

Supporting Information - Combining the platinum(II) drug candidate kiteplatin with 1,10-phenanthroline analogues

Benjamin J. Pages,^a Jennette Sakoff,^b Jayne Gilbert,^b Yingjie Zhang,^c James D. Hoeschele,^d Sharon M. Kelly,^e and Janice R. Aldrich-Wright.*^a

^a *Nanoscale Organisation and Dynamics Group, Western Sydney University, Campbelltown, NSW 2560, Australia*

^b *Calvary Mater Newcastle, Waratah, NSW 2298, Australia*

^c *Australian Nuclear Science and Technology Organisation, Locked Bag 2001, Kirrawee DC, NSW 2232, Australia*

^d *Department of Chemistry, Eastern Michigan University, Ypsilanti, MI 48197, USA*

^e *Institute of Molecular, Cell and Systems Biology, College of Medical, Veterinary and Life Sciences, University of Glasgow, Glasgow, G128QQ, United Kingdom.*

Table of Contents

Section S1 – UV Spectra	1
Section S2 – NMR Spectra.....	3
S2.1. ¹ H Spectra.....	3
S2.2. ¹ H- ¹⁹⁵ Pt HMQC spectra.....	4
Section S3 – ITC Data.....	5

Section S1 – UV Spectra

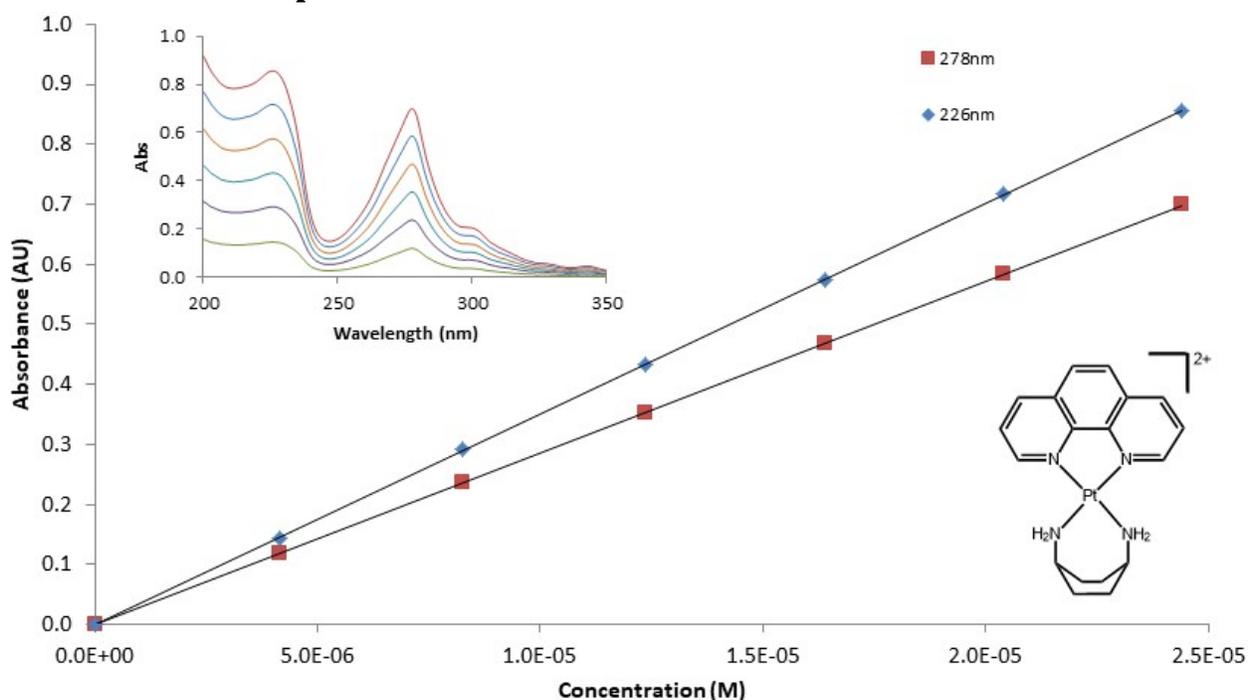


Figure S1.1. Standard absorbance plot of complex 1, obtained from the titration of the complex into water. Inset: the absorbance spectra recorded over the course of titrations.

