

Supplementary data for article:

Senerovic, L.; Zivkovic, M. D.; Veselinovic, A.; Pavic, A.; Djuran, M. I.; Rajkovic, S.; Nikodinovic-Runic, J. Synthesis and Evaluation of Series of Diazine-Bridged Dinuclear Platinum(II) Complexes through in Vitro Toxicity and Molecular Modeling: Correlation between Structure and Activity of Pt(II) Complexes. *Journal of Medicinal Chemistry* **2015**, 58 (3), 1442–1451. <https://doi.org/10.1021/jm5017686>

Supporting Information for

Synthesis and evaluation of series of diazine-bridged

dinuclear platinum(II) complexes through *in vitro* toxicity and

molecular modeling: Correlation between structure and

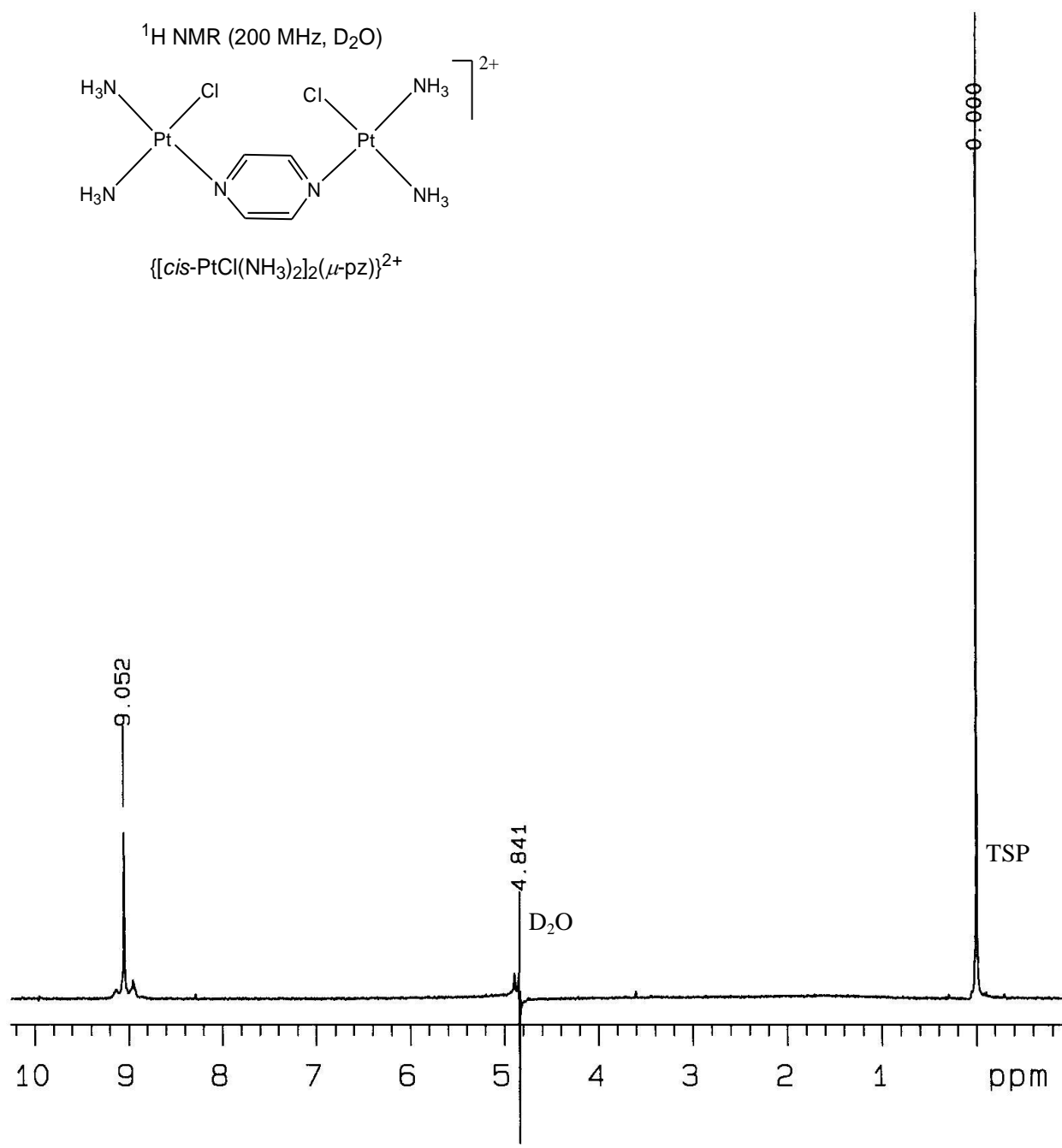
activity of Pt(II) complexes

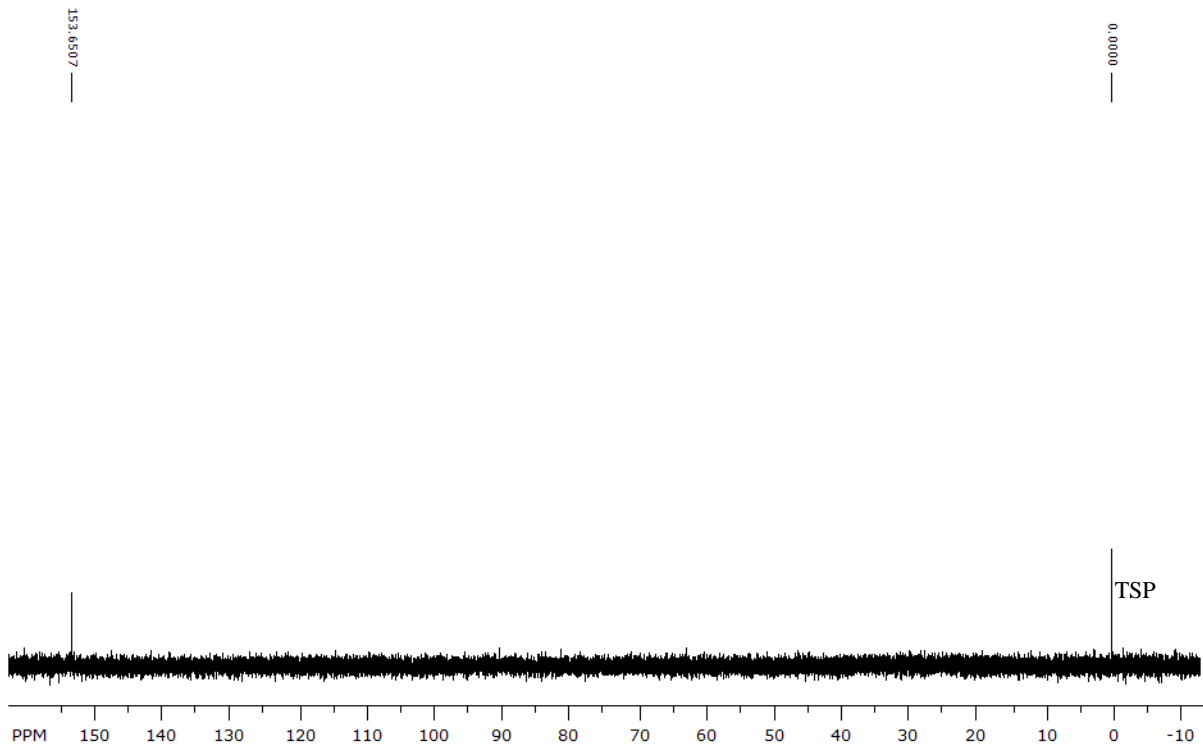
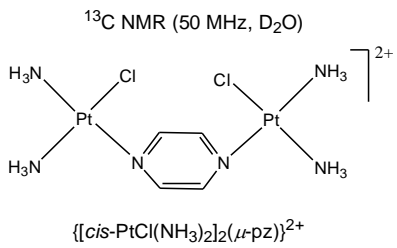
*Lidija Senerovic,<sup>†,#</sup> Marija D Zivkovic,<sup>‡,#</sup> Aleksandar Veselinovic,<sup>§</sup> Aleksandar Pavic,<sup>†</sup> Milos  
I Djuran,<sup>‡</sup> Snezana Rajkovic,<sup>‡,\*</sup> Jasmina Nikodinovic-Runic<sup>†\*</sup>*

