivalent atoms:

#1 x,y,z, #2 -x,1/2+y,-z

Table S10: Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for [PHENSS]Cl₂. The Anisotropic displacement factor exponent takes the form: -
 $2\pi^2[h^2a^*2U_{11}+\dots+2hka \times b \times U_{12}]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
Pt	12(1)	18(1)	13(1)	-1(1)	0(1)	1(1)
N(1)	15(1)	20(2)	22(1)	-4(3)	0(1)	-3(3)
N(2)	19(1)	18(2)	16(1)	3(3)	2(1)	-3(3)
C(1)	20(1)	26(2)	21(1)	1(4)	-1(1)	-1(3)
C(2)	30(2)	31(2)	21(1)	-1(4)	-6(1)	-9(4)
C(3)	41(2)	22(2)	15(1)	-1(3)	2(1)	-6(3)
C(4)	31(2)	14(3)	22(2)	-1(3)	7(1)	-1(3)
C(12)	20(1)	11(2)	20(1)	-3(3)	4(1)	1(2)
C(11)	17(1)	16(2)	23(1)	-4(3)	4(1)	0(3)
C(5)	36(2)	15(2)	25(2)	-1(3)	14(1)	-2(3)
C(6)	30(2)	25(3)	36(2)	-1(4)	18(1)	-2(4)
C(7)	22(1)	16(2)	36(2)	-6(3)	8(1)	-2(3)
C(8)	14(1)	27(2)	50(2)	-8(4)	6(1)	2(4)
C(9)	18(1)	30(2)	44(2)	-7(4)	-5(1)	0(4)
C(10)	19(1)	33(2)	24(2)	-10(4)	-3(1)	1(4)
N(3)	16(1)	23(2)	16(1)	2(3)	0(1)	0(3)
N(4)	21(1)	31(2)	15(1)	-7(3)	-1(1)	4(3)
C(13)	22(2)	24(2)	19(2)	2(1)	1(1)	2(1)
C(14)	35(2)	40(6)	15(2)	-3(2)	3(1)	-1(2)
C(15)	41(3)	62(4)	19(2)	4(2)	11(2)	-5(2)
C(16)	32(2)	52(4)	30(2)	0(4)	14(1)	2(4)
C(17)	20(1)	37(3)	26(2)	1(3)	7(1)	-2(3)
C(18)	24(2)	25(4)	14(2)	-1(2)	3(1)	3(2)
Cl(1)	38(1)	29(1)	40(1)	8(1)	-21(1)	-7(1)
Cl(2)	24(1)	24(1)	39(1)	0(1)	-9(1)	0(1)
W(1)	52(2)	33(2)	41(2)	6(2)	-3(2)	-2(2)

Table S11: Hydrogen Atom Coordinates ($\text{\AA}^2 \times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for [PHENSS]Cl₂.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	U(eq)
H(1)	6919	6909	289	34
H(2)	6991	6816	-1559	41
H(3)	8730	6980	-2342	39
H(5)	10966	7037	-2083	38
H(6)	12574	6877	-937	45
H(8)	13448	6846	998	45
H(9)	13125	6822	2794	46
H(10)	11260	6855	3373	38
H(3A)	6647	7604	2080	27
H(3B)	6757	5589	2360	27
H(4A)	9501	6130	4088	34
H(4B)	9073	8088	4093	34
H(13)	7742	4846	4165	33
H(14A)	7860	7874	5677	45
H(14B)	8347	5803	5894	45
H(15A)	6465	4525	5686	60
H(15B)	6488	6088	6587	60
H(16A)	5672	8326	5369	56
H(16B)	4854	6544	5422	56
H(17A)	5521	5357	3820	41

