

SUPPLEMENTARY INFORMATION AVAILABLE

Cytotoxic Properties of a New Organometallic Platinum(II) Complex and its Gold(I) Heterobimetallic Derivatives

Maria Serratrice, Laura Maiore, Antonio Zucca, Sergio Stoccoro, Ida Landini, Enrico Mini, Lara Massai, Giarita Ferraro, Antonello Merlino, Luigi Messori and Maria Agostina Cinellu

Table S1. Absorption characteristics of compounds **2** – **5-Cl** in various solvents. ^anegative deviation from Lambert-beer law.

Compound	λ_{\max} , nm (ϵ , Lmol ⁻¹ cm ⁻¹)			
	CH ₂ Cl ₂	CH ₃ CN	DMSO	BP 10 mM pH 7.4
pbiH	310	308 (74405)	313	227, 307
2	-	-	291 (9779) 328 sh (11598) 344 (13158)	-
3	240 sh (7935) 293 (3463) 346 (5565)	207 sh (9120) 237 sh (6034) 293 (2730) 341 (4258)	297 (2201) 345 (3990)	338
4-PF₆	238 (23033) 267 (9586) 275 (8905) 337 (15403)	215 (2168) 235 (^a) 267 (5998) 275 (5775) 329 (9804)	261 (8476) 268 (9858) 276 (9159) 342 (14060)	234 (-) 338 (-)
5-Cl	235 (22606) 294 sh (9142) 342 (15190)	208 (^a) 239 sh (20808) 335 (13478)	264 (8580) 296 (8890) 345 (14286)	232 (-) 338 (-)

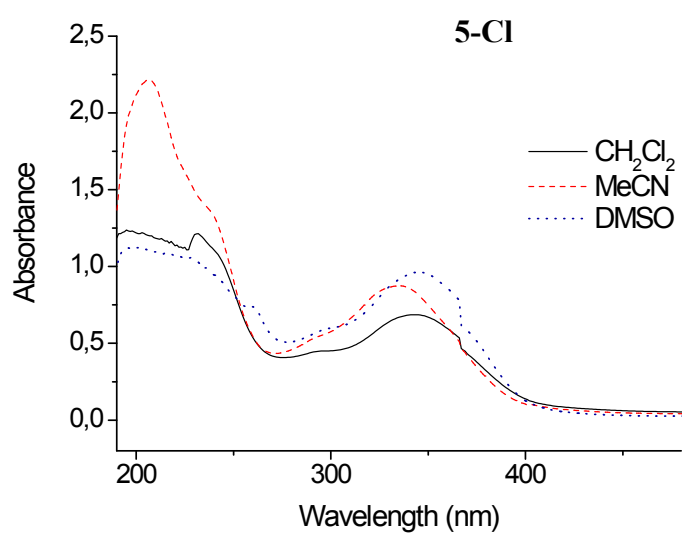
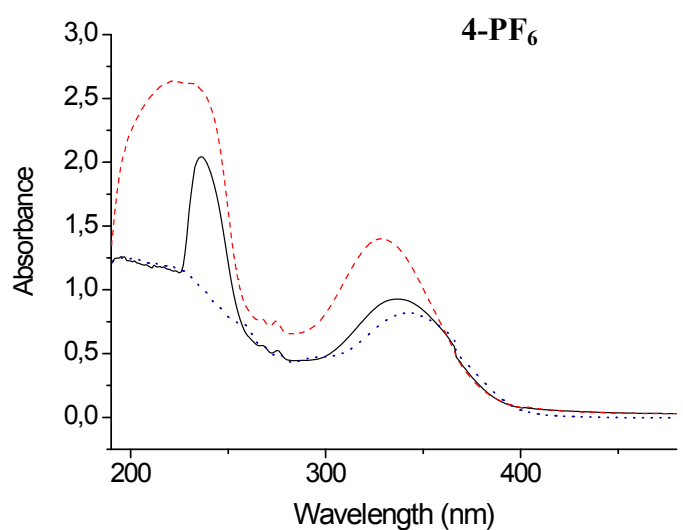
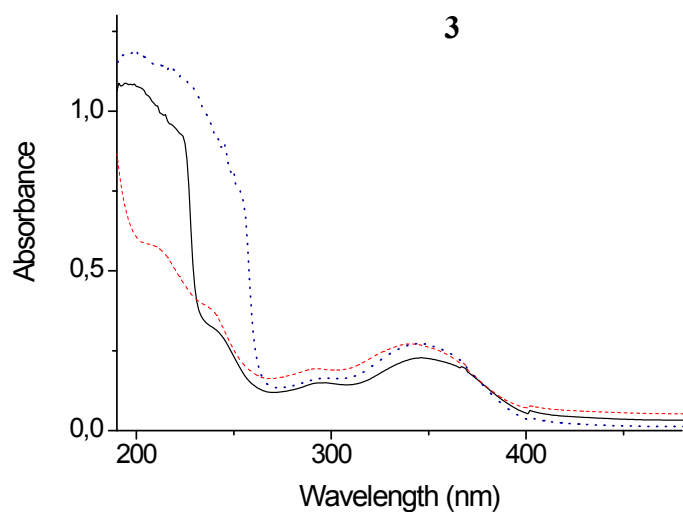


