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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Contents:

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

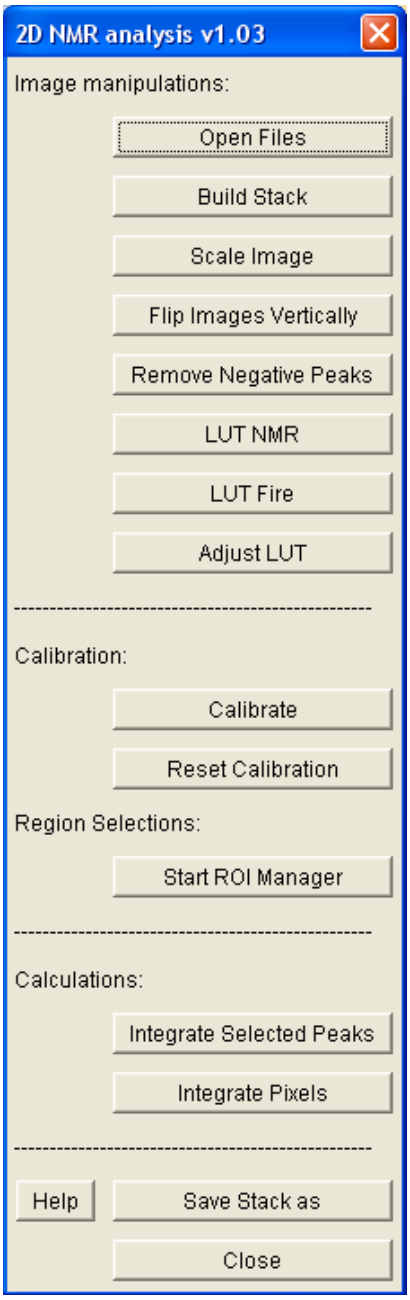

Figure S1. The '2D NMR Analysis' pop-up window that appears when loaded in ImageJ.

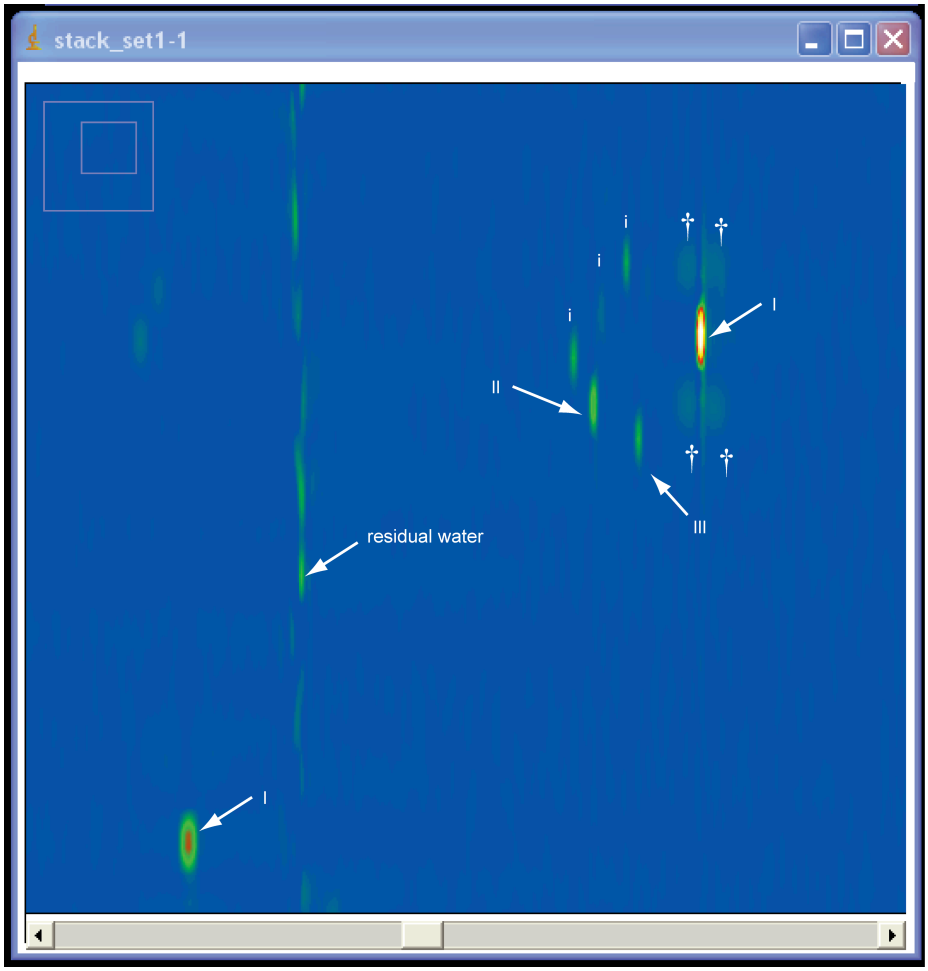

Figure S2. A snapshot of a 'stack' created using '2D NMR Analysis' for the aquation of **1** in the presence of 15 mM sulfate. Key: **I**: Pt-Cl, **II**: Pt-OH_2, **III**: Pt-SO_4. The roman numerals correspond to the mononuclear derivative of 1,1/*t*,*t*, [*trans*-$Pt(NH_3)_2(NH_2(CH_2)_6NH_2)Y]^{n+}$ where Y represents any other ligand. Peaks labeled 'i' are impurities from the ^{15}N-synthesis of 1,1/*t*,*t* and '†' are Pt satellites.

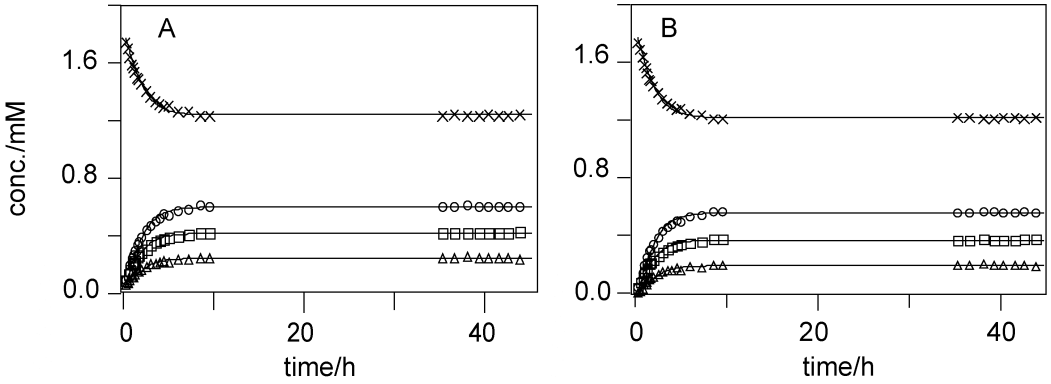

Figure S3. Plots of the time dependence of the species observed for the aquation of **1** in the presence of sulfate (15 mM, 298 K, pH 5.4) according to the kinetic model shown in Scheme 1 with data derived using '2D NMR Analysis' (A) and XWINNMR (B). Concentrations were calculated based on the mononuclear [*trans*-$Pt(NH_3)_2(NH_2(CH_2)_6NH_2)Y]^{n+}$ 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_H, k_{-H}, k_L and k_{-L} (see Scheme 2 and Table 2), were identical in both cases.