Table S12: Torsion Angles for [PHENSS]Cl₂.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
N2	PT	N1	C11	-1.48	C11	C7	C8	C9	-3.32
N2	PT	N1	C10	-177.96	C6	C7	C8	H8	1.23
N3	PT	N1	C11	53.08	C6	C7	C8	C9	-178.77
N3	PT	N1	C10	-123.4	C7	C8	C9	H9	-179.39
N4	PT	N1	C11	179.08	C7	C8	C9	C10	0.61
N4	PT	N1	C10	2.6	H8	C8	C9	H9	0.61
N1	PT	N2	C1	-178.5	H8	C8	C9	C10	-179.39
N1	PT	N2	C12	-1.56	C8	C9	C10	N1	0.14
N3	PT	N2	C1	2.79	C8	C9	C10	H10	-179.86
N3	PT	N2	C12	179.73	H9	C9	C10	N1	-179.86
N4	PT	N2	C1	-125.98	H9	C9	C10	H10	0.14
N4	PT	N2	C12	50.96	PT	N3	C18	C13	-41.31
N1	PT	N3	H3A	-99.56	PT	N3	C18	C17	-164.3
N1	PT	N3	H3B	19.11	PT	N3	C18	H18	75.07
N1	PT	N3	C18	139.77	H3A	N3	C18	C13	-161.97
N2	PT	N3	H3A	-45.19	H3A	N3	C18	C17	75.04
N2	PT	N3	H3B	73.48	H3A	N3	C18	H18	-45.59
N2	PT	N3	C18	-165.85	H3B	N3	C18	C13	79.36
N4	PT	N3	H3A	134.26	H3B	N3	C18	C17	-43.63
N4	PT	N3	H3B	-107.07	H3B	N3	C18	H18	-164.26
N4	PT	N3	C18	13.6	PT	N4	C13	H13	70.65
N1	PT	N4	H4A	-40.33	PT	N4	C13	C14	-168.9
N1	PT	N4	H4B	78.51	PT	N4	C13	C18	-44.78
N1	PT	N4	C13	-160.91	H4A	N4	C13	H13	-49.93
N2	PT	N4	H4A	-92.77	H4A	N4	C13	C14	70.52
N2	PT	N4	H4B	26.07	H4A	N4	C13	C18	-165.36
N2	PT	N4	C13	146.65	H4B	N4	C13	H13	-168.77
N3	PT	N4	H4A	138.39	H4B	N4	C13	C14	-48.32
N3	PT	N4	H4B	-102.77	H4B	N4	C13	C18	75.8
N3	PT	N4	C13	17.81	N4	C13	C14	H14A	56.44
PT	N1	C11	C12	4.23	N4	C13	C14	H14B	-63.03
PT	N1	C11	C7	178.14	N4	C13	C14	C15	176.7
C10	N1	C11	C12	-178.86	H13	C13	C14	H14A	176.88
C10	N1	C11	C7	-4.95	H13	C13	C14	H14B	57.42
PT	N1	C10	C9	178.27	H13	C13	C14	C15	-62.85
PT	N1	C10	H10	-1.73	C18	C13	C14	H14A	-63.77
C11	N1	C10	C9	1.94	C18	C13	C14	H14B	176.76
C11	N1	C10	H10	-178.07	C18	C13	C14	C15	56.49
PT	N2	C1	H1	0.35	N4	C13	C18	N3	55.58
PT	N2	C1	C2	-179.65	N4	C13	C18	C17	179.17
C12	N2	C1	H1	-176.46	N4	C13	C18	H18	-60.8
C12	N2	C1	C2	3.54	H13	C13	C18	N3	-59.85
PT	N2	C12	C4	179.53	H13	C13	C18	C17	63.74
PT	N2	C12	C11	4.3	H13	C13	C18	H18	-176.23
C1	N2	C12	C4	-3.19	C14	C13	C18	N3	-179.19
C1	N2	C12	C11	-178.42	C14	C13	C18	C17	-55.6
N2	C1	C2	H2	176.58	C14	C13	C18	H18	64.43
N2	C1	C2	C3	-3.42	C13	C14	C15	H15A	62.61
H1	C1	C2	H2	-3.42	C13	C14	C15	H15B	-179.1