Figure S1. UV-Vis spectra of compounds **3** – **5-Cl** in CH₂Cl₂, MeCN and DMSO solutions at $6 \cdot 10^{-5}$ mol/L.

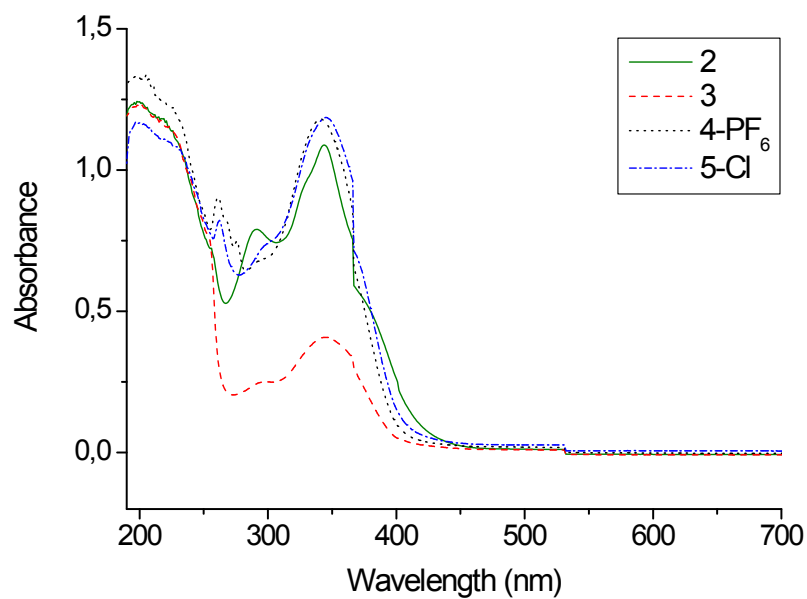


Figure S2. UV-Vis spectra of compounds **2**, **3**, **4-PF₆** and **5-Cl** in DMSO solution at $6 \cdot 10^{-5}$ mol/L.

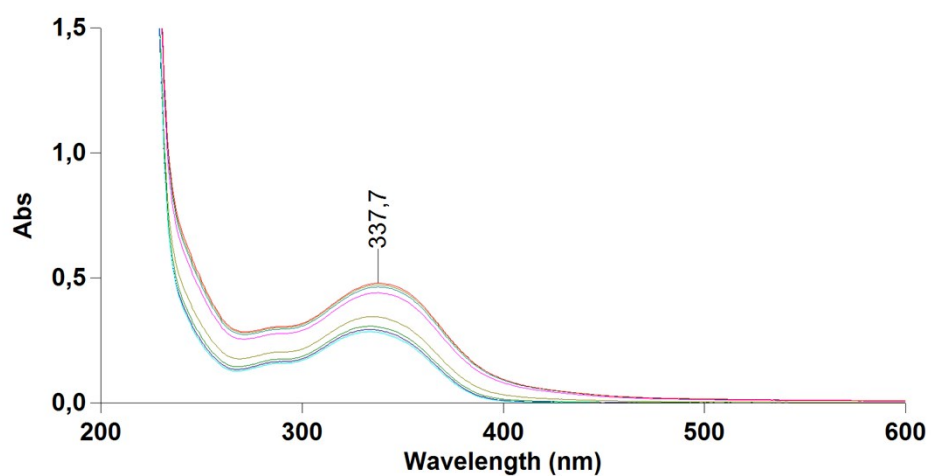


Figure S3. UV-Vis absorption spectral profiles of compounds **3** in 30 μ M phosphate buffered solution, 10 mM, pH 7.4. Spectra were recorded at different times over 24 hours at room temperature.

