

**Solution studies of dinuclear polyamine-linked platinum-based antitumor complexes**

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**Electronic Supplementary Information**

**Model S1.** Scientist equation used to fit the data for the aquation of **1** and **1'**.

// **1** or **1'** + H<sub>2</sub>O

IndVars: T

DepVars: A, B, Cl

Params: KAB, KBA

$A' = -KAB \cdot A + KBA \cdot B \cdot Cl$

$B' = KAB \cdot A - KBA \cdot B \cdot Cl$

$Cl' = KAB \cdot A - KBA \cdot B \cdot Cl$

// A=**1** or **1'**, B=**2** or **2'**, Cl=chloride concentration

// Initial conditions

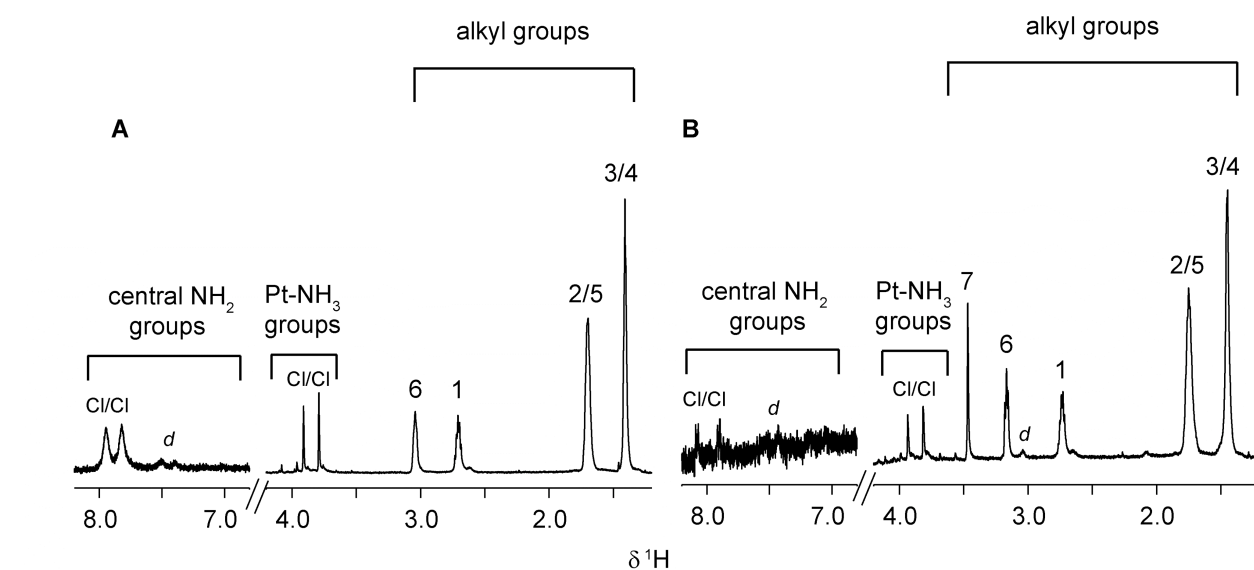
T=0.00

A=[**1** or **1'**]<sub>initial</sub>

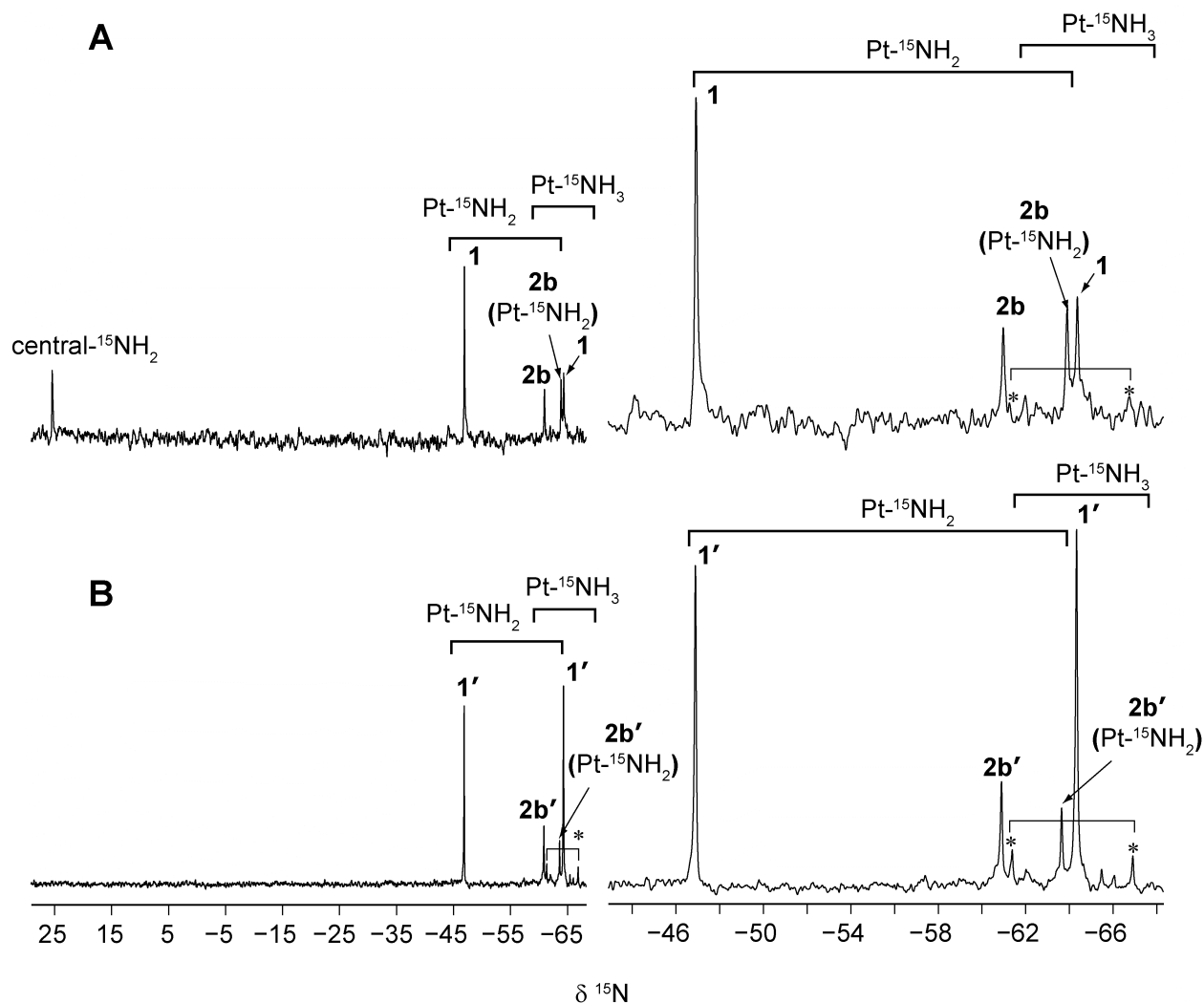
B=0.000

Cl=0.000

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**Fig. S1.**  $^1\text{H}$  NMR spectra of **1** (A) and **1'** (B) at pH 5.4 and 298 K (for numbering scheme see Scheme 1) in 15 mM sodium perchlorate. The chemical shifts for the alkyl  $\text{CH}_2$  groups have been tabulated in Table 3. For the doublet corresponding to the  $\text{Pt-}^{15}\text{NH}_3$  groups of **1** and **1'**  $^1J$  ( $^1\text{H-}^{15}\text{N}$ ) = 72 Hz. The resonance labeled '*d*' corresponds to the terminal