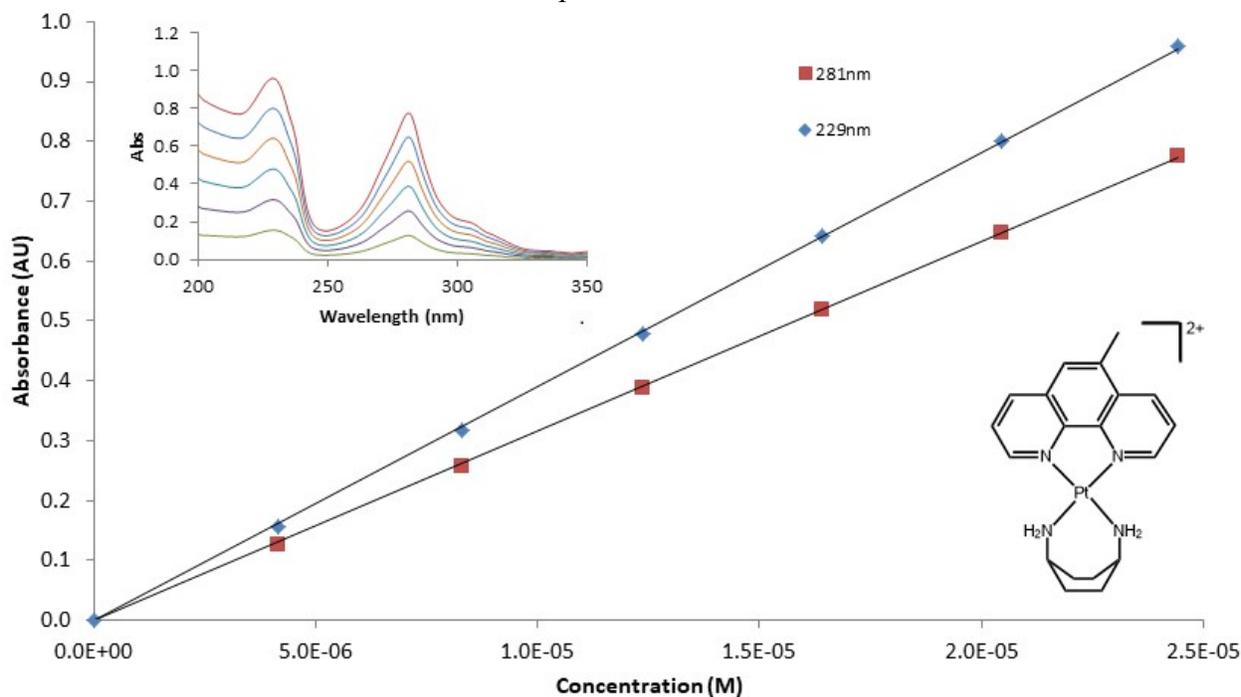


Figure S1.2. Standard absorbance plot of complex 2, obtained from the titration of the complex into water. Inset: the absorbance spectra recorded over the course of titrations.