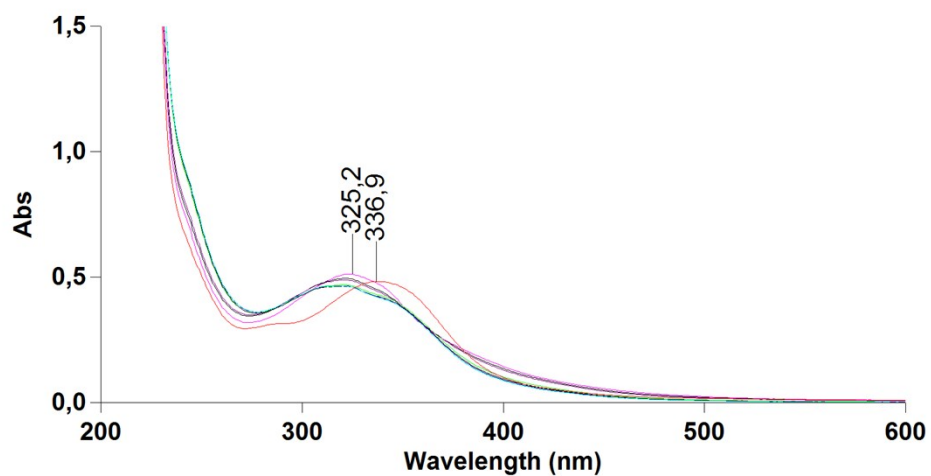
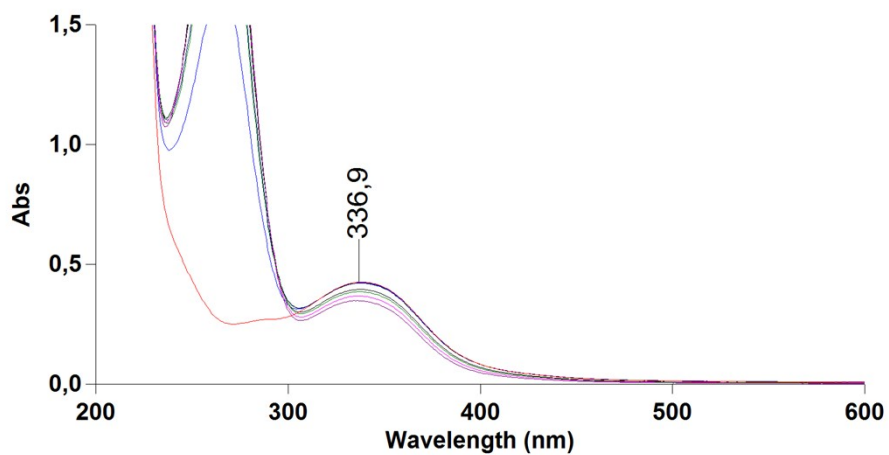
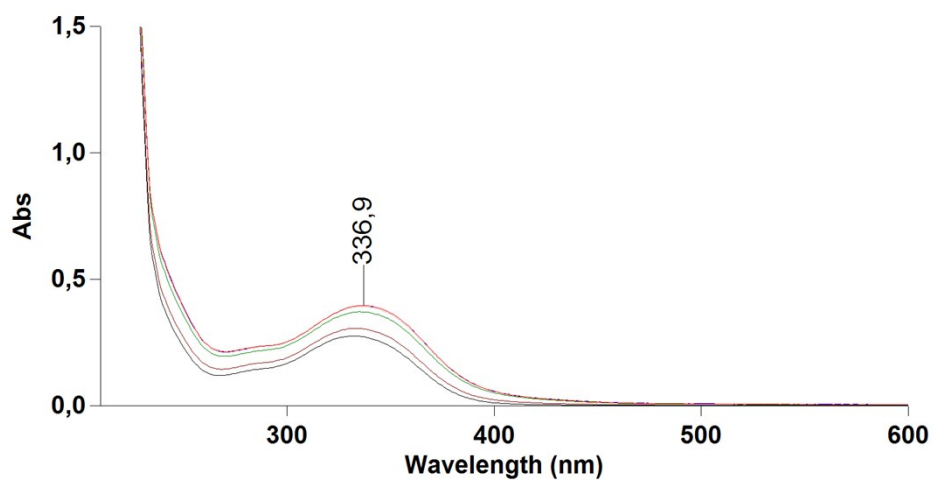
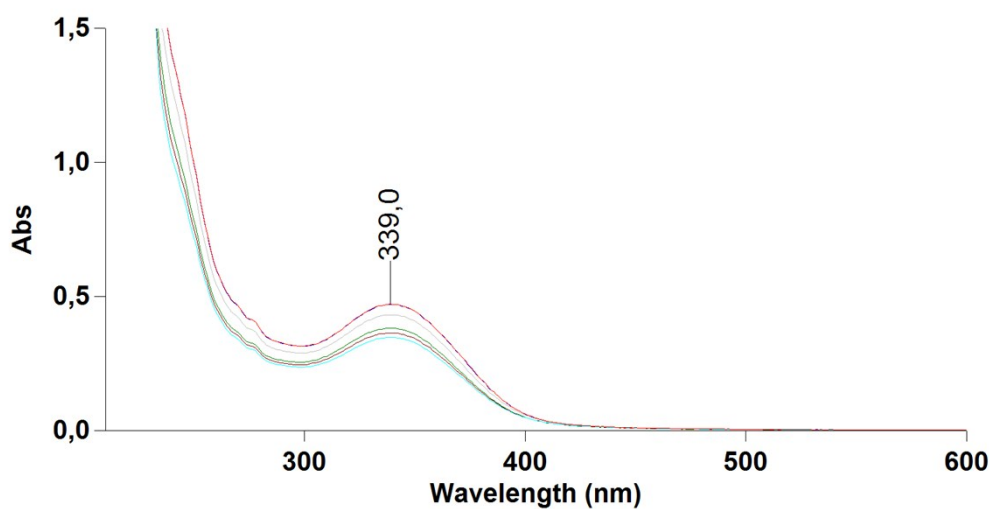