end of the dangling amine moiety of a Pt by-product (see main text). The equivalent peak for **1** is concealed beneath the resonance corresponding to the protons of  $\text{C}_6$  group in the alkyl linker. The central  $\text{NH}_2$  groups for **1'** are diminished in intensity due to exchange with the bulk water; the signal has been shown at a lower threshold for clarity. The  $\text{Pt-}^{15}\text{NH}_2$  groups are concealed underneath the residual  $^1\text{H}_2\text{O}$  resonance, which has been omitted for clarity.



**Fig. S2.**  $^{15}\text{N}$  { $^1\text{H}$ } DEPT NMR spectra of **1** (A) and **1'** (B) (15 mM sodium phosphate, pH 5.4, 298 K) shown on the same  $\delta$   $^{15}\text{N}$  scale – the spectra shown on the right are expansions of the region  $\sim \delta$  -45 to -66 ppm. Key (see Scheme 2): **1/1'**, dichloro species; **2b/2b'**, {PtN<sub>3</sub>O} end of the monoaqua monochloro species. The {PtN<sub>3</sub>Cl} moiety of the monoaqua monochloro species, **2a/2a'**, is concealed beneath the corresponding dichloro species, **1/1'**; see text. Peaks labeled '\*' are  $^{195}\text{Pt}$  satellites ( $^1J(^{195}\text{Pt}-^{15}\text{N}) = 334$  Hz) of the dichloro species, **1/1'**.