Contents:

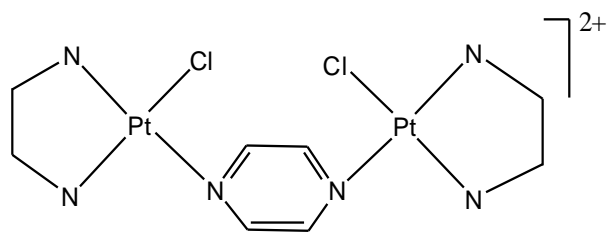
Spectral data for complexes **2-9**

Table S1.

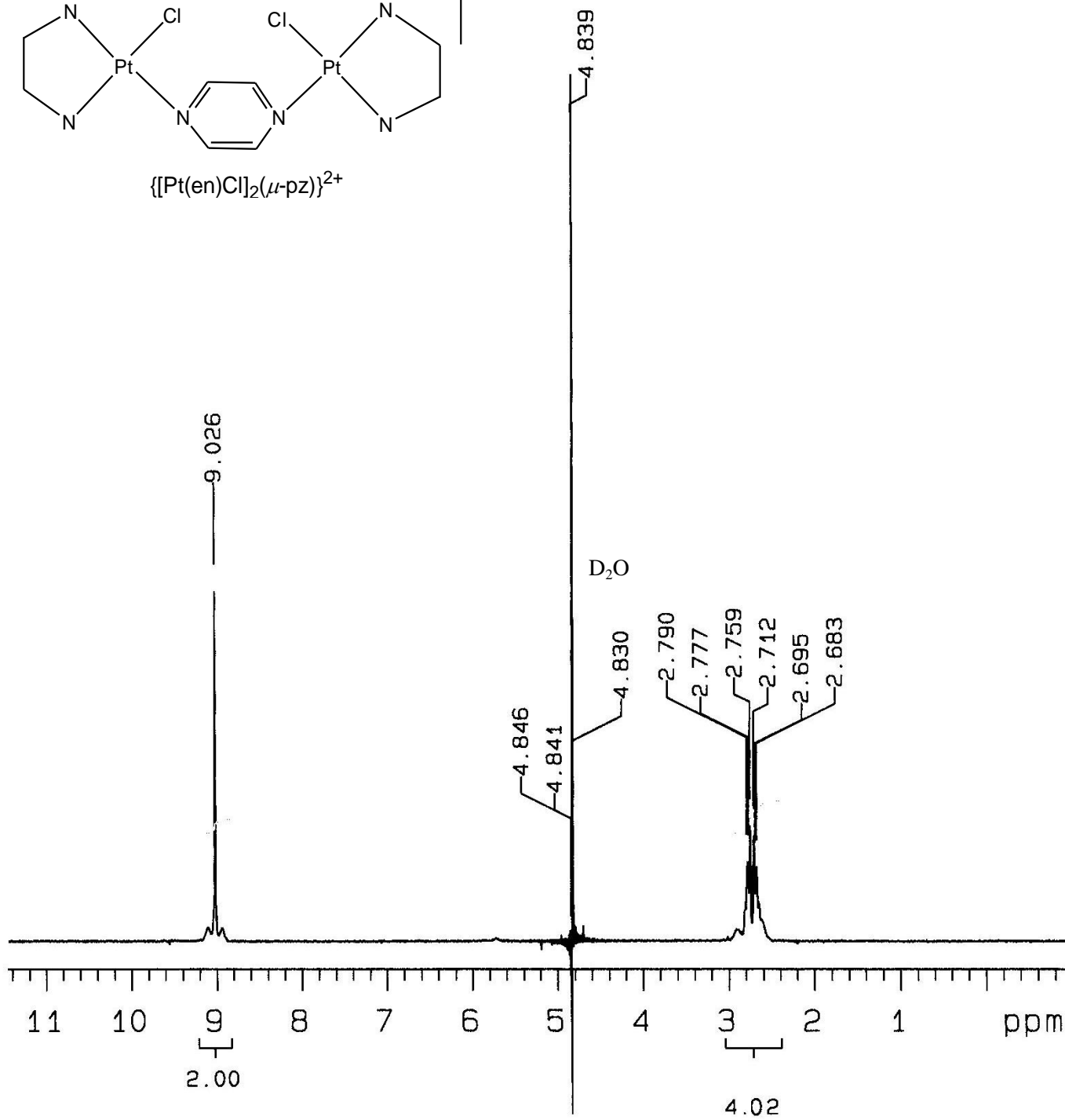


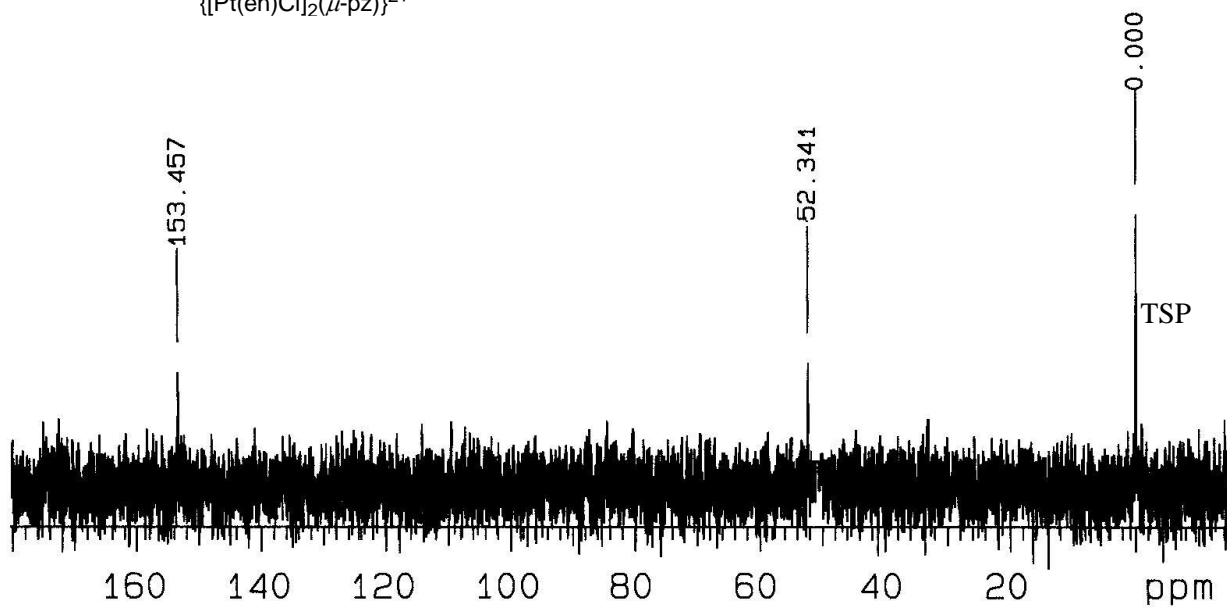
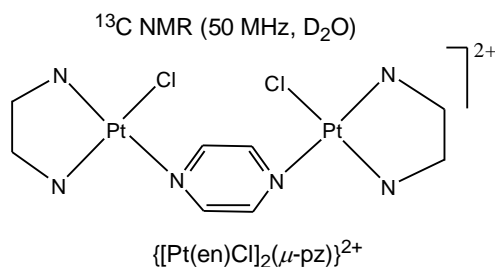


