Supplementary Material (ESI) for Dalton Transactions

Influence of amine ligands on the aquation and cytotoxicity of *trans* diamine platinum(II) anticancer complexes

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Supplementary Information

Fig. S1**:** Plots of the time dependence of species in the aquation of ^{15}N-**2** and -**3**

Scientist models

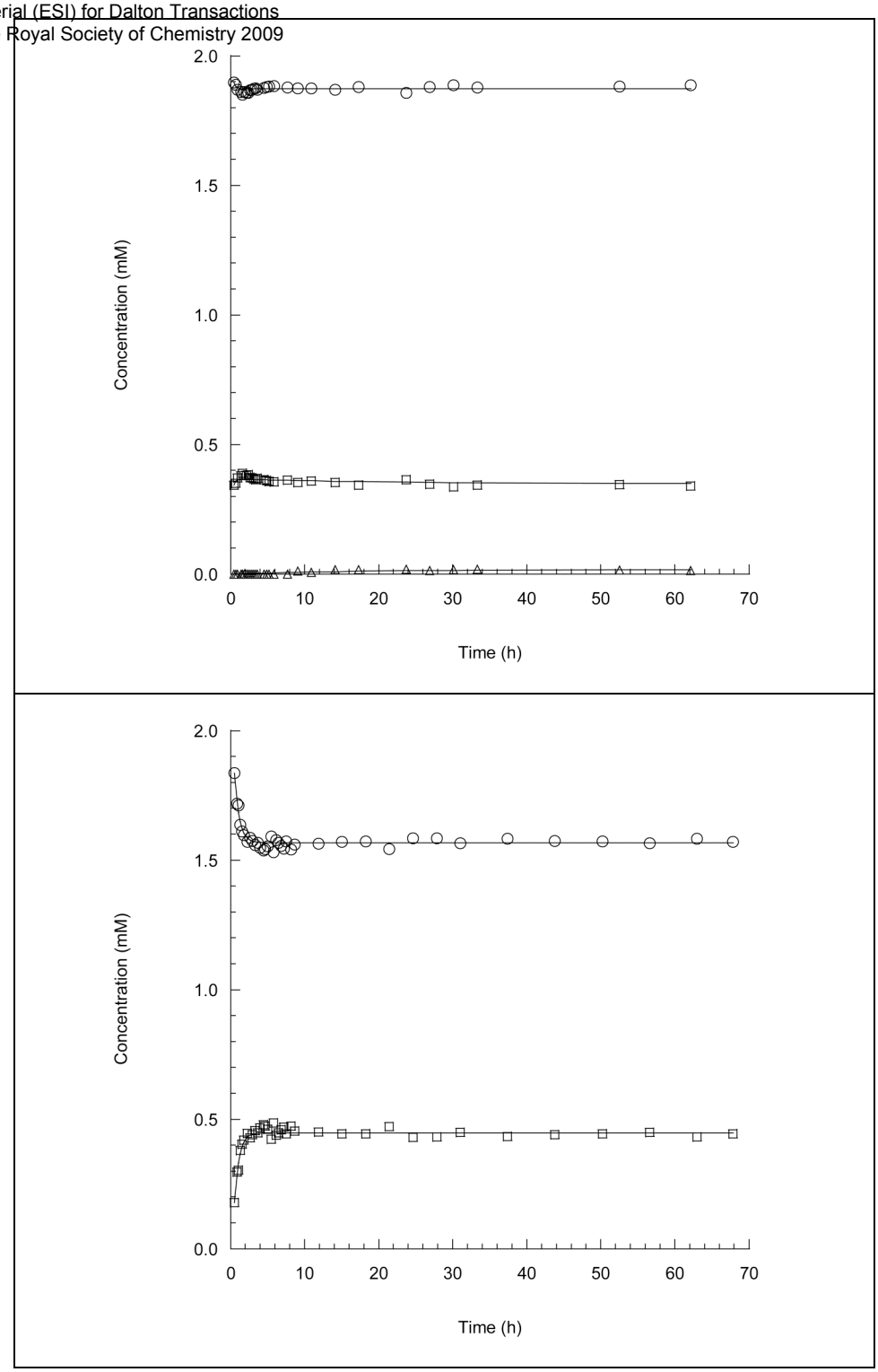

Fig S1. Plots of the time dependence of species in the aquation of (top) ^{15}N-**2** (pH 4.8) and bottom ^{15}N-**3** (pH 4.2), in 100 mM $NaClO_4$ (90% H_2O/10% D_2O) at 298 K. Labels: dichlorido, circles; monoaqua, squares; diaqua, triangles. The curves are computer best fits to the model shown in Scheme 1 and the rate constants are tabulated in Table 3.

Scientist Model:

Aquation of **1** (2.73 mM pH 4.4) and **2** (2.24 mM pH 4.2) in 100 mM $NaClO_4$, 298K

```
//MicroMath Scientist Model File
//Complex 1 hydrolysis second order reverse - equilibrium both aquation steps
IndVars: T
DepVars: A, B, C, Cl
Params: KAB, KBA, KBC, KCB
A'=-KAB*A+KBA*B*Cl
B'=KAB*A-KBA*B*Cl-B*KBC+C*KCB*Cl
C'=B*KBC-C*KCB*Cl
Cl'=KAB*A-KBA*B*Cl+B*KBC-C*KCB*Cl
//A= 1, B=aqua/Cl, C=diaqua, Cl=chloride
//Initial Conditions
T=1591
A=0.00249
B=0.00023987
C=0.0
Cl=0.00023987
***
```

Scientist Model:

Aquation of **3** (2.02 mM pH 4.2) in 100 mM $NaClO_4$, 298K

```
//MicroMath Scientist Model File
//Complex 3 hydrolysis pseudo first order reverse – first equilibrium step
IndVars: T
DepVars: A, B, Cl
Params: KAB, KBA
A'=-KAB*A+KBA*B*Cl
B'=KAB*A-KBA*B*Cl
Cl'=KAB*A-KBA*B*Cl
// A=3, B=aqua/Cl, Cl=chloride
// Initial Conditions
T=1818
A=0.0018364
B=0.00017861
Cl=0.00017861
***
```