Table S12: Torsion Angles for [PHENSS]Cl₂ continued.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
H1	C1	C2	C3	176.58	C13	C14	C15	C16	-58.24
C1	C2	C3	H3	-177.31	H14A	C14	C15	H15A	-177.12
C1	C2	C3	C4	2.69	H14A	C14	C15	H15B	-58.83
H2	C2	C3	H3	2.69	H14A	C14	C15	C16	62.03
H2	C2	C3	C4	-177.31	H14B	C14	C15	H15A	-57.65
C2	C3	C4	C12	-2.22	H14B	C14	C15	H15B	60.63
C2	C3	C4	C5	179.11	H14B	C14	C15	C16	-178.51
H3	C3	C4	C12	177.78	C14	C15	C16	H16A	-61.63
H3	C3	C4	C5	-0.89	C14	C15	C16	H16B	-179.72
C3	C4	C12	N2	2.51	C14	C15	C16	C17	59.32
C3	C4	C12	C11	177.55	H15A	C15	C16	H16A	177.51
C5	C4	C12	N2	-178.74	H15A	C15	C16	H16B	59.42
C5	C4	C12	C11	-3.71	H15A	C15	C16	C17	-61.53
C3	C4	C5	H5	1.74	H15B	C15	C16	H16A	59.22
C3	C4	C5	C6	-178.26	H15B	C15	C16	H16B	-58.87
C12	C4	C5	H5	-176.91	H15B	C15	C16	C17	-179.82
C12	C4	C5	C6	3.09	C15	C16	C17	H17A	64.97
N2	C12	C11	N1	-5.75	C15	C16	C17	H17B	-176.43
N2	C12	C11	C7	-179.85	C15	C16	C17	C18	-55.73
C4	C12	C11	N1	178.88	H16A	C16	C17	H17A	-174.07
C4	C12	C11	C7	4.78	H16A	C16	C17	H17B	-55.48
N1	C11	C7	C6	-178.63	H16A	C16	C17	C18	65.22
N1	C11	C7	C8	5.65	H16B	C16	C17	H17A	-55.98
C12	C11	C7	C6	-4.96	H16B	C16	C17	H17B	62.61
C12	C11	C7	C8	179.32	H16B	C16	C17	C18	-176.69
C4	C5	C6	H6	176.55	C16	C17	C18	N3	172.8
C4	C5	C6	C7	-3.45	C16	C17	C18	C13	53.45
H5	C5	C6	H6	-3.45	C16	C17	C18	H18	-66.57
H5	C5	C6	C7	176.55	H17A	C17	C18	N3	52.1
C5	C6	C7	C11	4.38	H17A	C17	C18	C13	-67.25
C5	C6	C7	C8	179.78	H17A	C17	C18	H18	172.73
H6	C6	C7	C11	-175.62	H17B	C17	C18	N3	-66.5
H6	C6	C7	C8	-0.22	H17B	C17	C18	C13	174.16
C11	C7	C8	H8	176.68	H17B	C17	C18	H18	54.13

General assignment of ancillary ligand in metallointercalators of the type $[\text{Pt}(\text{I}_L)(\text{DACP})]^{2+}$

The unambiguous assignment of all the proton resonances in the ^1H NMR of these metallointercalators can be difficult. Such difficulty arises from the spatial arrangement of the geminal protons being either in axial or equatorial positions (Fig. S1). A DEPT experiment was used to determine the primary ($-\text{CH}$) and secondary carbon ($-\text{CH}_2$) atoms (Fig. S2) of the RRDACP in $[\text{Pt}(\text{RRDACP})\text{Cl}_2]$. The two resonances were observed at 23 ppm which were assigned as $-\text{CH}_2$ of C3 and C5 as they were out of phase with the resonance at 67 ppm which was assigned $-\text{CH}$ (Table 13 and Fig. S2). Also of note for the DEPT spectra of RRDACP was that the signal at 26 ppm indicative of the C4. A small peak at 69 ppm and the small shoulder visible on the side of the two resonances at 23 ppm are attributed to uncoordinated RRDACP or exchange of the Cl ligand with the $\text{DMSO}-d_6$ solvent. C4 being further from the coordination appears to be coincident with the C4 of the coordinated RRDACP.

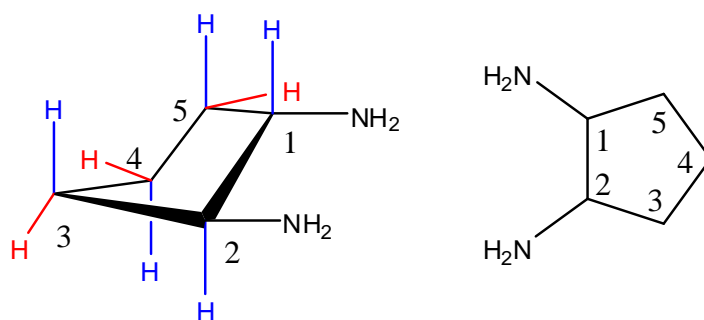


Fig. S1: The chemical structure and numbering system of DACP (right) showing half chair conformation and labelling of the proton resonances. Axial hydrogens are represented in blue and equatorial hydrogens are represented in red.