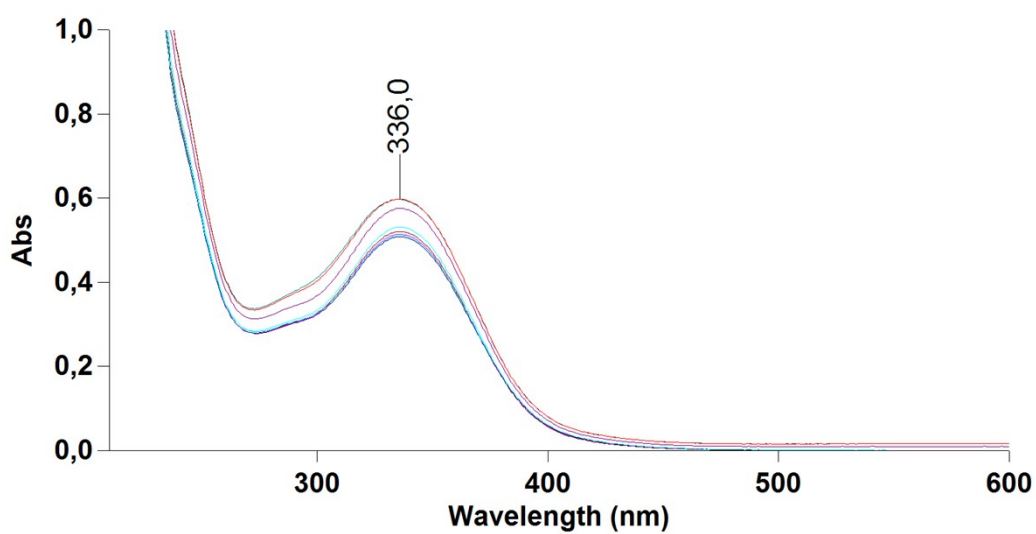
Figure S4. UV-Vis absorption spectral profiles of compounds **3** in 3×10^{-5} M phosphate buffered solution (10 mM, pH 7.4) before and after addition of Asc.Ac. (up) and GSH (down). Spectra were recorded at different times over 12 hours at room temperature.