$^1\text{H}$  NMR (200 MHz,  $\text{D}_2\text{O}$ )

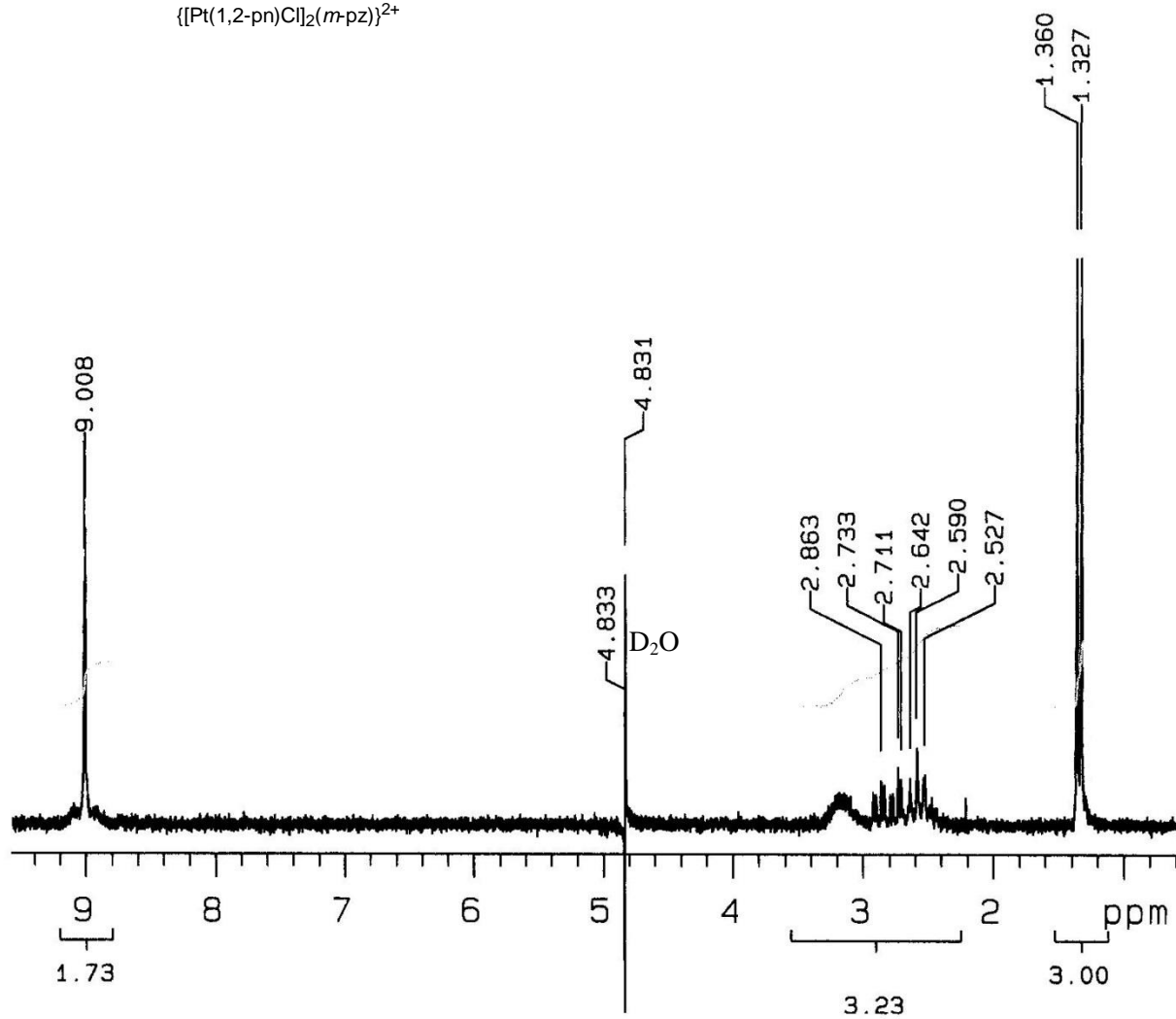
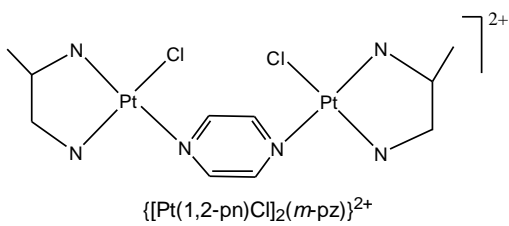


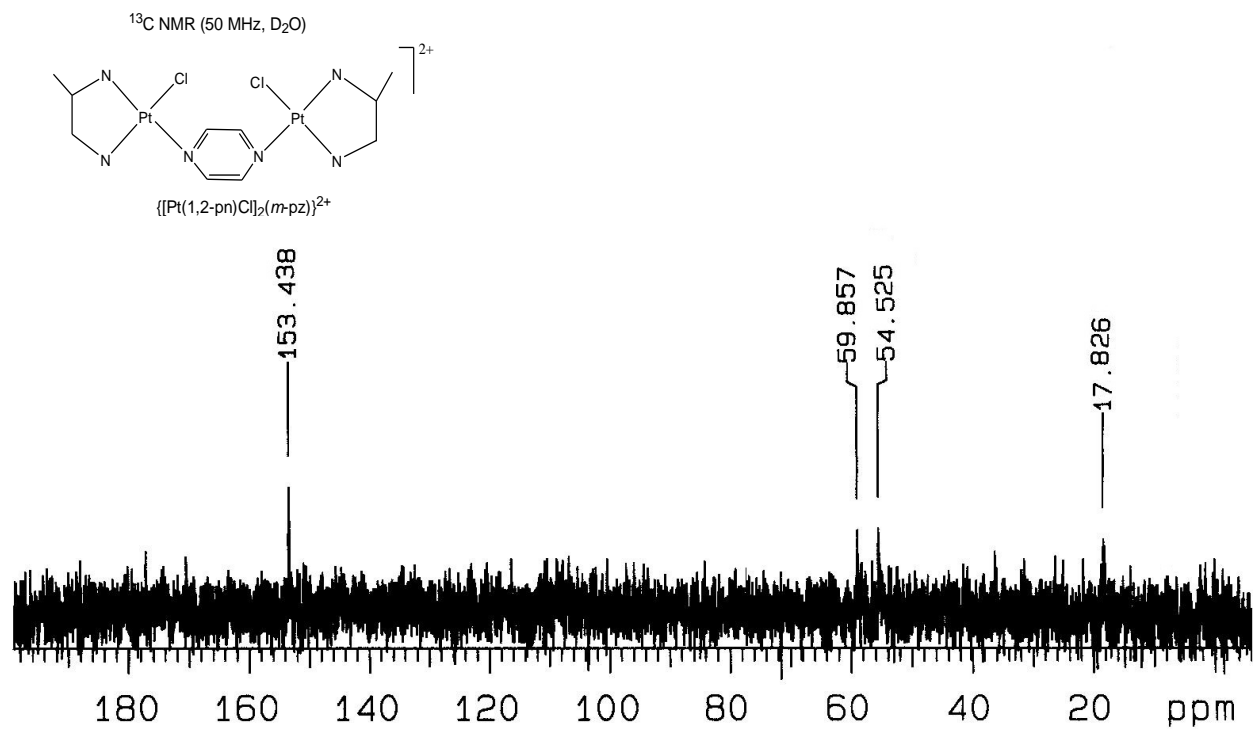
$\{[\text{Pt}(\text{en})\text{Cl}]_2(\mu\text{-pz})\}^{2+}$



