

Supplementary information

The death of the Job plot, transparency, open science and online tools, uncertainty estimation methods and other developments in supramolecular chemistry data analysis

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Results from fitting case study data (Tables 1-2):

The raw input data, the calculated fit, basic statistical information and associated information can be accessed via the www.supramolecular.org¹ database through the below unique URL: (copy-paste into a web-browser)

Table 1 data:

i) Results for 1:2 full Model:

<http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be>

ii) Results for noncooperative model:

<http://app.supramolecular.org/bindfit/view/ea706d9b-74fe-4ae1-a249-116e8087aef5>

iii) Results for additive model:

<http://app.supramolecular.org/bindfit/view/14b6fd08-602a-4829-a593-c300e0014756>

iv) Results for statistical model:

<http://app.supramolecular.org/bindfit/view/b7d25f27-9fb2-4cf8-b486-c27bfacf127a>

Table 2 data:

i) Results for Experiment 1 - 1:2 full Model (same as above in Table 1):

<http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be>

ii) Results for Experiment 2 - 1:2 full Model:

<http://app.supramolecular.org/bindfit/view/7f2321ad-757b-46ae-a6aa-86ec73eddf2b>

iii) Results for Experiment 3 - 1:2 full Model:

<http://app.supramolecular.org/bindfit/view/6280c6ca-f6b0-49b4-9ed7-4c0079c2523a>

Uncertainty calculations and results (Tables 2-3, Figs. 4-6).

All the Matlab m-files (software code) and mat-file (data files) in relations to the Standard Uncertainty (Asymptotic error), Model Comparison method and Monte Carlo calculations presented in Tables 2-3 and Figures 4-6 can be found at this URL (dropbox):

<https://www.dropbox.com/sh/ffxn6d8uie8efn6/AAAgKd7KA6twWREbUwamyS04a?dl=0>

The files are organised into the following folders:

i) *Table2andTable3Figure4_Data:*

Files that relate to the data shown in Table 2, Table 3 and Figure 4:

m-files:

<i>uncertaintyfor1to2example.m</i>	Main file – calculates all the uncertainties.
<i>"nmr1to2fitbindcal.m</i>	called by main file to calculate ycalc.
<i>"nmr1to2fitbind.m</i>	called by main file in the fitting process.
<i>"nmr1to2bbb.m</i>	helper file to solve cubic equations.

^aThese files are essentially identical to related files in the previously published *fittingprogram*.²

mat-files:

<i>CDCI3-CD3CN(1-1)_Mg-(ClO4)2_01.mat</i>	Input data experiment 1.
<i>CDCI3-CD3CN(1-1)_Mg-(ClO4)2_02.mat</i>	Input data experiment 2.
<i>CDCI3-CD3CN(1-1)_Mg-(ClO4)2_03.mat</i>	Input data experiment 3.
<i>mg1process.mat</i>	Output data experiment 1.
<i>mg2process.mat</i>	Output data experiment 2.
<i>mg3process.mat</i>	Output data experiment 3.

ii) *Figure5:*

m-files:

<i>MCfor1to1conc.m</i>	Main file – simulates all the Monte Carlo data.
<i>"nmr1to1fitbindcal.m</i>	called by main file to calculate ycalc.
<i>"nmr1to1fitbind.m</i>	called by main file in the fitting process.
<i>extract1to1MCdata.m</i>	Extracts key data from Monte Carlo results.
<i>plotmcbestka.m</i>	Plots the data in Fig. 5.

^aThese files are essentially identical to related files in the previously published *fittingprogram*.²

mat-files:

MCfor1to1concddata.mat

Output from Monte Carlo simulations (360 Mb!).

iii) *Figure6:*

m-files:

MCfor1to2conc.m

Main file – simulates all the Monte Carlo data.

^nmr1to2fitbindcal.m

called by main file to calculate ycalc.

^nmr1to2fitbind.m

called by main file in the fitting process.

^nmr1to2bbb.m

helper file to solve cubic equations.

extract1to2MCdata.m

Extracts key data from Monte Carlo results.

plotmcbestk1.m

Plots the K_1 (left panel) data in Fig. 6.

plotmcbestk2.m

Plots the K_2 (right panel) data in Fig. 6.