A

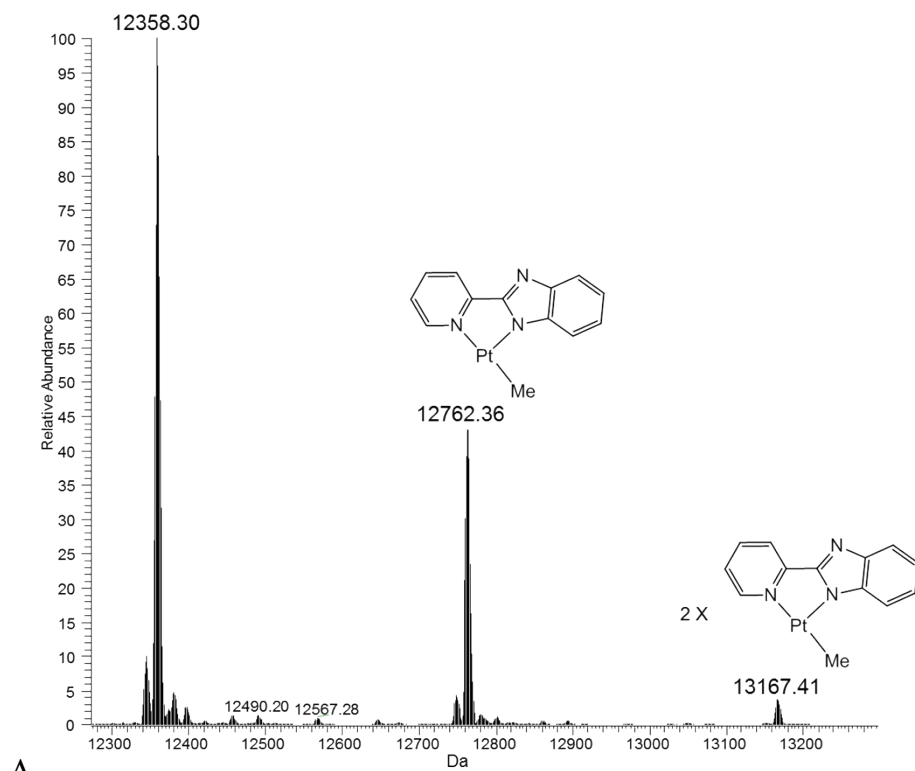


B

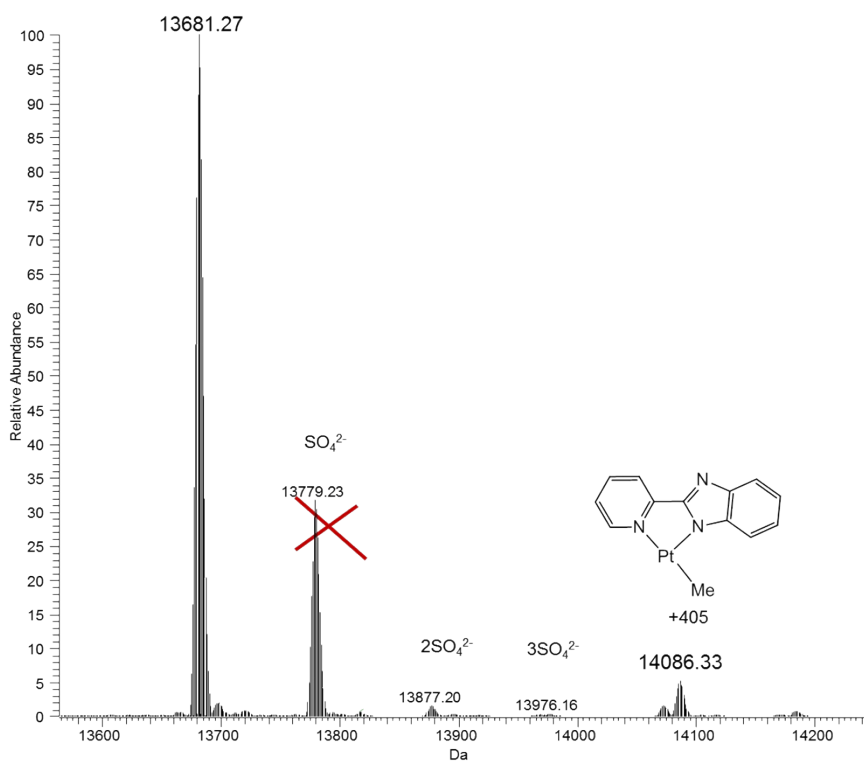


C

Figure S5. UV-Vis absorption spectral profiles of compounds 3 (A) 4-PF₆ (B) and 5-Cl (C) in Ammonium Acetate solution (20 mM, pH 6.8). Spectra were recorded at different times over 24 hours at room temperature.