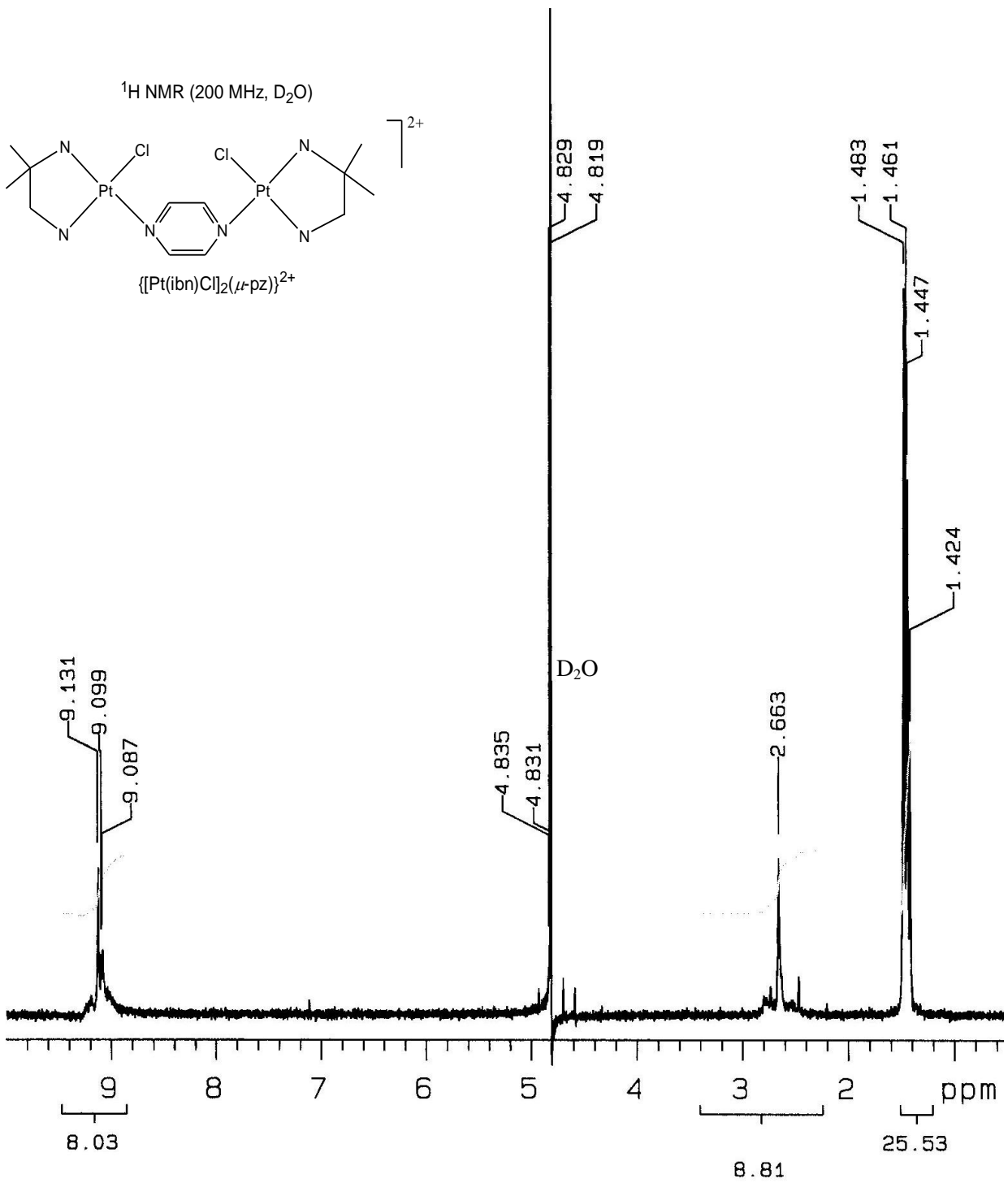


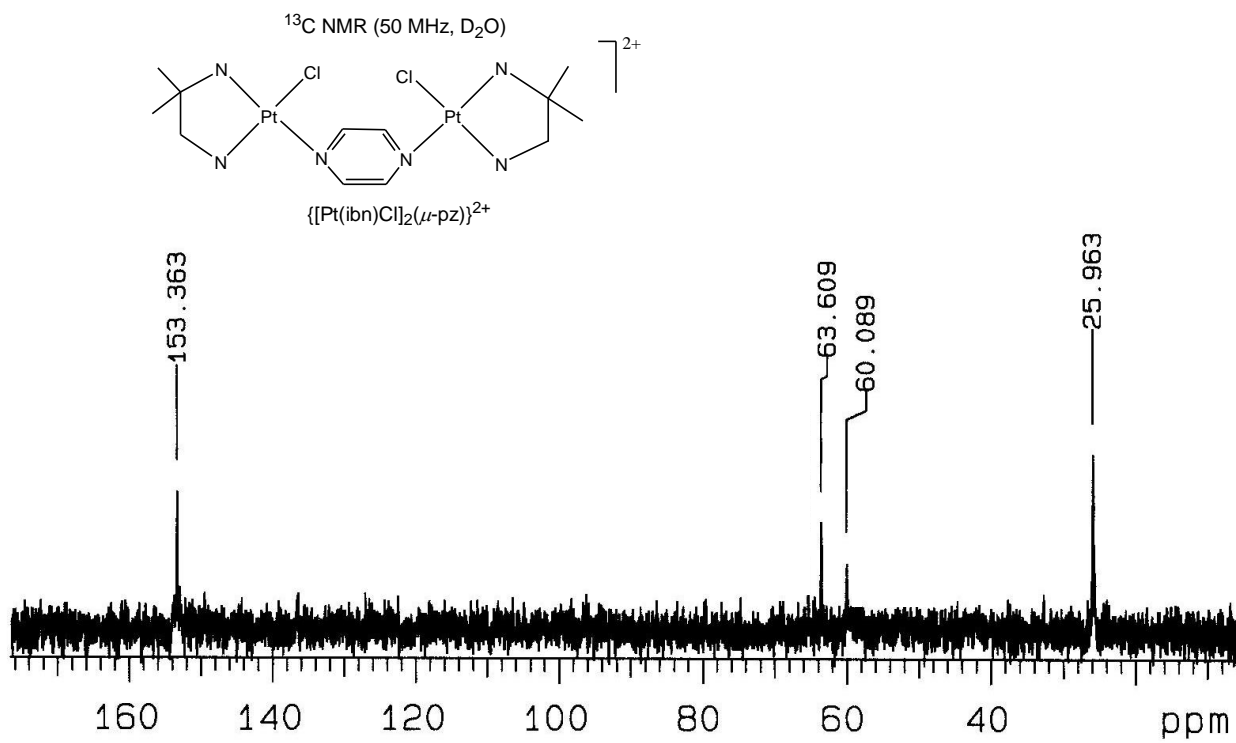
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