

Electronic Supporting Information

Cisplatin and Zoledronic acid: two drugs combined in a Pt(II) complex with potential antitumor activity towards bone tumors and metastases.

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- Elemental analysis and ¹⁹⁵Pt NMR data of the Pt precursor complexes *cis*-[PtI₂(NH₃)₂] and *cis*-[Pt(OSO₃)(OH₂)(NH₃)₂].
- Full ¹H NMR spectrum of Zoledronic Acid in D₂O.
- Table 1. pK_a values (calculated and experimental) for Zoledronic Acid.
- Figure S1. ESI-MS of compound **1** in water.
- Figure S2. Stereochemistry and Curve-fitted Pt4f XP spectrum of the Pt(III) complex [Pt₂Cl₂{N(H)C(Bu^t)O}₄].

Elemental analysis and ^{195}Pt NMR data of Pt precursor complexes

cis-[PtI₂(NH₃)₂]: Anal. Calcd. for H₆I₂N₂Pt: H, 1.25; N, 5.80%. Found: H, 1.51; N, 5.72%. ^{195}Pt NMR (DMF-d₇): -3199 ppm.

cis-[Pt(OSO₃)(OH₂)(NH₃)₂]: Anal. calcd for H₈N₂O₅PtS: H 2.34%, N 8.24. Found: H 2.45%, N 8.09%. ^{195}Pt NMR (D₂O): -1555 ppm.

Full ^1H NMR spectrum of Zoledronic Acid in D₂O. (* indicate TSP signals; # indicates residual H₂O signal)

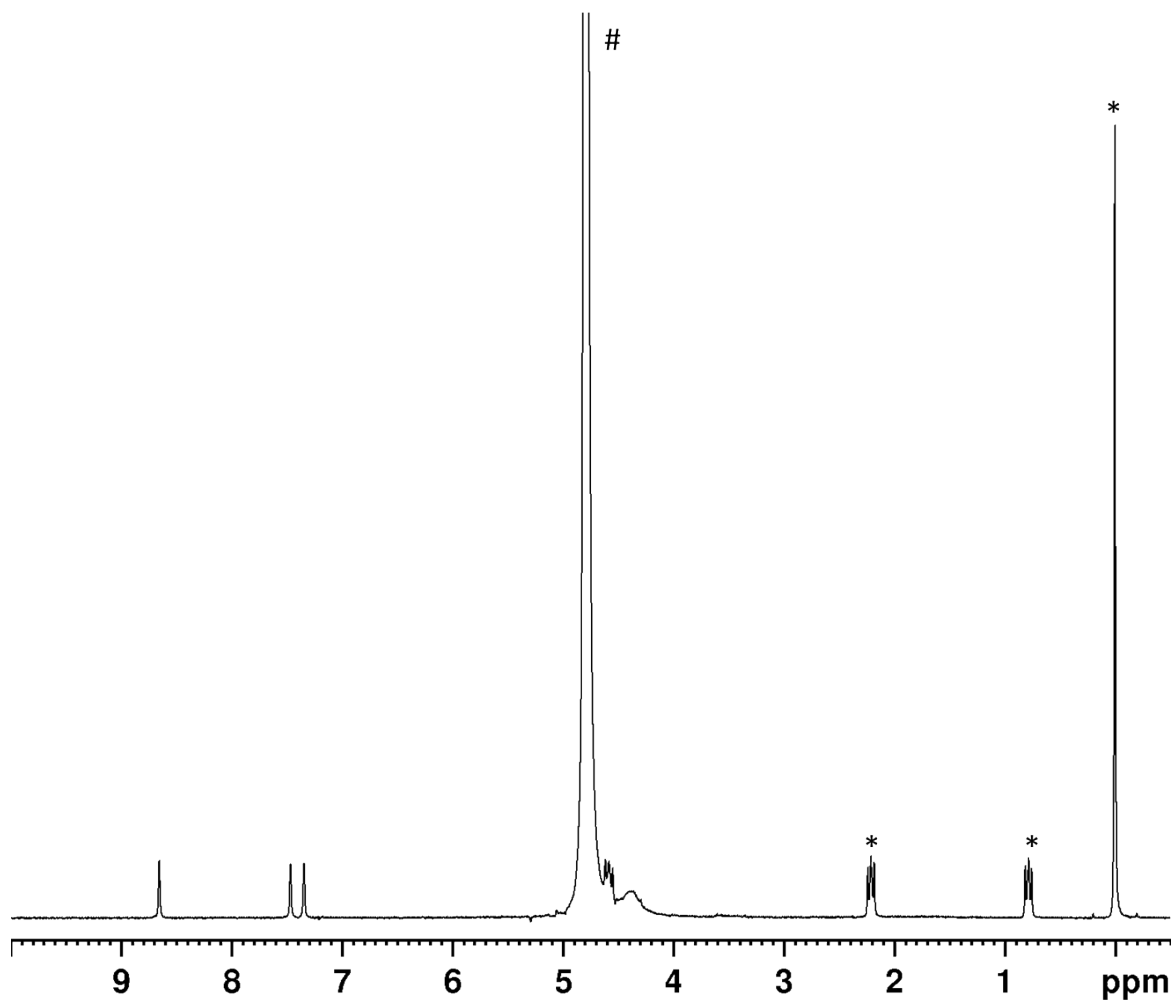
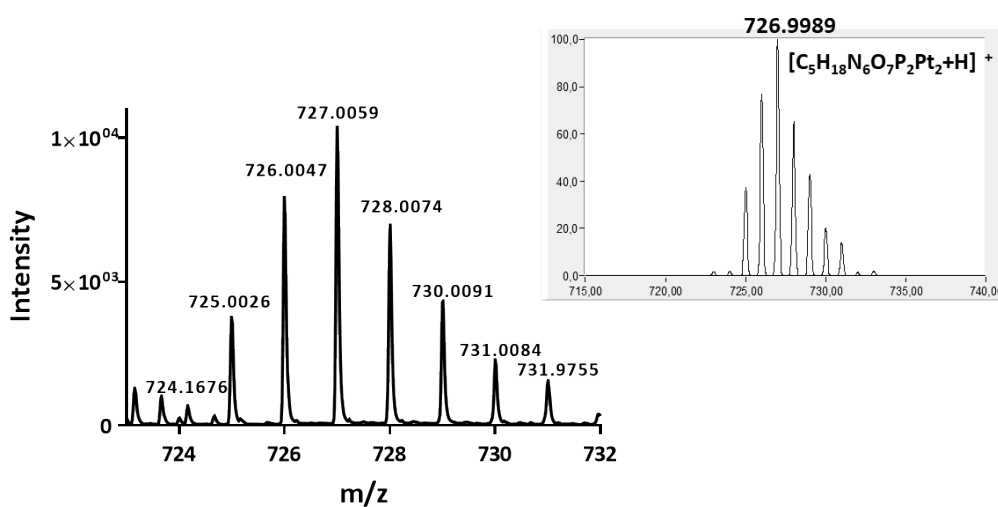