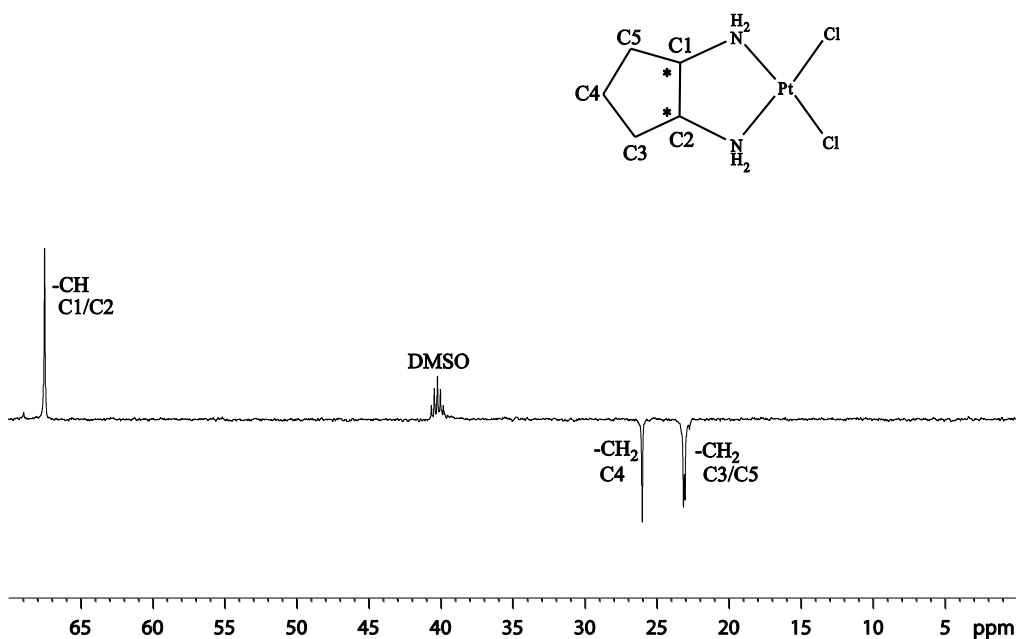


Fig. S2: The DEPT spectra and the chemical structure of $[\text{Pt}(\text{RRDACP})\text{Cl}_2]$ with carbon resonances labelled and the $-\text{CH}$ and $-\text{CH}_2$ resonances labelled.

Table S13: The summary of ^1H NMR data of complexes of the type $[\text{Pt}(\text{A}_L)\text{Cl}_2]$ showing chemical shift (ppm), multiplicity (s, d, dd, t, m and bs), integration and coupling constants (Hz) between the five complexes synthesised.

Resonance	$[\text{Pt}(\text{en})\text{Cl}_2]^{\#}$	$[\text{Pt}(\text{SSDACH})\text{Cl}_2]^{\#}$	$[\text{Pt}(\text{SSDACP})\text{Cl}_2]$	$[\text{Pt}(\text{RRDACP})\text{Cl}_2]$
$-\text{NH}_2$	6.4 (bs, 2H)	5.6 (bs, 2H)	5.2 (bs, 2H)	5.2 (bs, 2H)
$-\text{NH}_2$	6.1 (bs, 2H)	5.0 (bs, 2H)	5.0 (bs, 2H)	5.1 (bs, 2H)
H1'/H2'	2.61 (s, 4H)	2.2 (t, 2H, $J = 7.6$ Hz)	3.1 (bs, 2H)	3.0 (bs, 2H)
H3'/H6'	-	1.9 (d, 1H, $J = 12.1$ Hz)	-	-
H4'/H5'	-	1.5 (d, 1H, $J = 8.5$ Hz)	-	-
H3'/H6'	-	1.3 (d, 1H, $J = 8.9$ Hz)	-	-
H4'/H5'	-	1.0 (t, 1H, $J = 9.9$ Hz)	-	-
H4'/H4'	-	-	2.1 (m, 2H)	2.1 (m, 2H)
H3'/H5'	-	-	1.6 (m, 2H)	1.5 (m, 2H)
H3'/H5'	-	-	1.4 (m, 2H)	1.4 (m, 2H)
^{195}Pt	-3309	-3282	-3065	-3069

$\#$ included for comparison

Once the $-\text{CH}$ resonance was identified, it was then used in conjunction with the results of a ^1H - ^{13}C HMQC experiment to assign the proton label H1'/H2' to a resonance (Fig. S2). From this it was seen that the resonance that corresponded to the proton of the $-\text{CH}$ was the resonance that was the furthest downfield at 3.0 ppm. This is likely due to its

close proximity to the amine groups, causing them to be deshielded and hence producing a downfield shift.