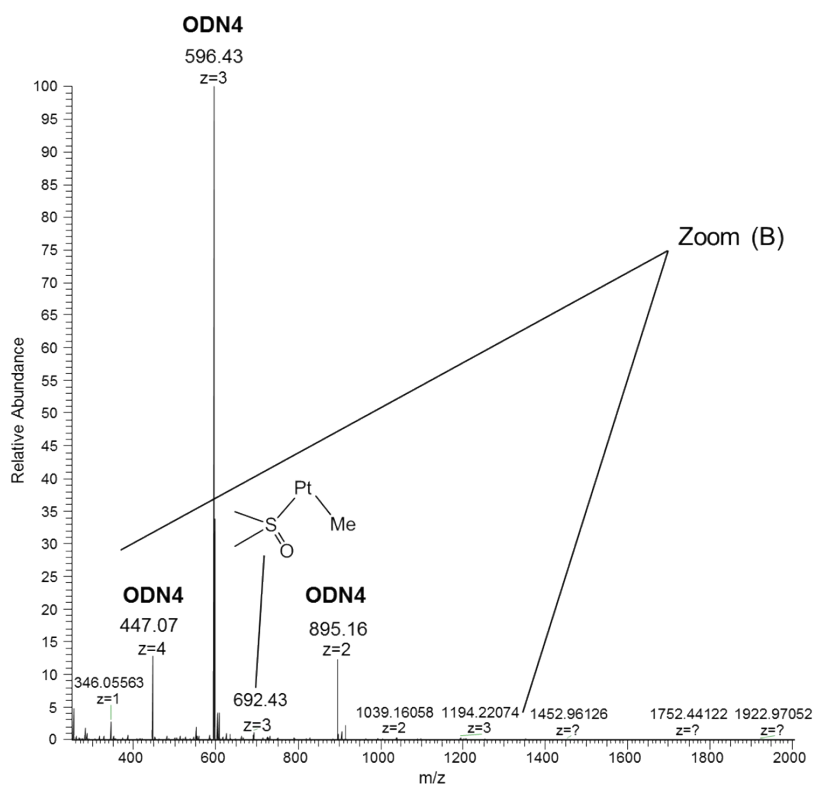


A

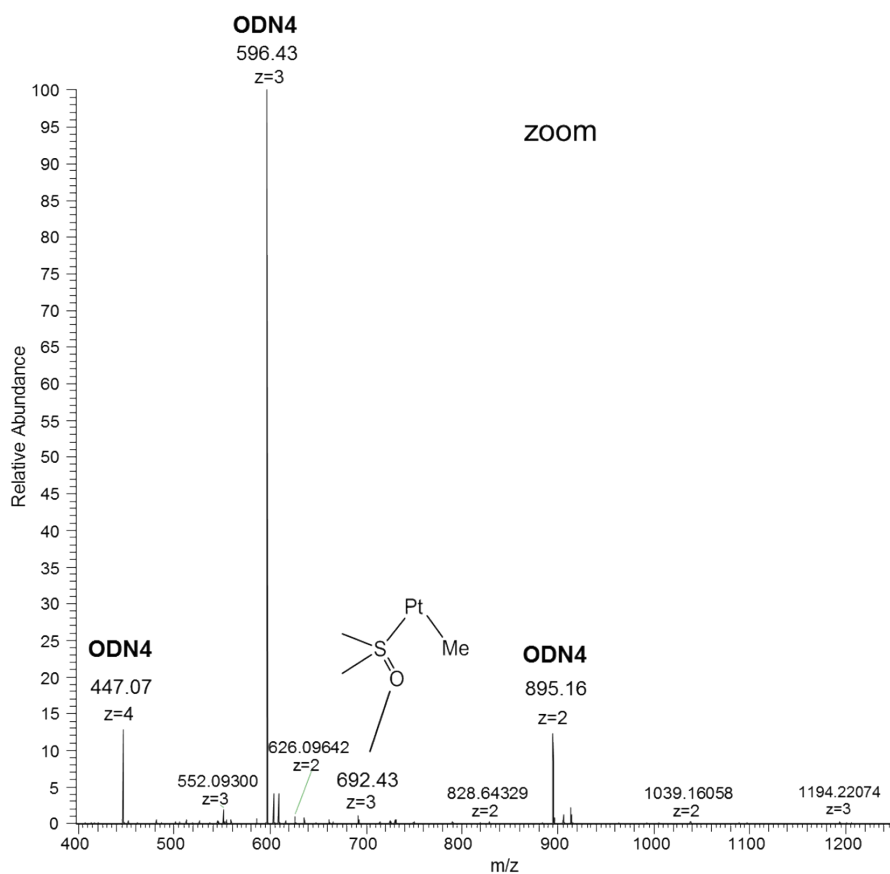


B

Figure S6 LTQ-Orbitrap ESI mass spectra of compound 3 in the presence of cytochrome c (A) and RNase (B) with a metallodrug-protein molar ratio of 3:1.



A



B

Figure S7 LTQ-Orbitrap ESI mass spectra of compound 3 in the presence of ODN4 with a metallodrug-oligonucleotide molar ratio of 3:1.