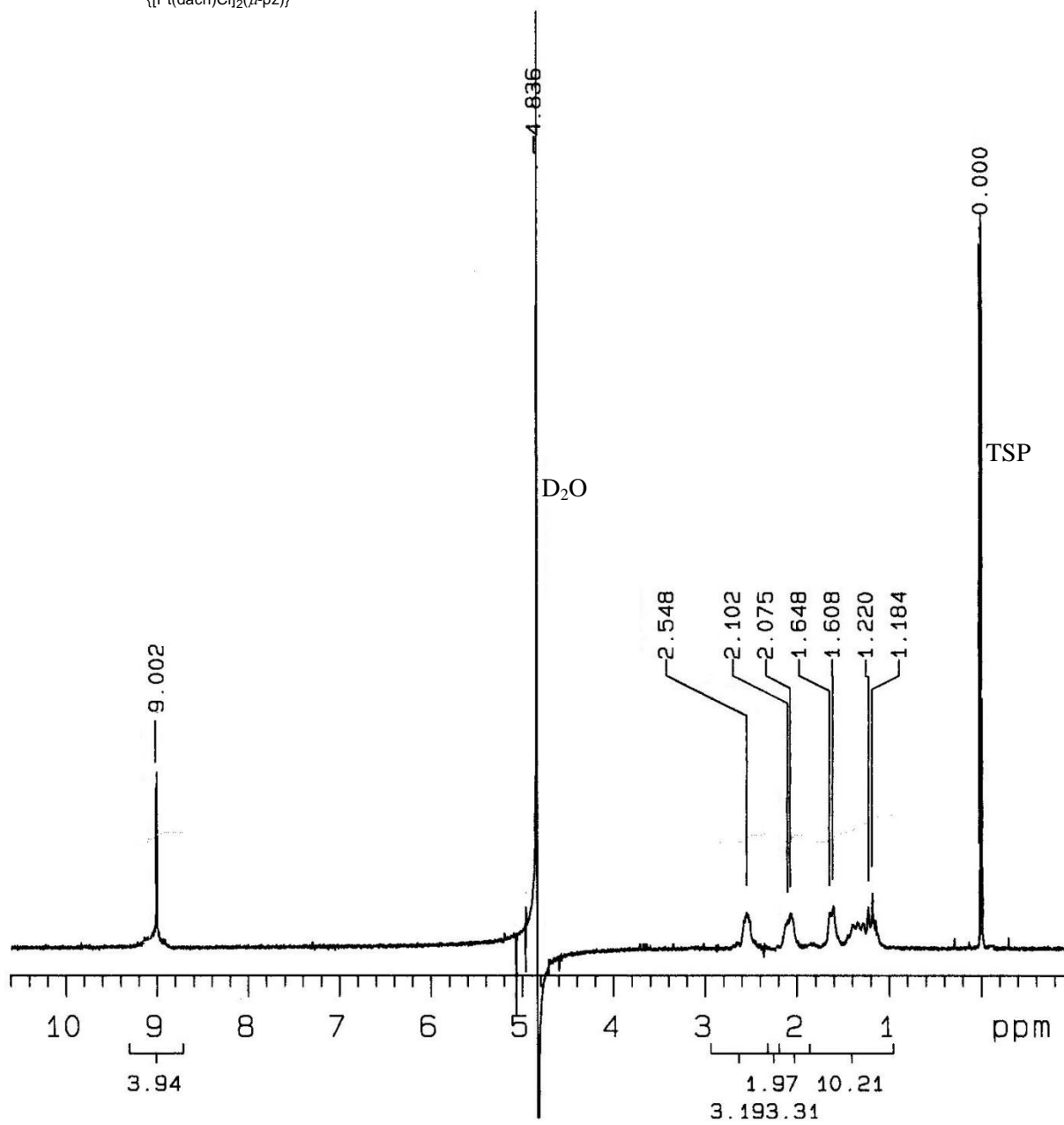
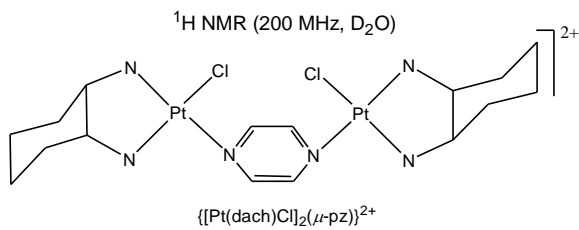


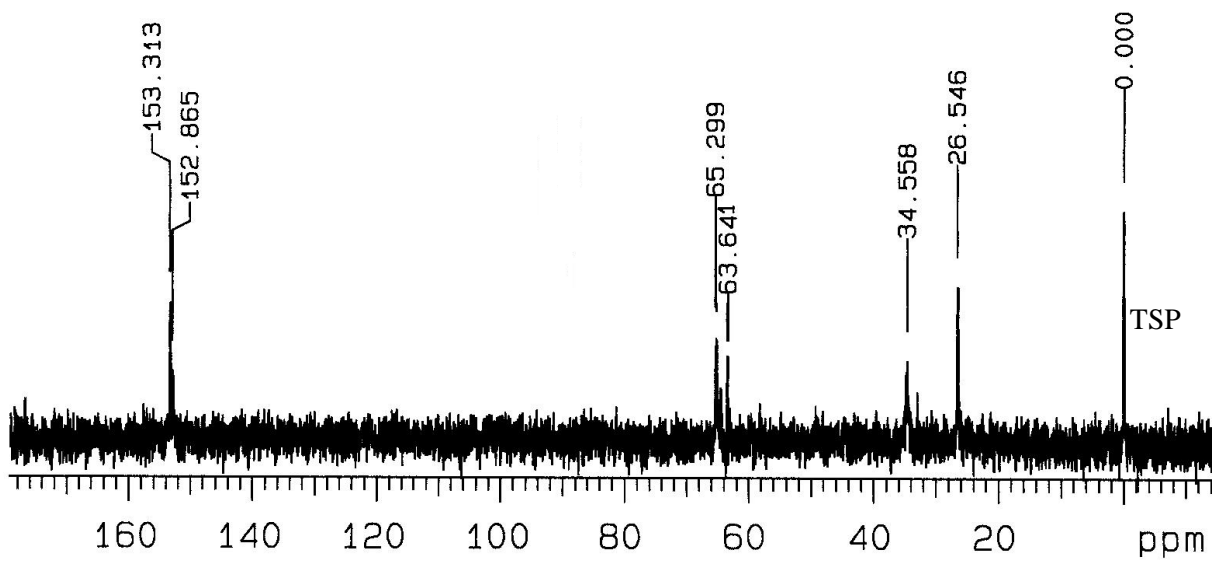
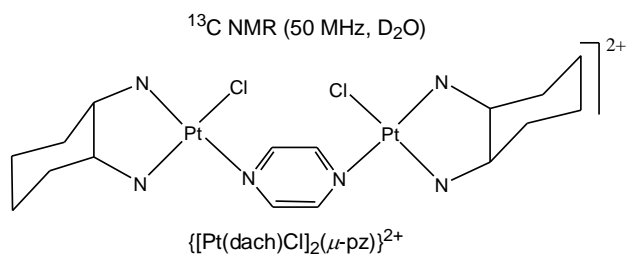