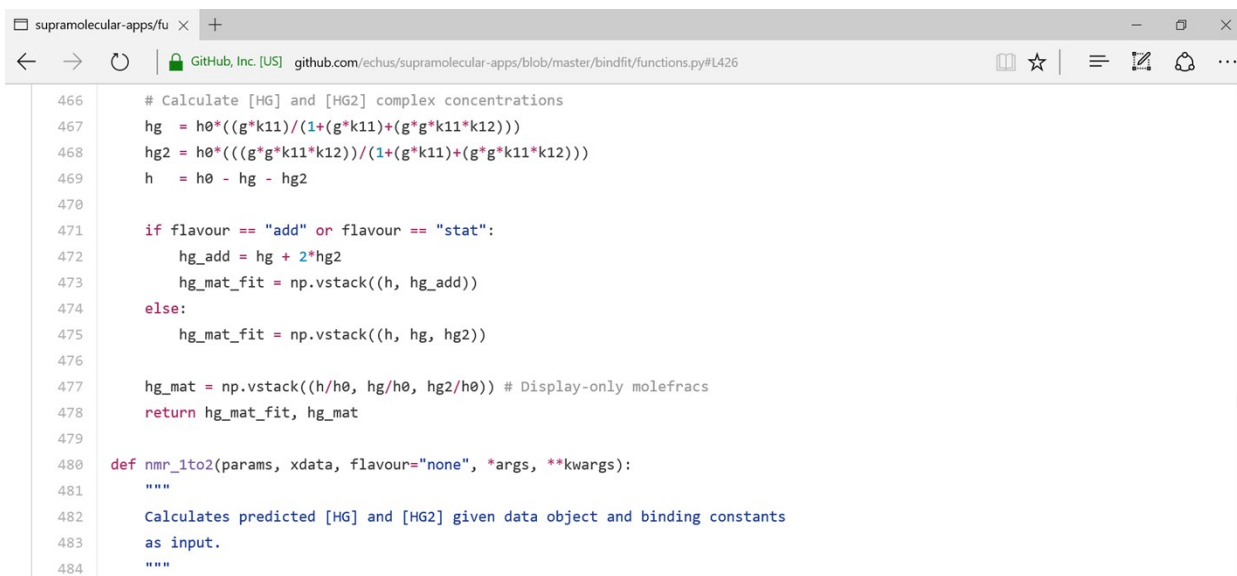
^aThese files are essentially identical to related files in the previously published *fittingprogram*.²

mat-files:

MCfor1to2concddata.mat

Output from Monte Carlo simulations (51 Mb!).

Additional Screenshots from supramolecular.org:

A screenshot of a web browser window displaying a GitHub repository page. The browser's address bar shows the URL: <https://github.com/echus/supramolecular-apps/blob/master/bindfit/functions.py#L426>. The page content shows a snippet of Python code from a file named `functions.py`. The code is as follows:

```
466 # Calculate [HG] and [HG2] complex concentrations
467 hg = h0*((g*k11)/(1+(g*k11)+(g*g*k11*k12)))
468 hg2 = h0*((g*g*k11*k12)/(1+(g*k11)+(g*g*k11*k12)))
469 h = h0 - hg - hg2
470
471 if flavour == "add" or flavour == "stat":
472     hg_add = hg + 2*hg2
473     hg_mat_fit = np.vstack((h, hg_add))
474 else:
475     hg_mat_fit = np.vstack((h, hg, hg2))
476
477 hg_mat = np.vstack((h/h0, hg/h0, hg2/h0)) # Display-only molefracs
478 return hg_mat_fit, hg_mat
479
480 def nmr_1to2(params, xdata, flavour="none", *args, **kwargs):
481     """
482     Calculates predicted [HG] and [HG2] given data object and binding constants
483     as input.
484     """
```

Fig. S1 Screenshot from a small part of the source code for supramolecular.org¹ website on github (supramolecular-apps) at

<https://github.com/echus/supramolecular-apps/blob/master/bindfit/functions.py#L426>

N.b. This url might NOT be permanent – to find the latest url for the source code visit the help->Source code sectin on supramolecular.org website: <http://supramolecular.org/help-and-guides/source-code/>