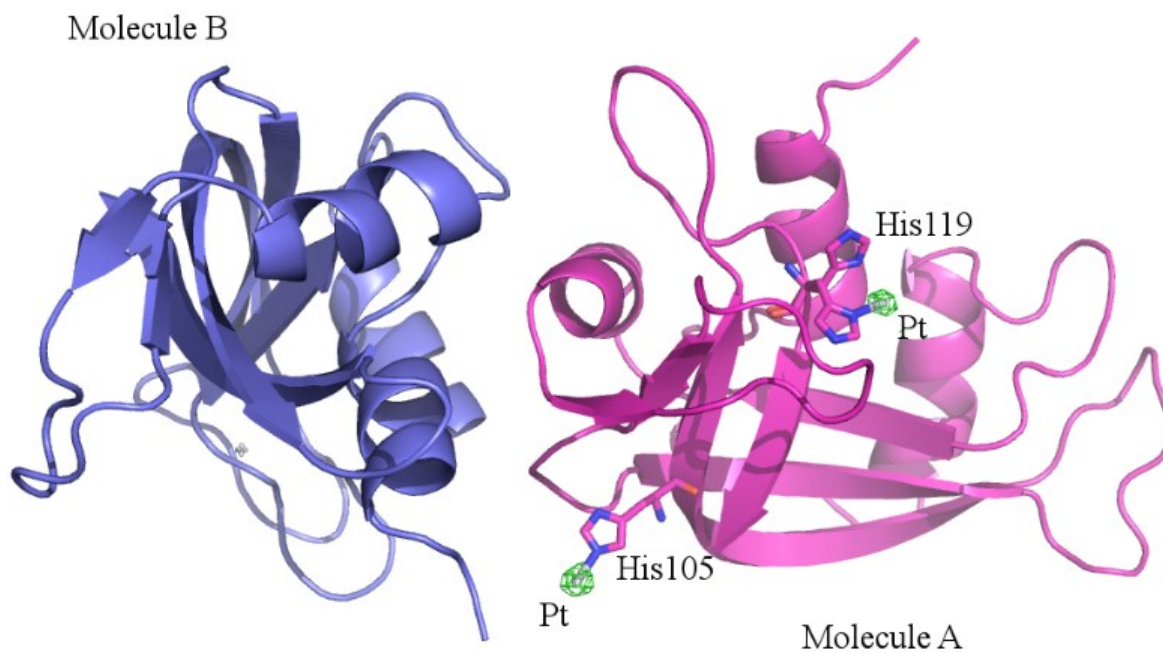
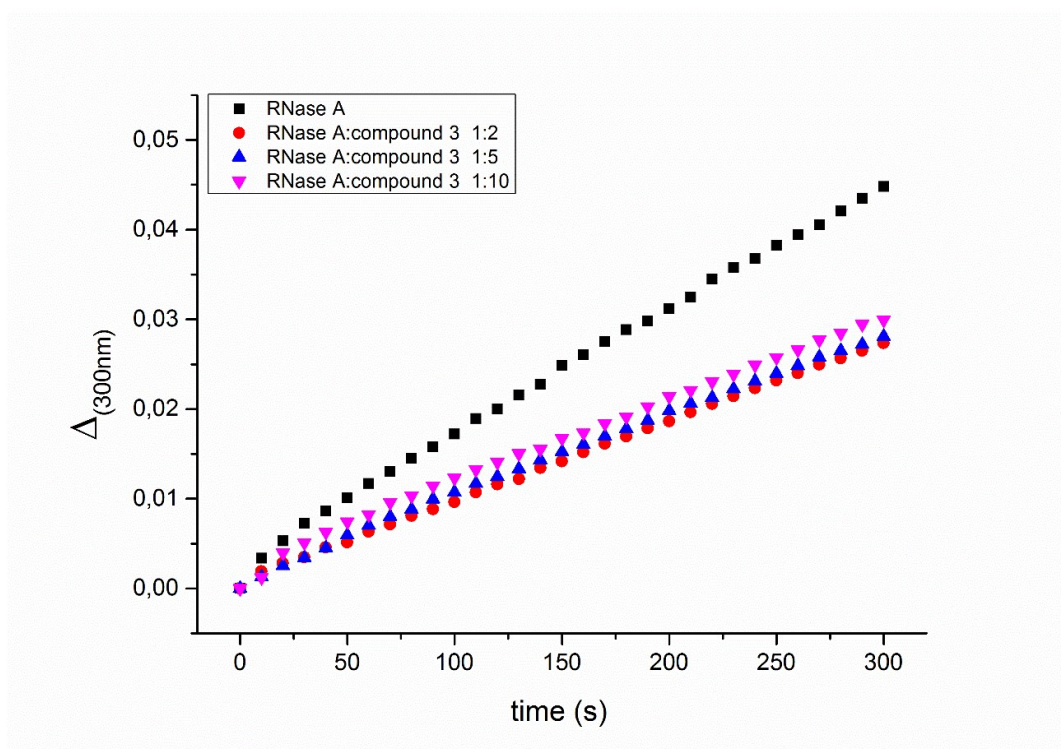
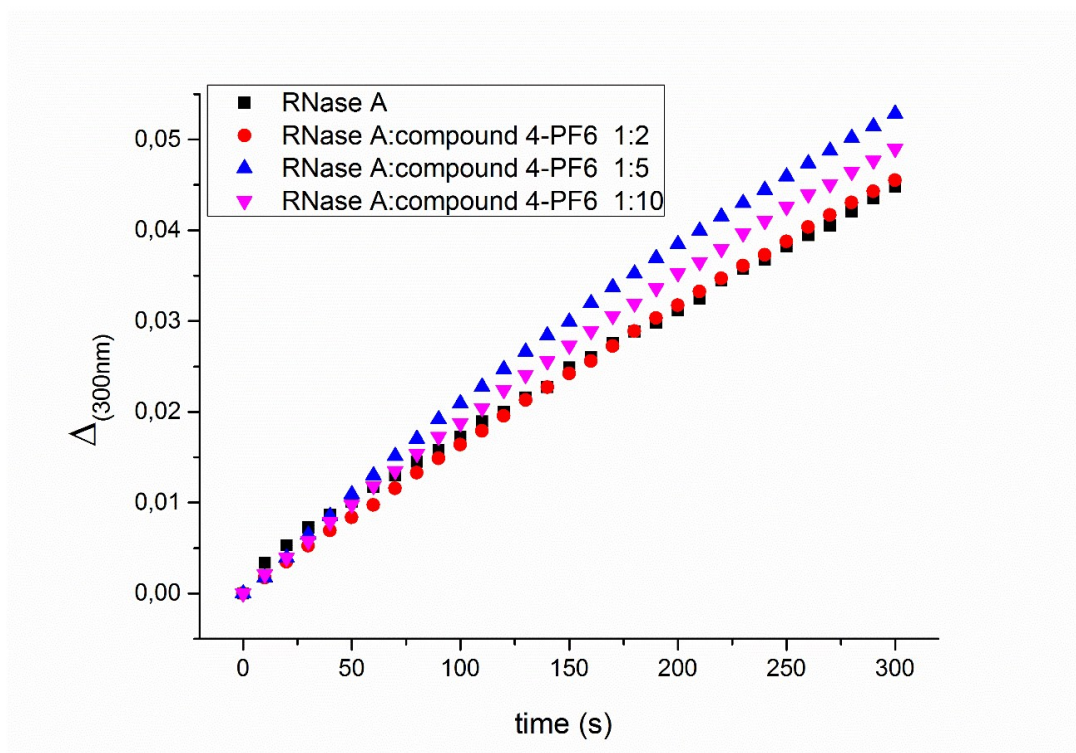