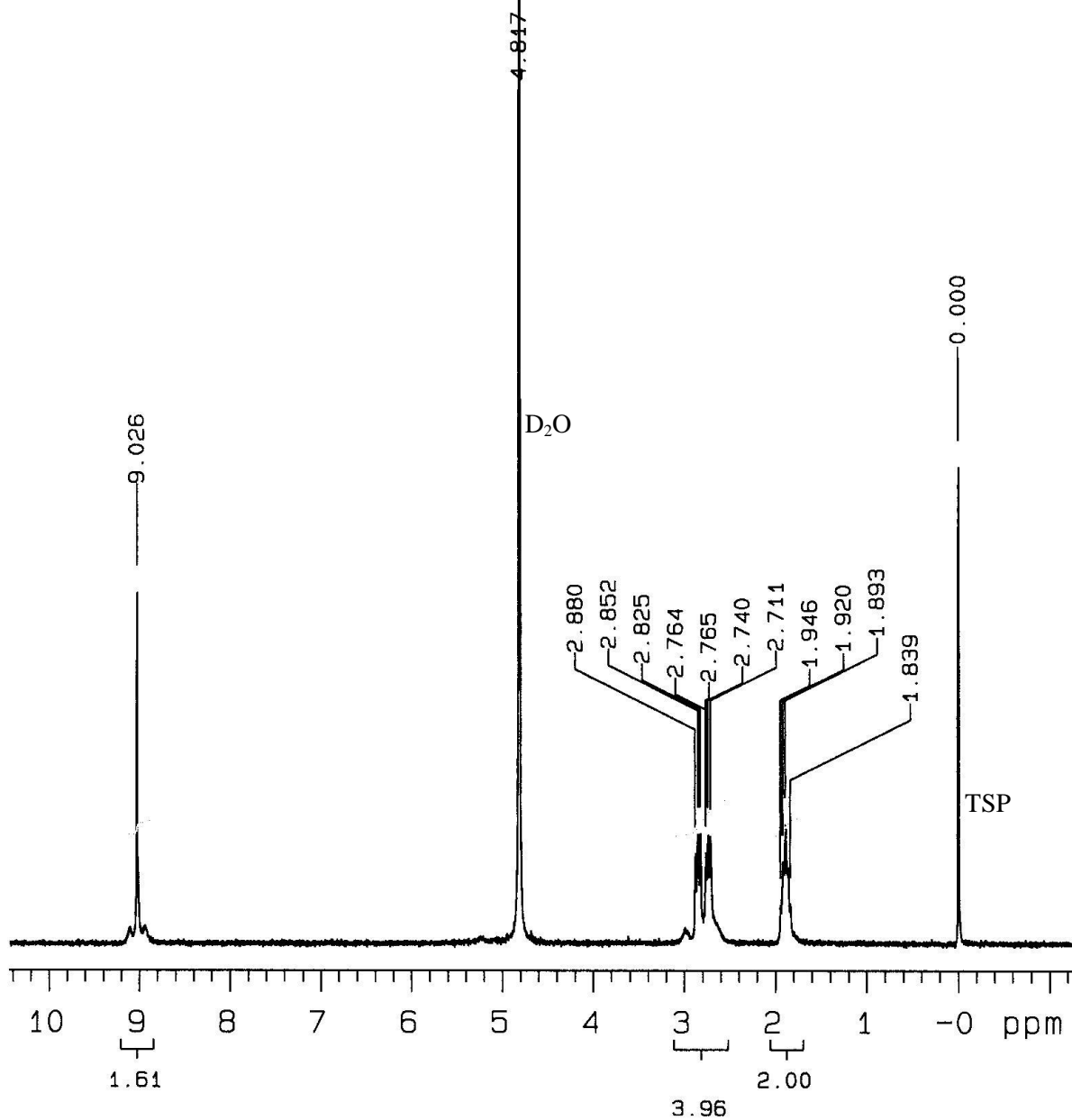
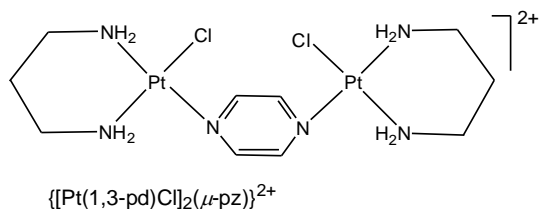




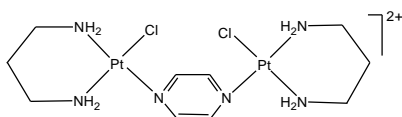




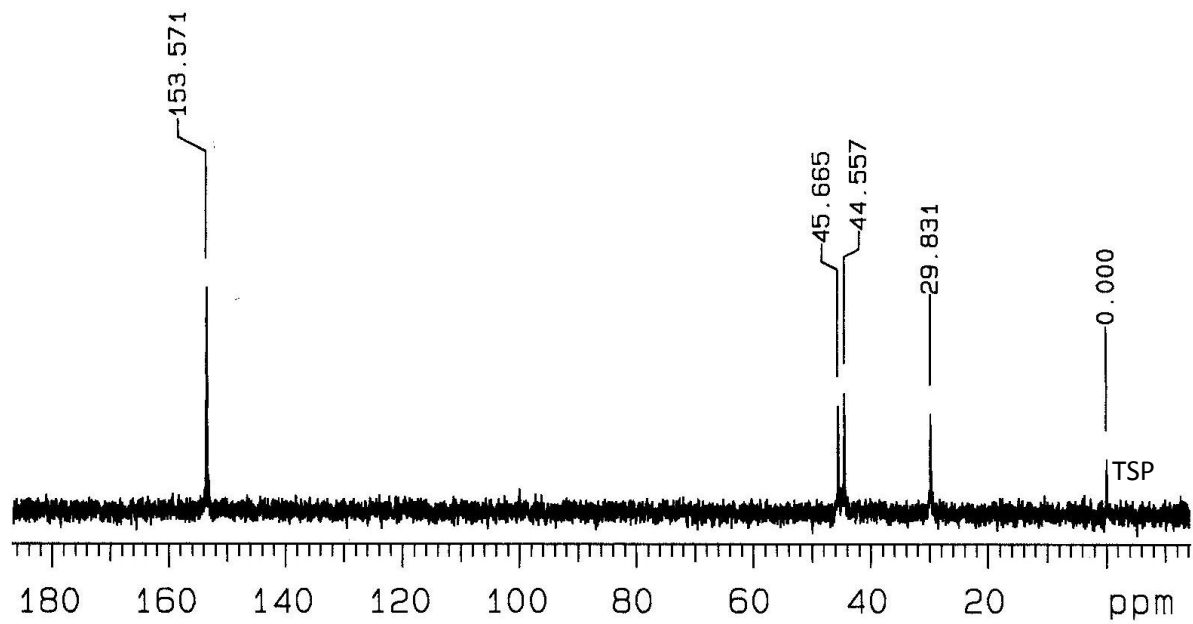
$^1\text{H}$  NMR (200 MHz,  $\text{D}_2\text{O}$ )