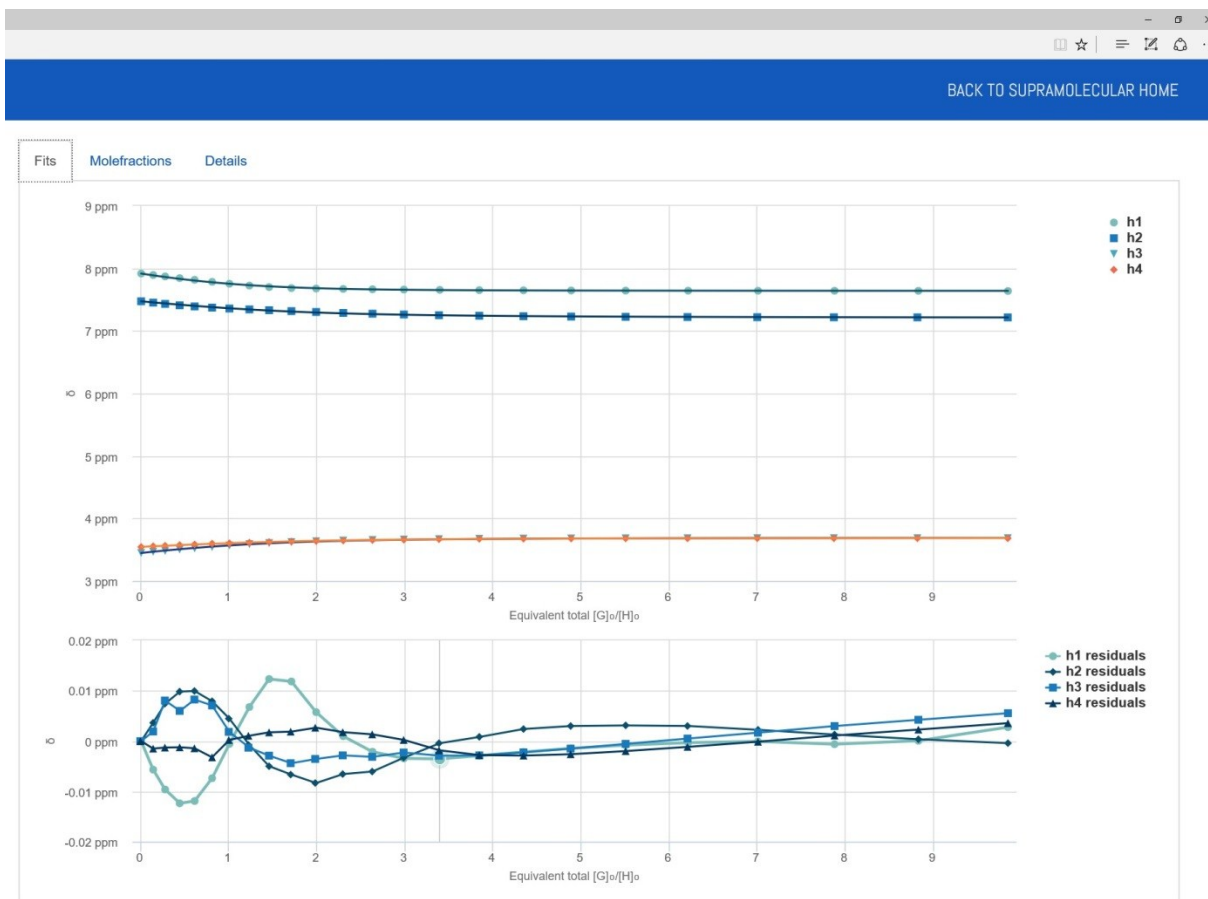


Fig. S2 Screenshot from the result window of *supramolecular.org*¹ from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be> which was fitted to 1:2 NMR binding data. This screenshot shows the raw vs. fitted data (top) and the corresponding residual plot.

