Supporting Information

Determination of the Kinetic Profile of a Dinuclear Platinum Anticancer Complex in the Presence of Sulfate: Introducing a New Tool for the Expedited Analysis of 2D [$^1$H, $^{15}$N] HSQC NMR Spectra.

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Model S1. Scientist equation used to fit the data for the aquation of 1 in the presence of sulfate.

// Micromath Scientist Model File
// 1,1/t,t in 15 mM sodium sulfate
IndVars: T
DepVars: A, B, Cl, C, S
Params: KAB, KBA, KBC, KCB
A'=-KAB*A+KBA*B*Cl
B'=KAB*A-KBA*B*Cl-KBC*B*S+KCB*C
C'=KBC*B*S-KCB*C
Cl'=KAB*A-KBA*B*Cl
S'=-KBC*B*S+KCB*C
//A = 1,1/t,t, B = aqua, C = sulfato, S = sulfate concentration, Cl = chloride concentration
// Initial Conditions
T=0.0
A=0.001772
B=0.0
C=0.0
Cl=0.0
S=0.015
Figure S1. The '2D NMR Analysis' pop-up window that appears when loaded in ImageJ.
Figure S2. A snapshot of a 'stack' created using '2D NMR Analysis' for the aquation of 1 in the presence of 15 mM sulfate. Key: I: Pt-Cl, II: Pt-OH₂, III: Pt-SO₄. The roman numerals correspond to the mononuclear derivative of 1,1/t,t, [trans-Pt(NH₃)₃(NH₂(CH₂)₆NH₂)₂]ⁿ⁺ where Y represents any other ligand. Peaks labeled 'i' are impurities from the ¹⁵N-synthesis of 1,1/t,t and '†' are Pt satellites.
Figure S3. Plots of the time dependence of the species observed for the aquation of 1 in the presence of sulfate (15 mM, 298 K, pH 5.4) according to the kinetic model shown in Scheme 1 with data derived using '2D NMR Analysis' (A) and XWINNMR (B). Concentrations were calculated based on the mononuclear \([\text{trans-Pt(NH}_3)_2\text{(NH}_2\text{CH}_2\text{CH}_2\text{NH}_2)Y}]^{n+}\) species (see main text) where Y is any other ligand. Key: I : x; Cl\(^-\) : open circles (○), II : open squares (□); III : open triangles (Δ). The derived rate constants, \(k_\text{H}, k_\text{H}, k_\text{L}\) and \(k_\text{L}\) (see Scheme 2 and Table 2), were identical in both cases.