Synthesis, characterization and antiproliferative activity on mesothelioma cell lines of bis(carboxylato)platinum(IV) complexes based on picoplatin.

Mauro Ravera[a] • Elisabetta Gabano[a] • Ilaria Zanellato[a] • Ilaria Bonarrigo[a] • Esther Escribano[b] • Virtudes Moreno[b] • Mercè Font-Bardia[c,d] • Teresa Calvet[c] • Domenico Osella*[,a]

[a] *Dipartimento di Scienze dell'Ambiente e della Vita, Università del Piemonte Orientale "Amedeo Avogadro", Viale Michel 11, 15121, Alessandria, Italy. E-mail: domenico.osella@mfn.unipmn.it*

[b] *Departament de Química Inorgànica, Universitat de Barcelona, Martí i Franquès 1-11, 08028, Barcelona, Spain*

[c] *Cristal·lografia, Mineralogia i Dipòsits Minerals, Universitat de Barcelona, Martí i Franquès s/n, 08028 Barcelona, Spain*

[d] *Unitat de Difracció de RX, Centre Científic i Tecnològic de la Universitat de Barcelona (CCITUB), Solé i Sabarís 1-3, 08028 Barcelona, Spain*

SUPPLEMENTARY MATERIAL

Content:

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Table S5 Hydrogen bonds for complex **2** (Å and º).

Table S1 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **2**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	**y**	**z**	**U(eq)**
Pt	2621(1)	1886(1)	4758(1)	33(1)
Cl(1)	560(1)	621(1)	4258(1)	45(1)
Cl(2)	3191(1)	97(1)	4111(1)	48(1)
O(1)	1783(3)	3389(4)	3886(2)	44(1)
O(2)	3302(3)	188(3)	5547(1)	42(1)
O(3)	3619(3)	4302(4)	3888(2)	55(1)
O(4)	4620(4)	1977(4)	6416(2)	54(1)
N(1)	2037(3)	3448(4)	5334(2)	38(1)
N(2)	4485(3)	2826(4)	5168(2)	40(1)
C(1)	2422(4)	4152(6)	3605(2)	50(1)
C(2)	1513(6)	4866(10)	2877(3)	82(2)
C(3)	1834(18)	6550(20)	2718(9)	88(4)
C(3')	2281(16)	5740(20)	2559(8)	92(4)
C(4)	4203(3)	578(5)	6220(2)	39(1)
C(5)	4611(5)	-931(7)	6699(3)	64(1)
C(6)	5818(7)	-629(10)	7404(3)	93(2)
C(7)	2115(4)	5122(5)	5379(2)	43(1)
C(8)	1576(4)	5990(6)	5746(2)	48(1)
C(9)	1004(4)	5146(6)	6079(2)	53(1)
C(10)	956(4)	3418(6)	6048(2)	48(1)
C(11)	1472(4)	2617(5)	5671(2)	44(1)
C(12)	2748(5)	6114(6)	5046(3)	60(1)

Table S2 Bond lengths (Å) and angles (º) for complex **2**.

Pt-O(2)	2.006(3)
Pt-O(1)	2.025(3)
Pt-N(2)	2.033(3)
Pt-N(1)	2.087(3)
Pt-Cl(2)	2.3012(10)
Pt-Cl(1)	2.3151(13)
O(1)-C(1)	1.312(5)
O(2)-C(4)	1.340(4)
O(3)-C(1)	1.217(5)
O(4)-C(4)	1.207(5)
N(1)-C(7)	1.339(5)
N(1)-C(11)	1.362(5)
N(2)-H(2A)	0.8900
N(2)-H(2B)	0.8900
N(2)-H(2C)	0.8900
C(1)-C(2)	1.504(7)
C(2)-C(3)	1.477(17)
C(2)-C(3')	1.529(17)
C(2)-H(2D)	0.9700
C(2)-H(2E)	0.9700
C(2)-H(2D')	0.9700
C(2)-H(2E')	0.9700
C(3)-H(3A)	0.9610
C(3)-H(3B)	0.9594
C(3)-H(3C)	0.9606
C(3)-H(3A')	1.2796
C(3)-H(3B')	1.0053
C(3')-H(3A)	1.2610
C(3')-H(3C)	0.9419
C(3')-H(3A')	0.9605
C(3')-H(3B')	0.9589
C(3')-H(3C')	0.9606
C(4)-C(5)	1.502(6)
C(5)-C(6)	1.494(8)
C(5)-H(5A)	0.9700
C(5)-H(5B)	0.9700
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(7)-C(8)	1.403(5)
C(7)-C(12)	1.479(7)
C(8)-C(9)	1.365(6)
C(8)-H(8)	0.9300
C(9)-C(10)	1.381(7)
C(9)-H(9)	0.9300