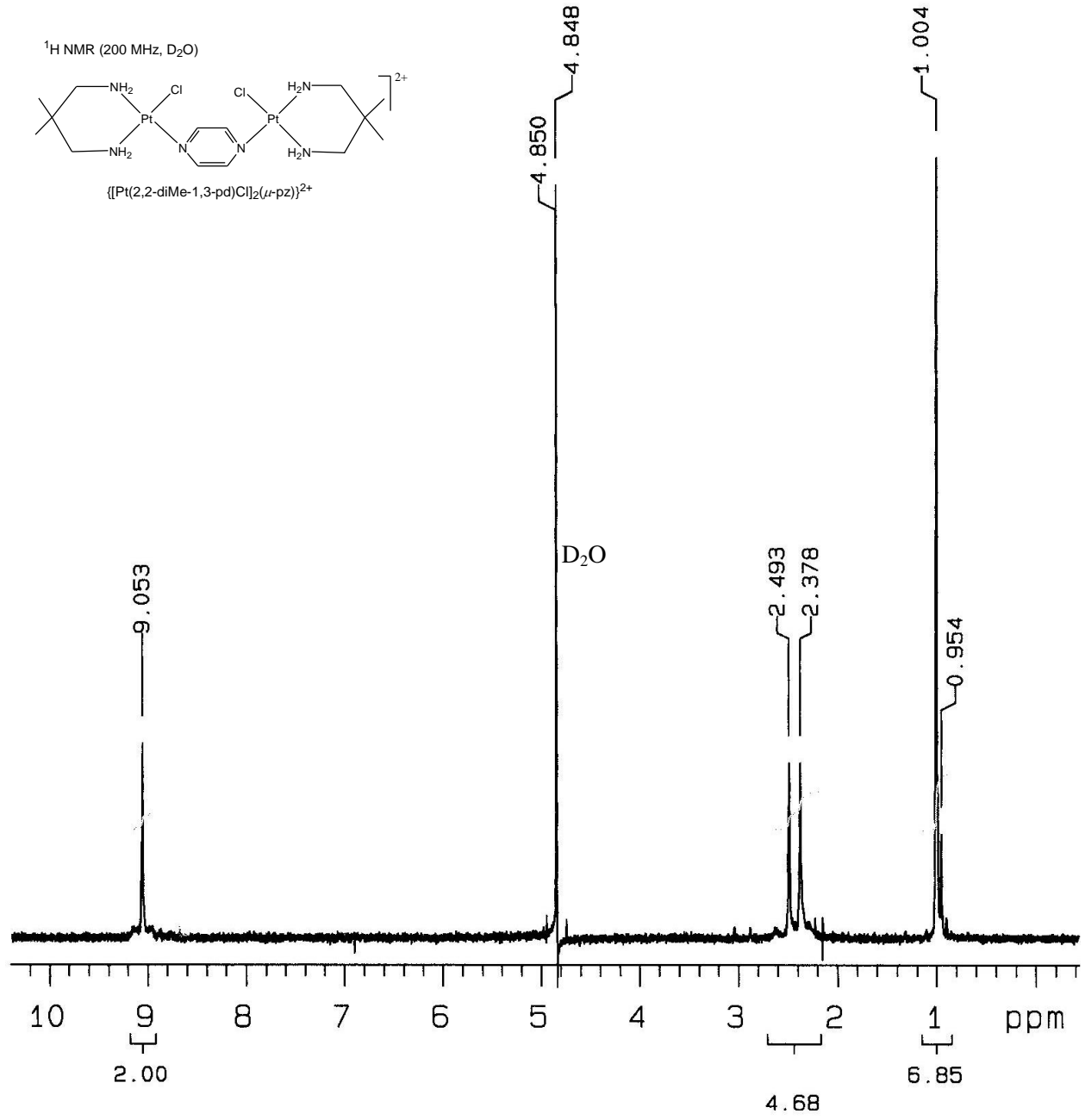


<sup>13</sup>C NMR (50 MHz, D<sub>2</sub>O)

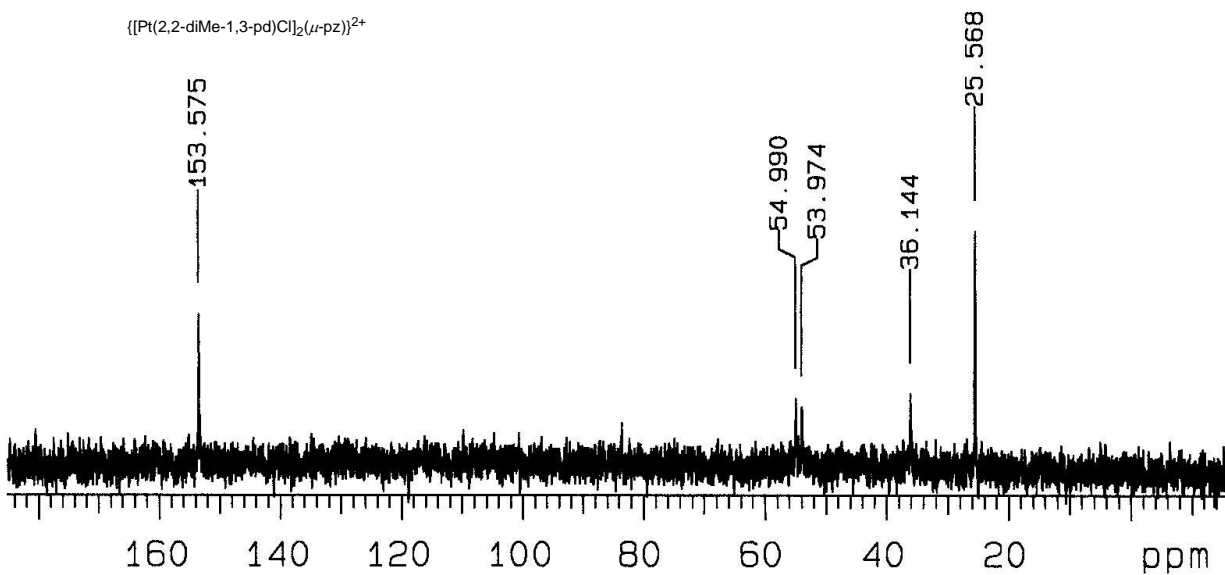
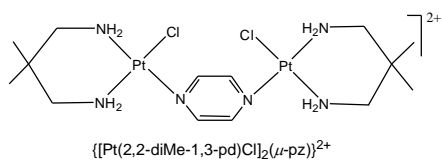