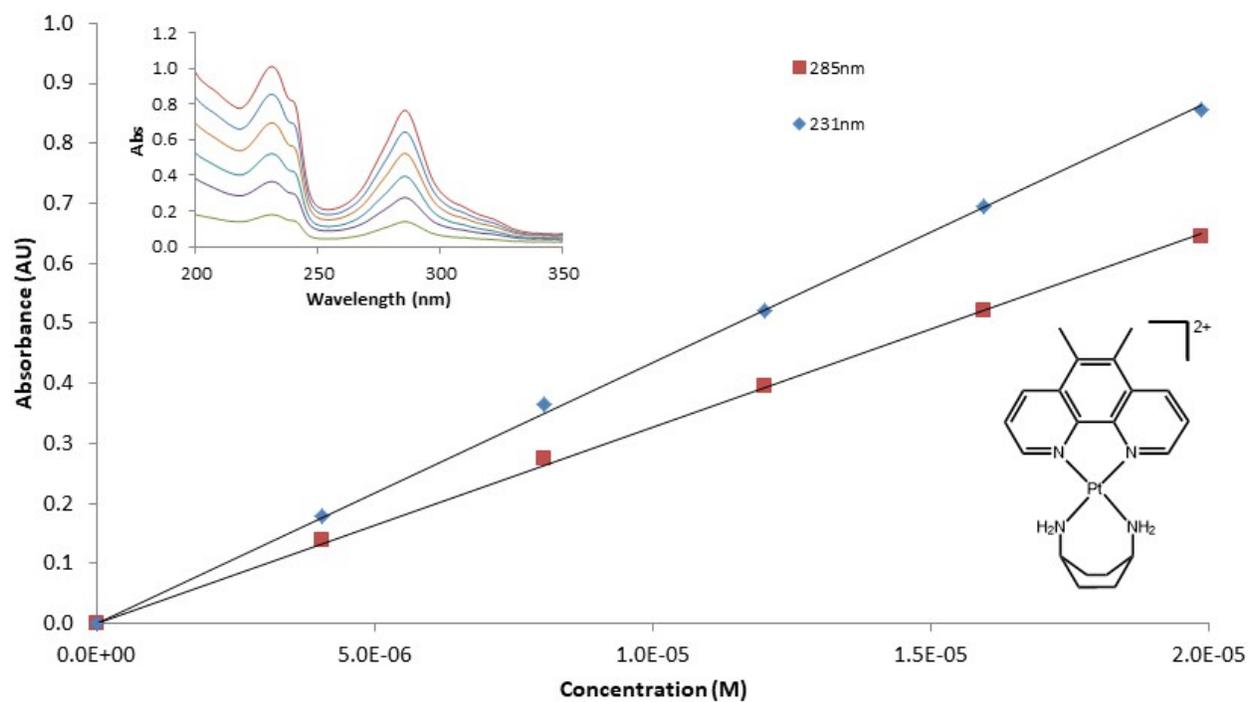


Figure S1.2. Standard absorbance plot of complex **3**, obtained from the titration of the complex into water. Inset: the absorbance spectra recorded over the course of titrations.

Section S2 – NMR Spectra

S2.1. ^1H Spectra

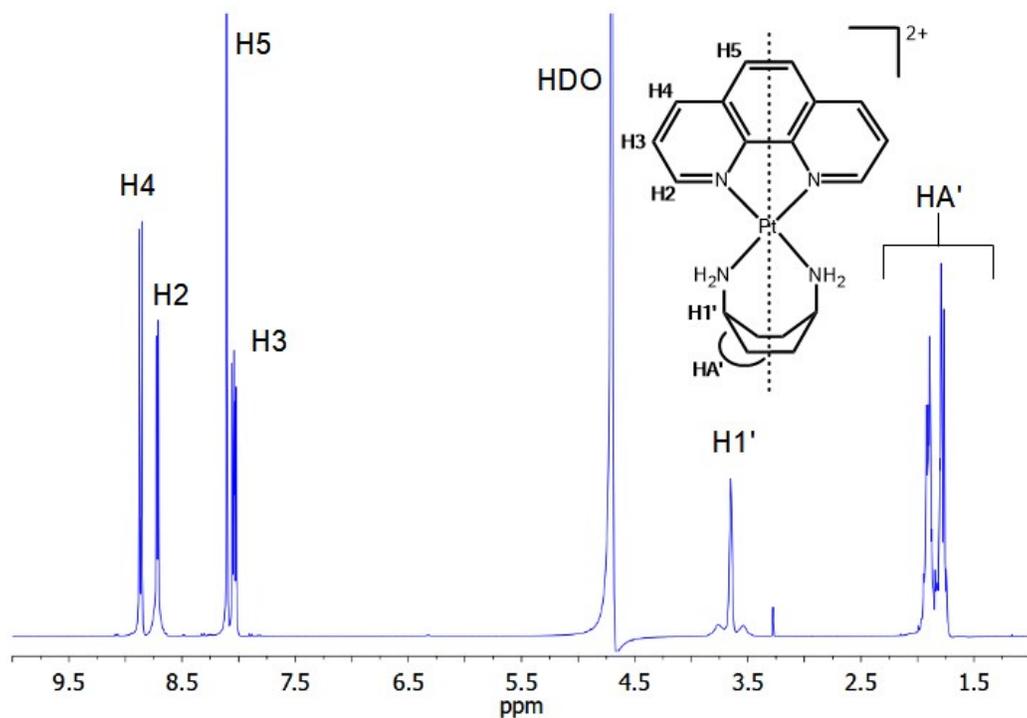


Figure S2.1.1. The ^1H NMR spectrum of Complex 1 in D_2O , showing proton labels.