C(10)-C(11)	1.375(5)
C(10)-H(10)	0.9300
C(11)-H(11)	0.9300
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
O(2)-Pt-O(1)	173.23(11)
O(2)-Pt-N(2)	89.31(12)
O(1)-Pt-N(2)	96.28(12)
O(2)-Pt-N(1)	90.60(12)
O(1)-Pt-N(1)	92.61(12)
N(2)-Pt-N(1)	96.06(13)
O(2)-Pt-Cl(2)	88.86(8)
O(1)-Pt-Cl(2)	87.69(9)
N(2)-Pt-Cl(2)	86.18(10)
N(1)-Pt-Cl(2)	177.68(9)
O(2)-Pt-Cl(1)	89.22(8)
O(1)-Pt-Cl(1)	84.89(9)
N(2)-Pt-Cl(1)	175.13(10)
N(1)-Pt-Cl(1)	88.59(9)
Cl(2)-Pt-Cl(1)	89.15(4)
C(1)-O(1)-Pt	125.3(3)
C(4)-O(2)-Pt	122.0(2)
C(7)-N(1)-C(11)	118.7(3)
C(7)-N(1)-Pt	127.5(3)
C(11)-N(1)-Pt	113.7(3)
Pt-N(2)-H(2A)	109.5
Pt-N(2)-H(2B)	109.5
H(2A)-N(2)-H(2B)	109.5
Pt-N(2)-H(2C)	109.5
H(2A)-N(2)-H(2C)	109.5
H(2B)-N(2)-H(2C)	109.5
O(3)-C(1)-O(1)	125.2(4)
O(3)-C(1)-C(2)	121.9(4)
O(1)-C(1)-C(2)	112.9(4)
C(3)-C(2)-C(1)	117.2(8)
C(1)-C(2)-C(3')	111.8(7)
C(3)-C(2)-H(2D)	108.0
C(1)-C(2)-H(2D)	108.0
C(3)-C(2)-H(2E)	108.0
C(1)-C(2)-H(2E)	108.0
H(2D)-C(2)-H(2E)	107.3
C(1)-C(2)-H(2D')	109.3
C(3')-C(2)-H(2D')	109.3
C(1)-C(2)-H(2E')	109.3

C(3')-C(2)-H(2E')	109.3
C(2D')-C(2)-H(2E')	107.9
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.6
H(3A)-C(3)-H(3B)	109.4
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.4
H(3B)-C(3)-H(3C)	109.5
C(2)-C(3)-H(3B')	110.5
H(3A)-C(3)-H(3B')	107.9
H(3B)-C(3)-H(3B')	109.9
C(2)-C(3')-H(3C)	106.7
C(2)-C(3')-H(3A')	109.5
C(2)-C(3')-H(3B')	109.4
H(3A')-C(3')-H(3B')	109.5
C(2)-C(3')-H(4C')	109.4
H(3A')-C(3')-H(4C')	109.4
H(3B')-C(3')-H(4C')	109.5
O(4)-C(4)-O(2)	123.9(3)
O(4)-C(4)-C(5)	124.4(4)
O(2)-C(4)-C(5)	111.7(3)
C(6)-C(5)-C(4)	112.9(5)
C(6)-C(5)-H(5A)	109.0
C(4)-C(5)-H(5A)	109.0
C(6)-C(5)-H(5B)	109.0
C(4)-C(5)-H(5B)	109.0
H(5A)-C(5)-H(5B)	107.8
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
N(1)-C(7)-C(8)	120.1(4)
N(1)-C(7)-C(12)	122.0(4)
C(8)-C(7)-C(12)	117.9(4)
C(9)-C(8)-C(7)	120.8(4)
C(9)-C(8)-H(8)	119.6
C(7)-C(8)-H(8)	119.6
C(8)-C(9)-C(10)	119.1(4)
C(8)-C(9)-H(9)	120.5
C(10)-C(9)-H(9)	120.5
C(11)-C(10)-C(9)	118.3(4)
C(11)-C(10)-H(10)	120.9
C(9)-C(10)-H(10)	120.9
N(1)-C(11)-C(10)	123.1(4)