$\{[Pt(1,3-pd)Cl]_2(\mu-pz)\}^{2+}$

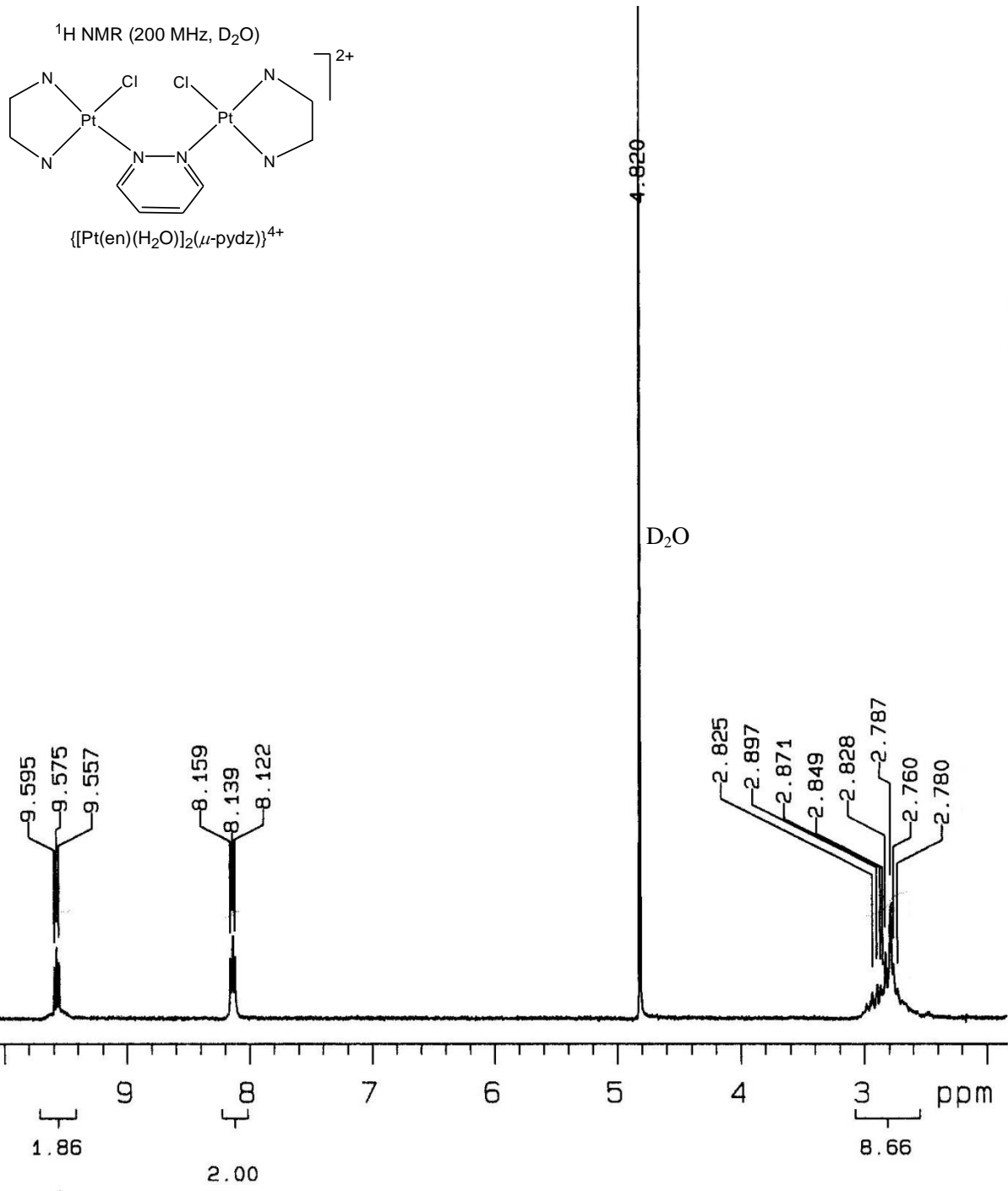


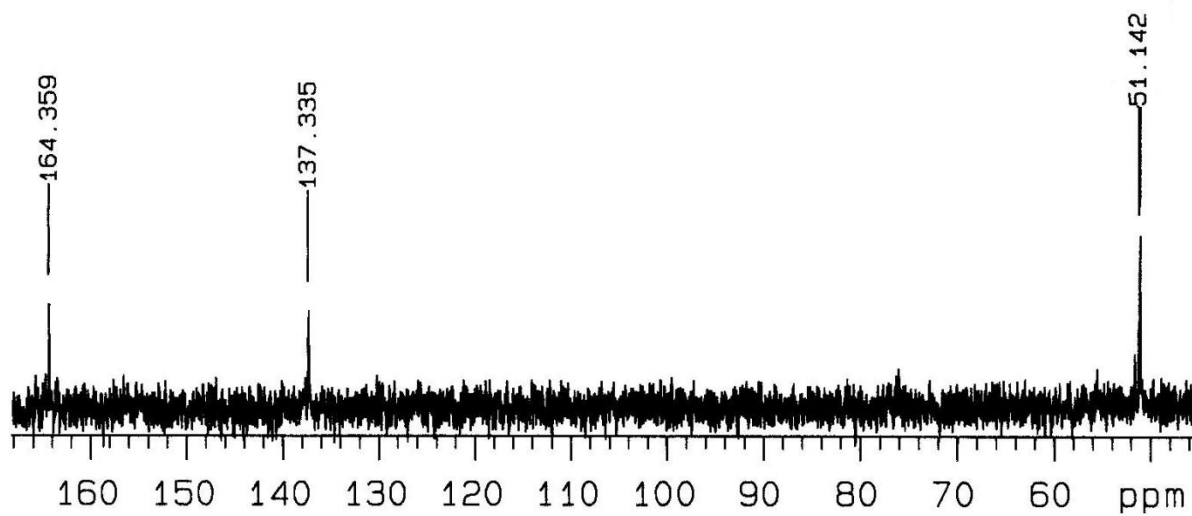
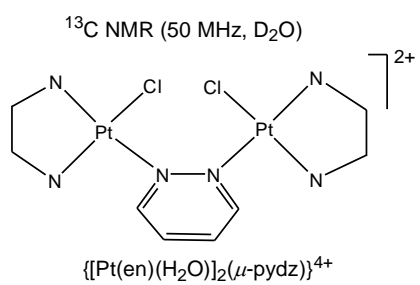


$^{13}\text{C}$  NMR (50 MHz,  $\text{D}_2\text{O}$ )









**Table S1.** Lethal and teratogenic effects observed in zebrafish (*Danio rerio*) embryos at different hours post fertilization (hpf).

Category	Developmental endpoints	Exposure time			
		24 h	48 h	72 h	96 h
Lethal effect	Egg coagulation <sup>a</sup>	•	•	•	•
	Tail not detached	•	•	•	•
	No somite formation	•	•	•	•
	No heart-beat		•	•	•
Teratogenic effect	Malformation of head	•	•	•	•
	Malformation of eyes <sup>b</sup>	•	•	•	•
	Malformation of sacculi/otoliths <sup>c</sup>	•	•	•	•
	Malformation of chorda	•	•	•	•
	Malformation of tail <sup>d</sup>	•	•	•	•
	Scoliosis	•	•	•	•
	Yolk deformation	•	•	•	•
Growth retardation <sup>e</sup>	•	•	•	•	

<sup>a</sup> No clear organs structure are recognized

<sup>b</sup> Malformation of eyes was recorded for the retardation in eye development and abnormality in shape and size.

<sup>c</sup> Presence of no, one or more than two otoliths per sacculus, as well as reduction and enlargement of otoliths and/or sacculi (otic vesicles).

<sup>d</sup> Tail malformation was recorded when the tail was bent, twisted or shorter than to control embryos as assessed by optical comparison.

<sup>e</sup> Growth retardation was recorded by comparing with the control embryos in development or size (before hatching, at 24 hpf and 48 hpf) or in a body length (after hatching, at and onwards 72 hpf).