A COSY experiment was used to assign the proton resonances (Fig. S3) of [Pt(RRDACP)Cl₂] complex. The resonance at 3.03 ppm corresponds to the –CH resonance in the DEPT spectra and as such was assigned to represent the proton H1'/H2' of the RRDACP ancillary ligand. The resonance H1'/H2' shares a cross-peak with the resonances at 1.5 and 1.4 ppm. The two resonances being associated with two different protons can also be seen in the HMQC spectra. In this case the two different carbon resonances at 23 ppm correlated to the resonance at 1.5 and 1.4 ppm. The resonance at 1.5 ppm was assigned to the proton H3'/H5' and the resonance at 1.4 ppm assigned as H3'/H5'. Both H3'/H5' and H3'/H5' share a cross-peak with the resonance at 2.1 ppm and as such it was assigned as H4'.

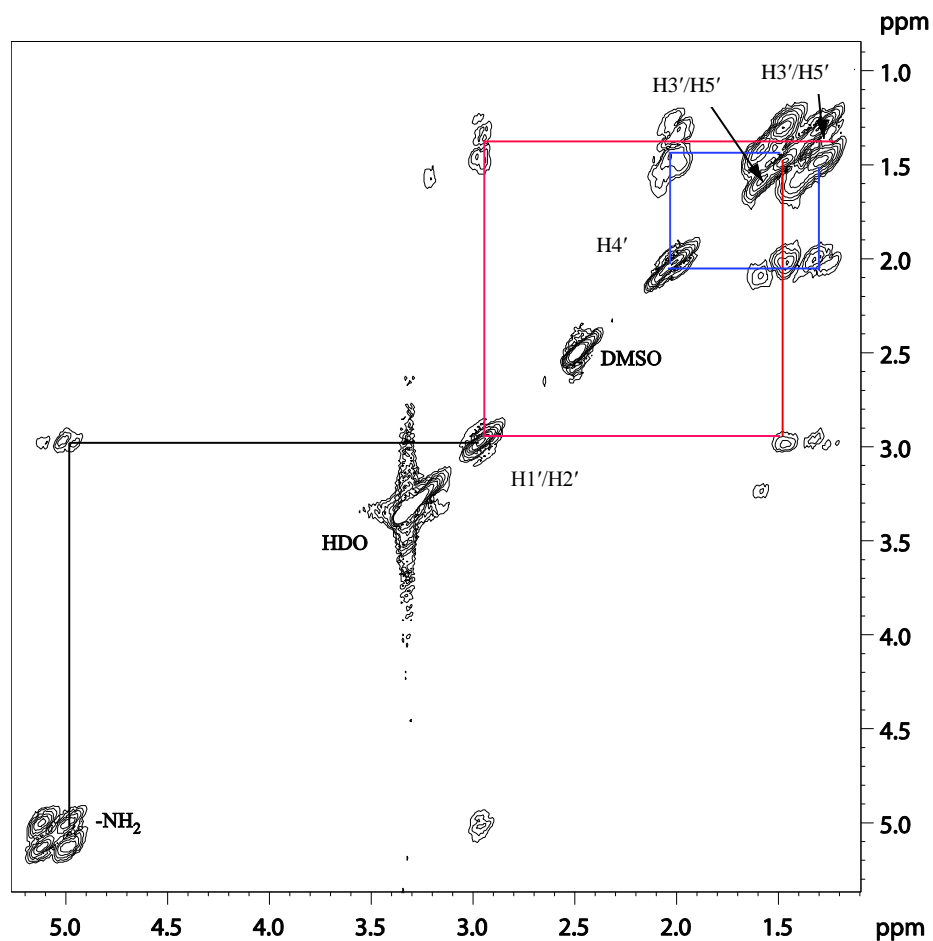


Fig. S3: An expansion of the 2D COSY spectrum of [Pt(RRDACP)Cl₂] obtained at 35 °C in DMSO-*d*₆ and referenced to the residual solvent peak showing the labelling of cross-peak correlation between resonances.