N(1)-C(11)-H(11)	118.5
C(10)-C(11)-H(11)	118.5
C(7)-C(12)-H(12A)	109.5
C(7)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(7)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5

Table S3 Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **2**. 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	33(1)	32(1)	36(1)	0(1)	18(1)	0(1)
Cl(1)	42(1)	44(1)	49(1)	-4(1)	22(1)	-5(1)
Cl(2)	51(1)	47(1)	48(1)	-2(1)	26(1)	5(1)
O(1)	44(1)	44(1)	43(1)	4(1)	20(1)	4(1)
O(2)	44(1)	37(1)	43(1)	1(1)	21(1)	-2(1)
O(3)	57(2)	59(2)	55(2)	7(1)	31(1)	-1(1)
O(4)	60(2)	49(2)	50(2)	-4(1)	25(1)	-5(1)
N(1)	38(1)	37(1)	42(1)	-1(1)	21(1)	2(1)
N(2)	37(1)	39(2)	44(2)	1(1)	19(1)	-2(1)
C(1)	52(2)	48(2)	48(2)	6(2)	24(2)	2(2)
C(2)	76(4)	92(5)	66(3)	18(3)	27(3)	-3(3)
C(3)	96(11)	69(9)	82(9)	7(7)	32(8)	-7(8)
C(3')	88(10)	107(13)	68(7)	22(8)	27(7)	1(8)
C(4)	35(2)	45(2)	36(2)	2(1)	18(1)	1(1)
C(5)	70(3)	62(3)	53(2)	7(2)	25(2)	-2(2)
C(6)	90(4)	101(6)	69(3)	17(3)	23(3)	-7(4)
C(7)	41(2)	40(2)	48(2)	-5(1)	21(2)	-1(1)
C(8)	44(2)	43(2)	55(2)	-7(2)	24(2)	2(2)
C(9)	49(2)	55(3)	56(2)	-8(2)	28(2)	1(2)
C(10)	46(2)	54(2)	45(2)	-5(2)	24(2)	-2(2)
C(11)	45(2)	40(2)	51(2)	-1(2)	27(2)	2(2)
C(12)	66(3)	44(3)	80(3)	-4(2)	43(2)	-1(2)

Table S4 Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for complex **2**.

	x	y	z	U(eq)
H(2A)	4481	3678	4899	48
H(2B)	5026	2028	5172	48
H(2C)	4763	3182	5612	48
H(2D)	1493	4093	2523	98
H(2E)	625	4904	2815	98
H(2D')	914	5662	2912	98
H(2E')	984	3970	2560	98
H(3A)	1341	6747	2212	105
H(3B)	1604	7380	2962	105
H(3C)	2765	6613	2875	105
H(3A')	1670	6192	2099	111
H(3B')	2802	6630	2870	111
H(4C')	2853	4946	2508	111
H(5A)	3886	-1255	6779	77
H(5B)	4782	-1854	6462	77
H(6A)	6046	-1636	7684	140
H(6B)	5643	251	7652	140
H(6C)	6540	-306	7330	140
H(8)	1609	7155	5763	57
H(9)	652	5727	6323	63
H(10)	585	2811	6276	57
H(11)	1432	1453	5644	53
H(12A)	3065	5374	4810	91
H(12B)	3476	6738	5407	91
H(12C)	2111	6875	4703	91

Table S5 Hydrogen bonds for complex **2** (Å and º).

	D-H···A				d(D-H)	d(H···A)	d(D···A)	<(DHA)
Intra	N2	--H2A	O3		0.89	1.96	2.691(5)	139
Intra	N2	--H2C	O4		0.89	2.05	2.692(5)	128
Inter	N2	--H2B	Cl2	[1-x,1-y,-z]	0.89	2.53	3.317(4)	148
Inter	N2	--H2C	O3	[1-x,1-y,-z]	0.89	2.59	3.135(5)	120