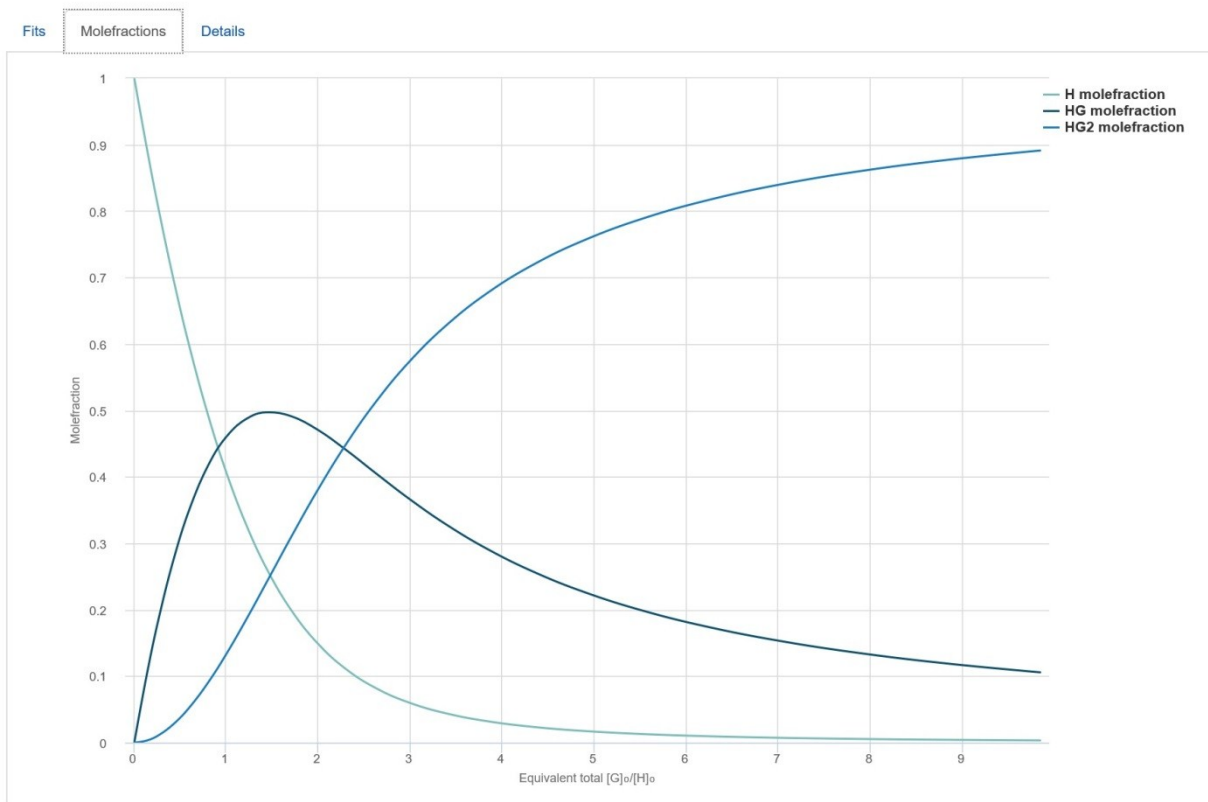


Fig. S3 Screenshot from the result window of *supramolecular.org*¹ from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be> which was fitted to 1:2 NMR binding data. This screenshot shows the calculated molefractions.

Fits Molefractions **Details**

Quality of fit

Fit	RMS	Covariance
h1	6.1150e-3	4.6269e-3
h2	5.0733e-3	3.7663e-3
h3	3.9578e-3	2.4817e-3
h4	1.9157e-3	1.7454e-3
Total	4.5405e-3	6.5464e-4

Coefficients

Fit	H	HG	HG2
h1	7.9173	7.6436	7.6399
h2	7.4733	7.3104	7.2033
h3	3.4498	3.6392	3.6980
h4	3.5467	3.6330	3.6961

Fig. S4 Screenshot from the result window of *supramolecular.org*¹ from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be> which was fitted to 1:2 NMR binding data. This screenshot shows some the additional calculated parameters from the data fitting process.

BindFit v0.5 | Supramole × +

← → ↻ | app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be

bindfit FITTER SEARCH

Input Summary **Metadata** Edit

Experiment

Name	Value
Author(s)	Pall Thordarson
Experiment name	Mg binding no 1
Experiment date	Tuesday, September 25, 2012 12:00 AM
Fit date	Tuesday, May 3, 2016 10:42 PM
Lab book reference	EH-4-133
Host species	Pyromellitimide-crown
Guest species	MgClO4
Solvent	1:1 CD3CN:CDCl3
Temperature	25 C
Notes	Published in http://dx.doi.org/10.1021/ja503383e

Bindfit

Name	Value
Fit ID	8a658114-0b28-4c63-92c0-09a7a976f0be
Searchable	Yes

Fig. S5 Screenshot from the result window of *supramolecular.org*¹ from data archived at the unique url: <http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be> which was fitted to 1:2 NMR binding data. This screenshot shows some of the metadata (labels) that can be added to the data.

References.

- 1 <http://supramolecular.org>. (Accessed 9th May 2016).
- 2 P Thordarson, *Chem. Soc. Rev.*, 2011, **40**, 1305-1323.