The ¹H NMR spectrum of [Pt(RRDACP)Cl₂] was assigned according to the proton labelling system as shown in Fig. S4. The spectrum was initially recorded in DMSO-*d*₆ to observe the amine resonance. A drop of D₂O was added, causing the amine resonances to disappear due to exchange of the protons (not shown). The broad resonance at 5.1 ppm was assigned to represent the amines of the [Pt(RRDACP)Cl₂]. The protons H1' and H2' were observed at 3.0 ppm, which had shifted upfield when compared to the uncoordinated ancillary ligand as a result of the coordination of the adjacent amines. The proton H4' was observed at 2.1 ppm. The protons H3'/H5' were observed at 1.5 ppm and 1.4 ppm. The amine resonances shared a cross-peak with the resonance at 3.0 ppm and were hence assigned to represent the protons H1'/H2'. Cross-peak correlation was

observed from the resonance assigned H1'/H2' with resonances at 1.5 and 1.4 ppm of the H3'/H5' protons. The H3'/H5' protons both shared cross-peaks with the resonance at 2.1 ppm and was therefore assigned to represent the proton H4'.

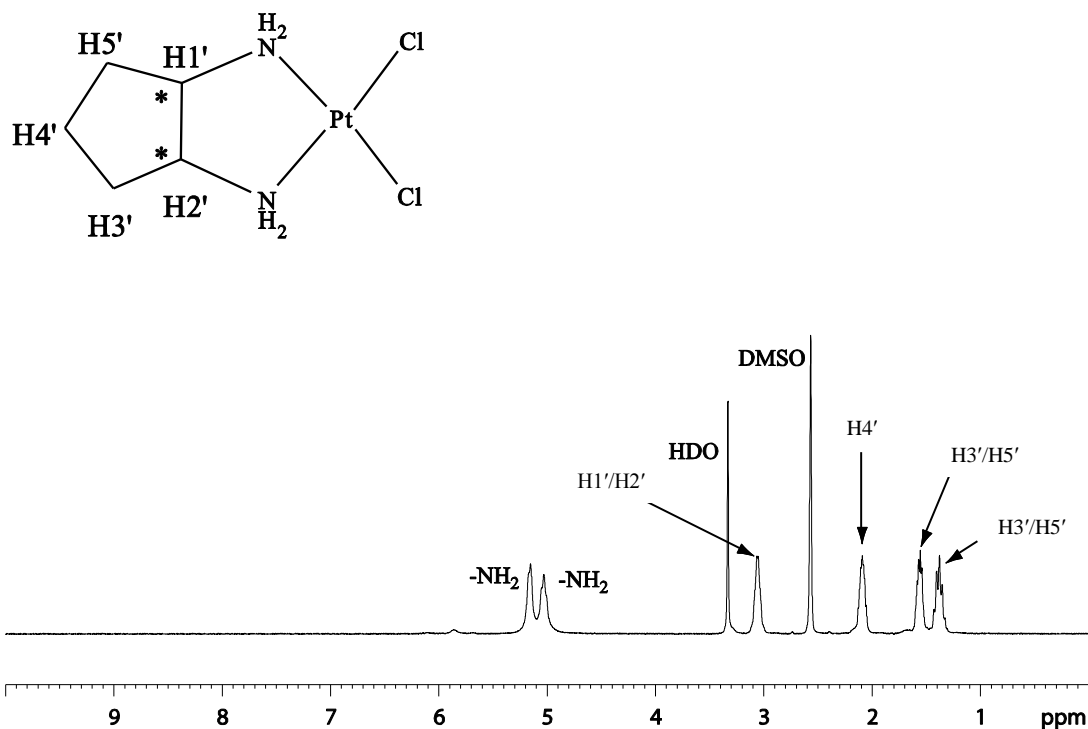


Fig. S4: The chemical structure and ¹H NMR spectrum of [Pt(RRDACP)Cl₂] obtained at 35 °C in DMSO-*d*₆ showing the proton labelling system and assignment of proton resonances.