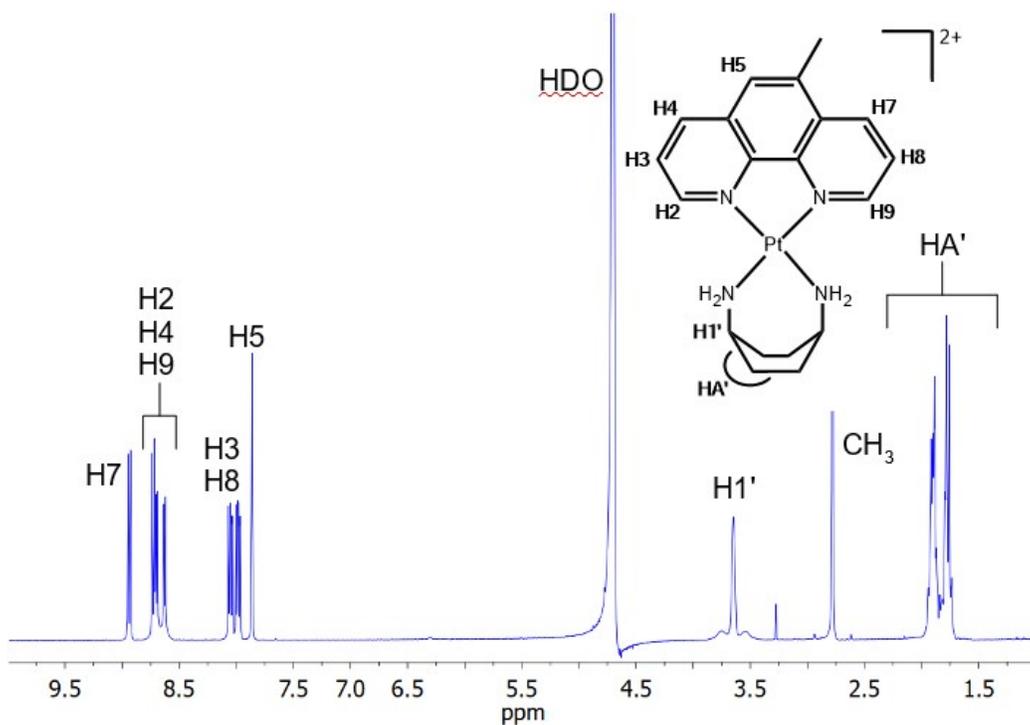


Figure S2.1.2. The ^1H NMR spectrum of Complex 2 in D_2O , showing proton labels.

S2.2. ^1H - ^{195}Pt HMQC spectra

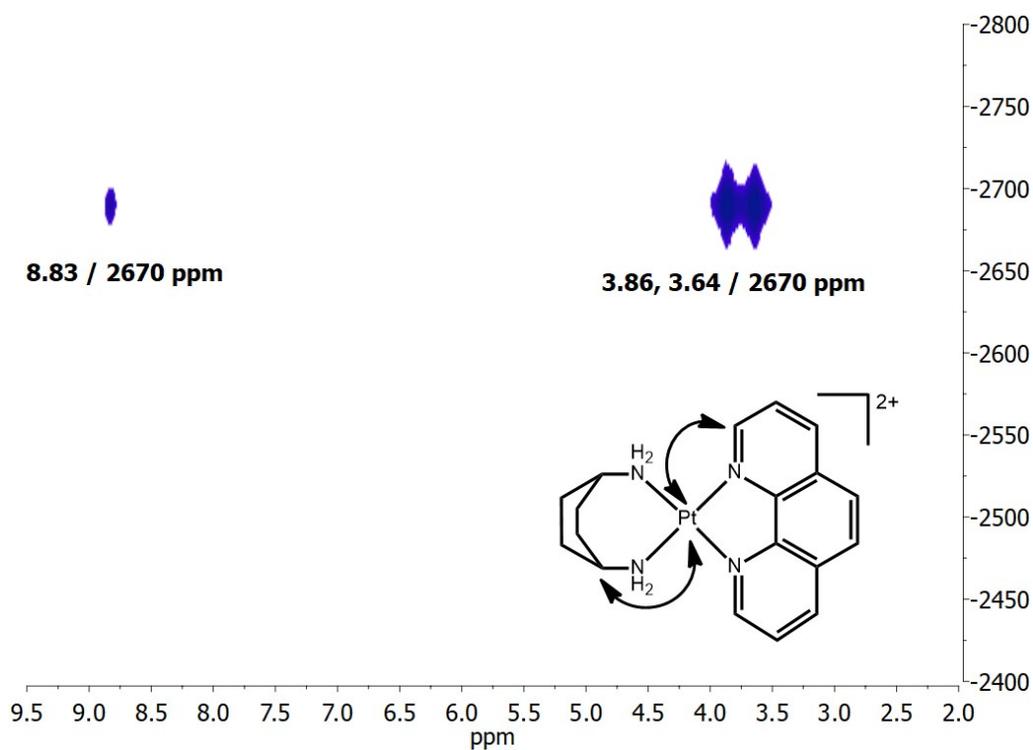


Figure S2.2.1. The ^1H - ^{195}Pt HMQC spectrum of complex **1** in D_2O , showing cross-peaks.