Table 1. pK_a values (calculated and experimental) for Zoledronic Acid.

	Experimental (¹ H and ³¹ P NMR)	Calculated with ACD pKa LABS
pK _{a1}	-	0.76
pK _{a2}	1.25	0.76
pK _{a3}	2.32	0.76
pK _{a4}	7.38	0.76
pK _{a5}	7.9	6.43
pK _{a6}	12.08	9.14

Figure S1. ESI-MS of compound **1** in water. The calculated isotope mass distribution for the specified molecular formula is shown in the inset.



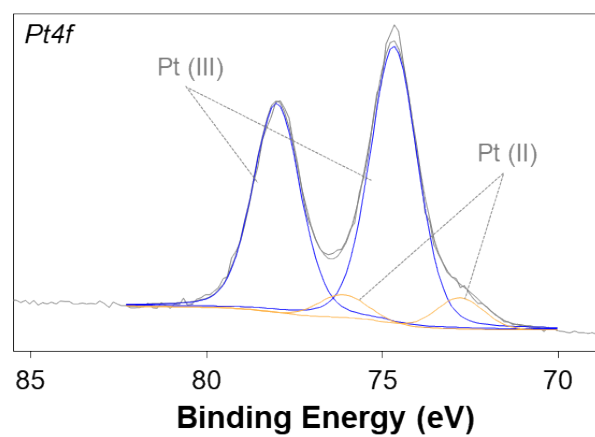
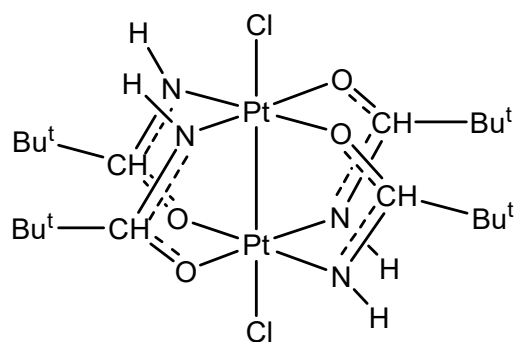


Figure S2. Stereochemistry and Curve-fitted Pt4f XP spectrum of the Pt(III) complex $[\text{Pt}_2\text{Cl}_2\{\text{N}(\text{H})\text{C}(\text{Bu}^t)\text{O}\}_4]$.