Figure S8. Overall content of the asymmetric unit of RNase A/3. The two RNase A chains denoted as molecule A and molecule B are coloured in pink and violet, respectively. Pt binding occurs only in molecule A. Anomalous electron density map is coloured in green and contoured at 3.0σ level.



A



B

Figure S9. Hydrolysis of yeast RNA by RNase A free and in complex with 3 (panel A) and 4-PF₆ (panel B) in different protein:metal compound ratios. Experiments have been performed using the

Table S2. Data collection and refinement statistics

Kunitz method in 50 mM sodium acetate pH 5.0 (see SI for details). The values are the average of three independent experiments.

	RNase A/ 3	RNase A/ 4-PF₆
Data collection		
Space group	C2	C2
Unit cell parameter		
a/b/c (Å), β (°)	100.4/32.7/72.5, 89.9°	99.5/31.2/69.0 Å, 90.7°
Observed reflections	55531	56875
Unique reflections	16494	23228
Resolution (Å)	72.5-1.98 (2.01-1.98)	69.0-1.68 (1.71-1.68)
Completeness (%)	98.8 (100.0)	95.0 (88.4)
Rmerge	0.087 (0.408)	0.097 (0.296)
I/ σ (I)	4.8 (2.6)	6.5 (2.0)
Multiplicity	3.4 (3.2)	2.4 (1.6)
Refinement		
Resolution (Å)	72.5-1.98	69.0-1.68
number of reflections in working set	15652	22040
number of reflections in test set	834	1188
R factor/R _{free} /R _{all} (%)	0.195/0.254/0.192	0.183/0.234/0.186
Number of non-hydrogen atoms	2111	2118
Mean Overall B-value(Å ²)	34.3	30.2
R.m.s.d. bonds (Å)	0.019	0.019
R.m.s.d. angles (°)	1.92	1.92
Estimated overall coordinate error		
based on R value/R free/maximum likelihood (Å)	0.211/0.189/0.155	0.126/0.126/0.102