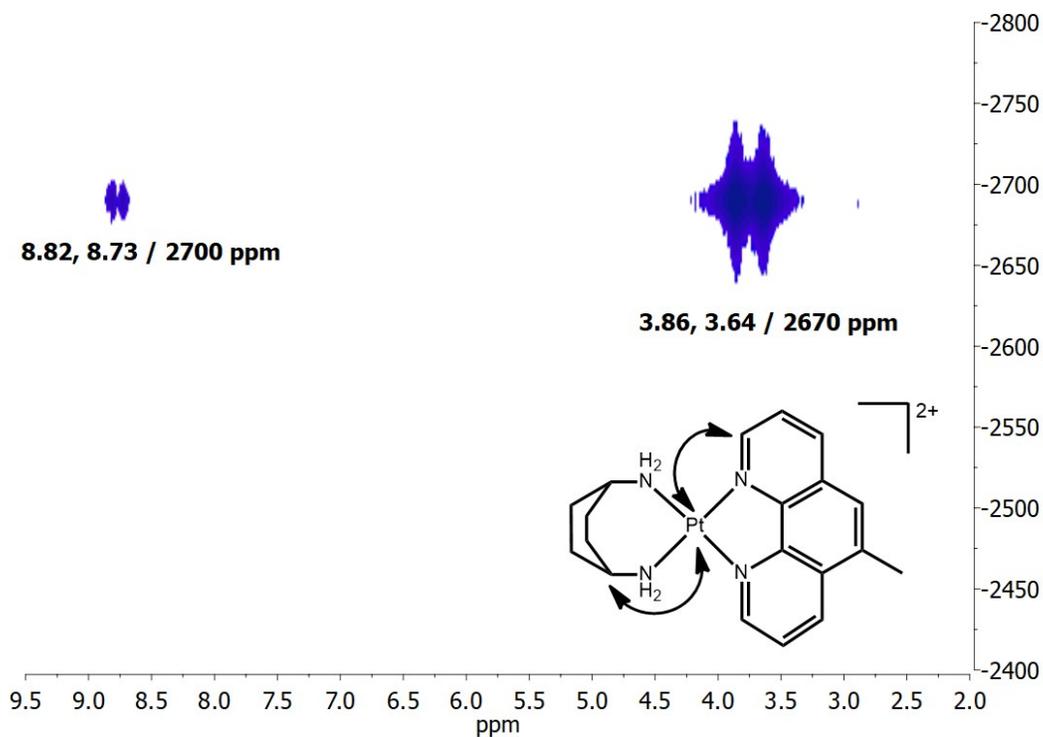


Figure S2.2.2. The ^1H - ^{195}Pt HMQC spectrum of complex **2** in DMSO-d_6 , showing cross-peaks.