The ^{195}Pt NMR spectrum of the complex $[\text{Pt}(\text{RRDACP})\text{Cl}_2]$ (Fig. S5) shows one broad resonance at -3065 ppm indicating the presence of only one platinum species. The platinum resonance was in accordance with the expected shift of a nuclei coordinated to both chloride and amine ligands. When compared to the starting material which has a chemical shift of -1650 ppm a good indication is provided that the coordination sphere has changed. This process was used to assign both enantiomers of the DACP ligand coordinated to the platinum nuclei.

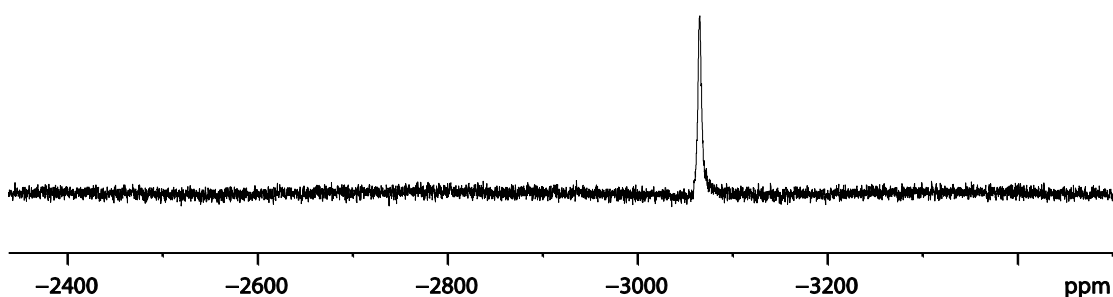


Fig. S5: The ^{195}Pt NMR spectrum of $[\text{Pt}(\text{RRDACP})\text{Cl}_2]$ obtained at 35 °C in $\text{DMSO-}d_6$.

General assignment of I_L for $[\text{Pt}(\text{I}_L)(\text{A}_L)]^{2+}$

COSY spectra (Fig. S6) of metallointercalators were used in combination with J -coupling constants and resonance multiplicity to assign protons to their corresponding resonances in the ^1H NMR spectra. The numbering system for the proton resonances of I_L are shown in Fig. S1. The methodology for assigning all protons of the DACP complexes is illustrated using **9**. The change in chemical shift between the complexes RRDACP , $[\text{Pt}(\text{RRDACP})\text{Cl}_2]$ and **9** is shown graphically in Fig. S8.

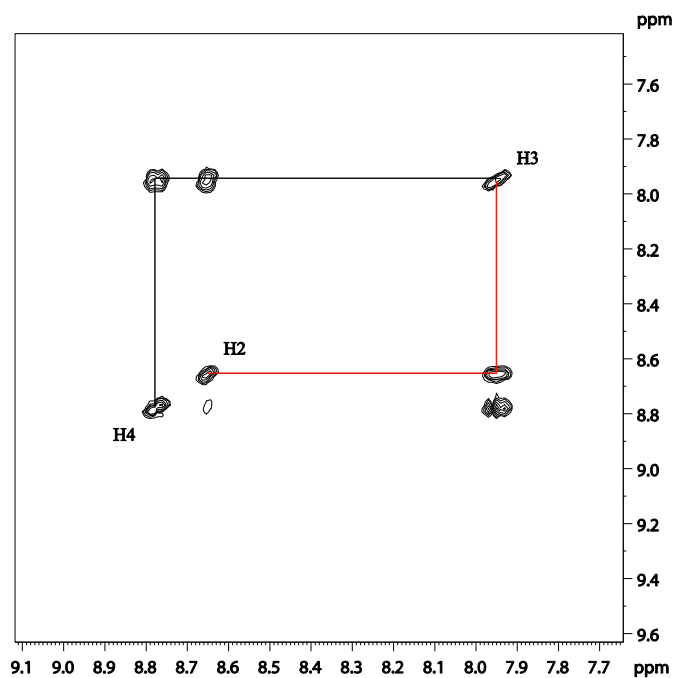


Fig. S6: An expansion of the 2D COSY spectrum of **9** obtained at 25 °C in D₂O and referenced to the residual solvent peak showing the labelling of cross-peak correlation between resonances.