Section S3 - ITC Data

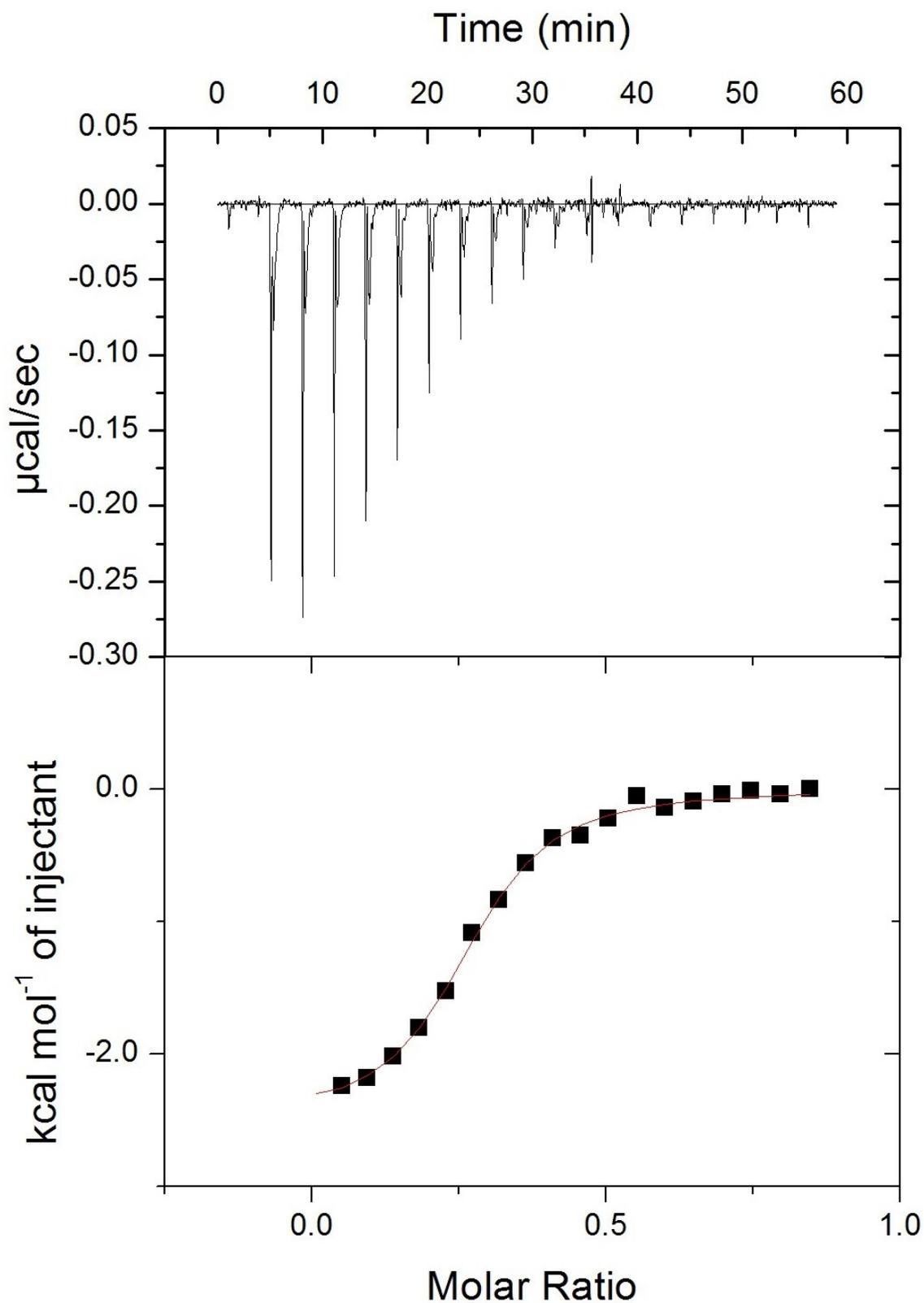


Figure S3.1. ITC trace and binding curve of the titration of PHENKITE or complex **1** ($750 \mu\text{M}$) into CT-DNA ($160 \mu\text{M}$). Fits were obtained using a one-site binding model.