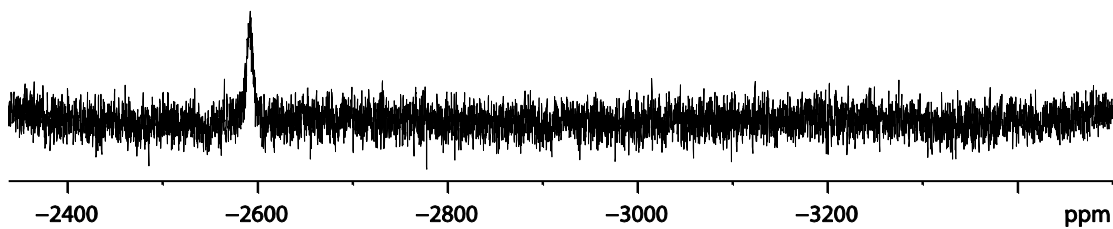


Fig. S7: The ¹⁹⁵Pt NMR spectrum of **9** obtained at 25 °C in D₂O.

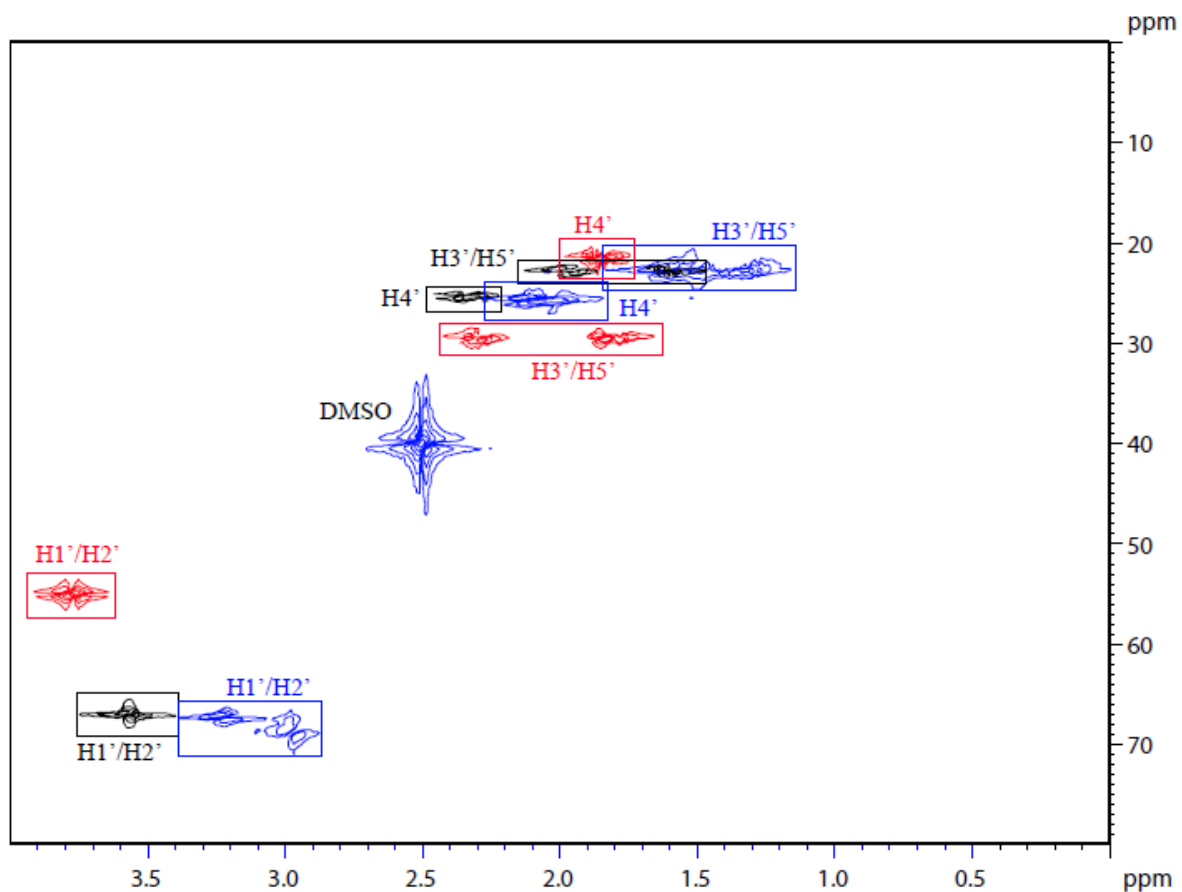


Fig. S8: HMQC comparison of RRDACP (red), [Pt(RRDACP)Cl₂] (blue) and **9** (black) showing the shift in resonance that occur once the ancillary and intercalating ligands have coordinated to the platinum.