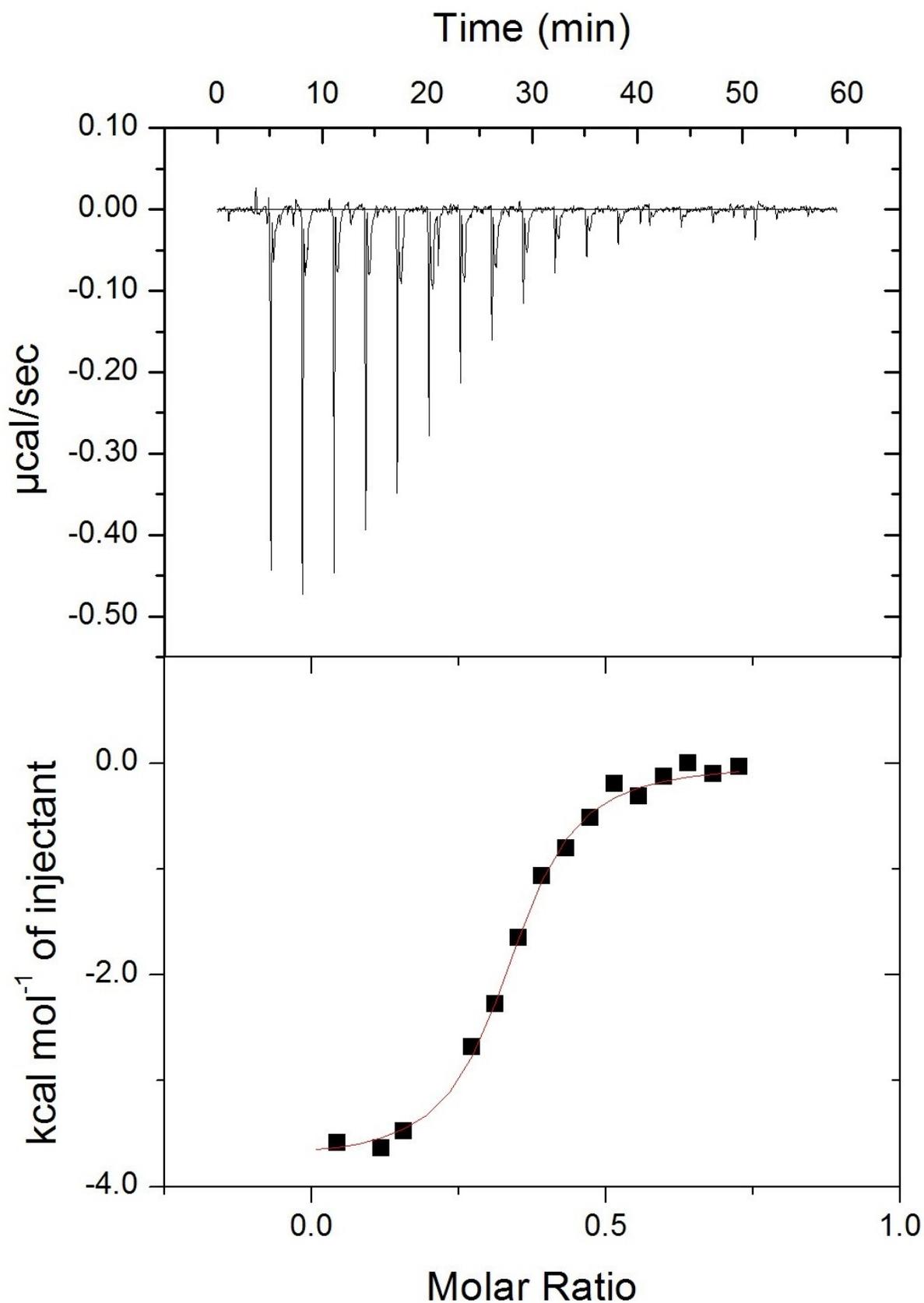


Figure S3.2. ITC trace and binding curve of the titration of 5KITE or complex 2 (600 μM) into CT-DNA (160 μM). Fits were obtained using a one-site binding model.

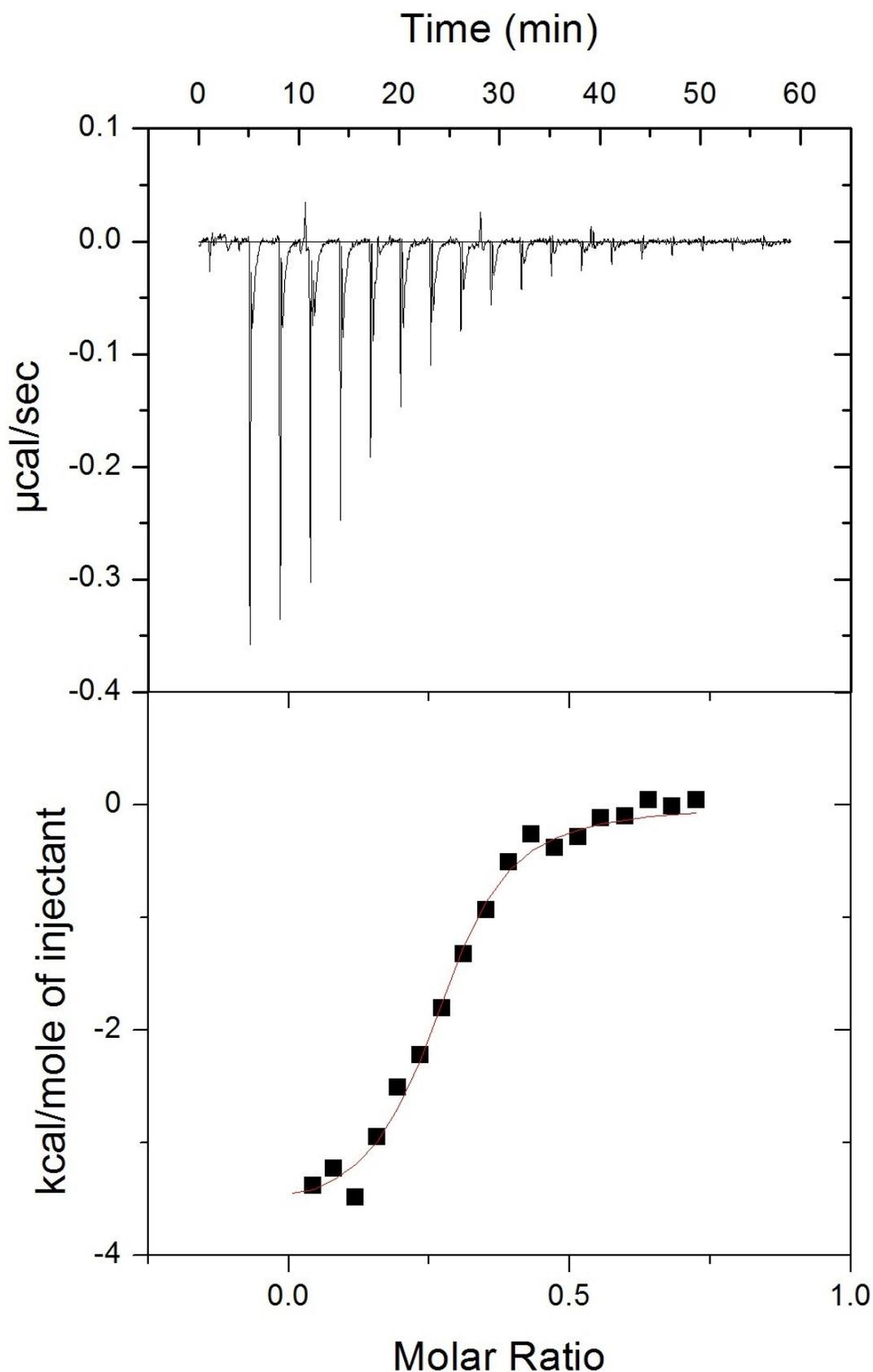


Figure S3.3. ITC trace and binding curve of the titration of 5MESS chloride or complex **5** (600 μM) into CT-DNA (160 μM). Fits were obtained using a one-site binding model.

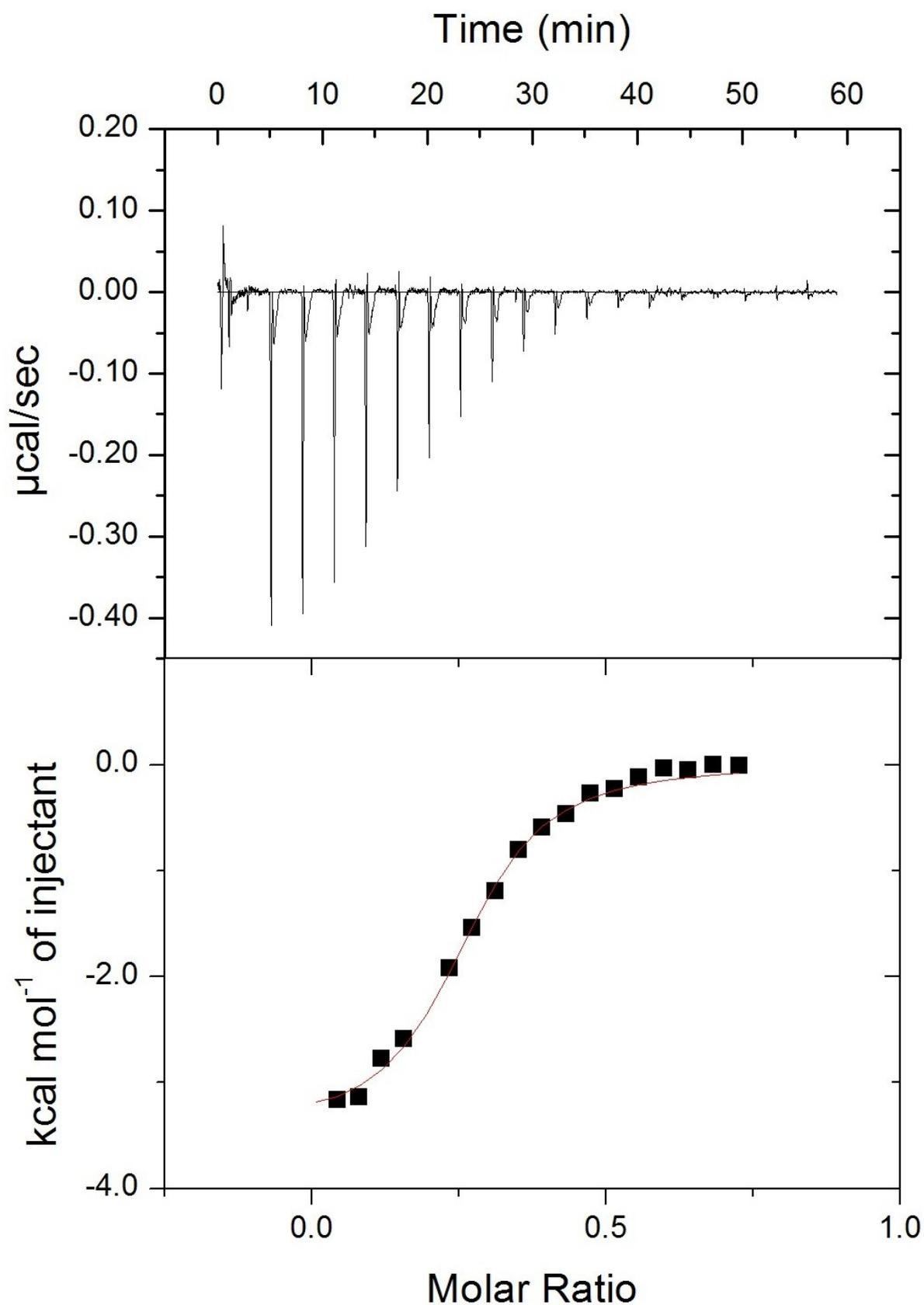


Figure S3.4. ITC trace and binding curve of the titration of 5MESS nitrate or complex **5a** ($600 \mu\text{M}$) into CT-DNA ($160 \mu\text{M}$). Fits were obtained using a one-site binding model.