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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Contents

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.org[1] 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 noncoopertive 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:

uncertaintyfor1to2example.m	Main file – calculates all the uncertainties.
[a]nmr1to2fitbindcal.m	called by main file to calculate ycalc.
[a]nmr1to2fitbind.m	called by main file in the fitting process.
[a]nmr1to2bbb.m	helper file to solve cubic equations.

[a]These files are essentially identical to related files in the previously published *fittingprogram.*[2]

mat-files:

CDCl3-CD3CN(1-1)_Mg-(ClO4)2_01.mat	Input data experiment 1.
CDCl3-CD3CN(1-1)_Mg-(ClO4)2_02.mat	Input data experiment 2.
CDCl3-CD3CN(1-1)_Mg-(ClO4)2_03.mat	Input data experiment 3.
mg1process.mat	Output data experiment 1.
mg2process.mat	Output data experiment 2.
mg3process.mat	Output data experiment 3.

ii) Figure5:

m-files:

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

[a]These files are essentially identical to related files in the previously published *fittingprogram.*[2]

mat-files:

MCfor1to1concdata.mat	Output from Monte Carlo simulations (360 Mb!).

iii) Figure6:

m-files:

MCfor1to2conc.m	Main file – simulates all the Monte Carlo data.
[a]***nmr1to2fitbindcal.m***	called by main file to calculate ycalc.
[a]***nmr1to2fitbind.m***	called by main file in the fitting process.
[a]***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.

[a]These files are essentially identical to related files in the previously published *fittingprogram.*[2]

mat-files:

MCfor1to2concdata.mat	Output from Monte Carlo simulations (51 Mb!).

Additional Screenshots from supramolecular.org:

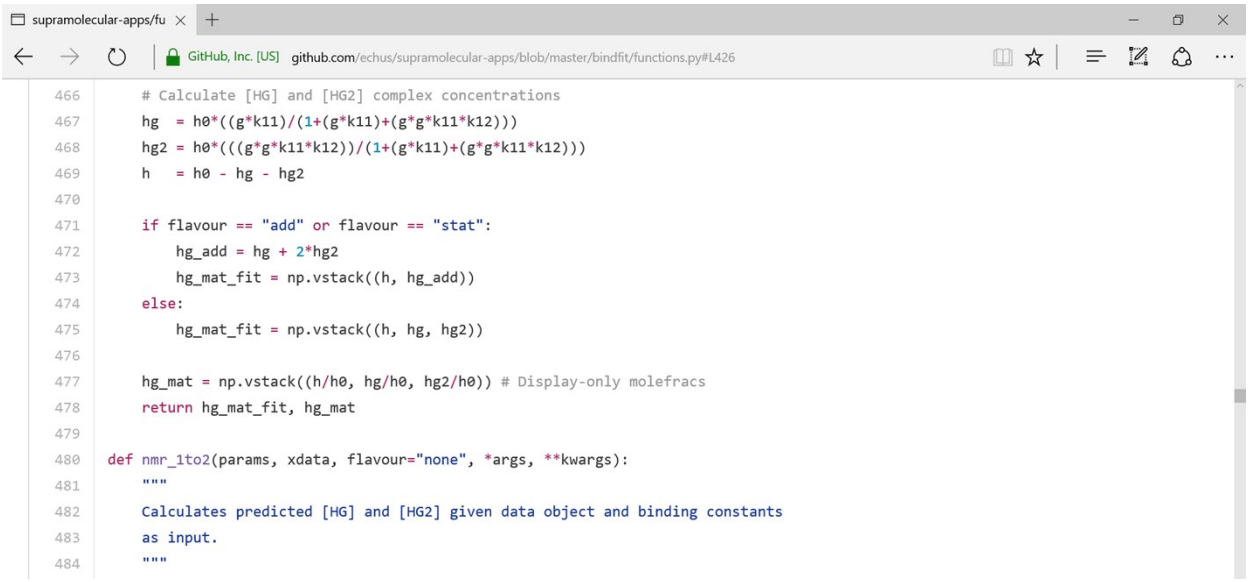

Fig. S1 Screenshot from a small part of the source code for *supramolecular.org*[1] website on github (supramolecular-apps) at

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/

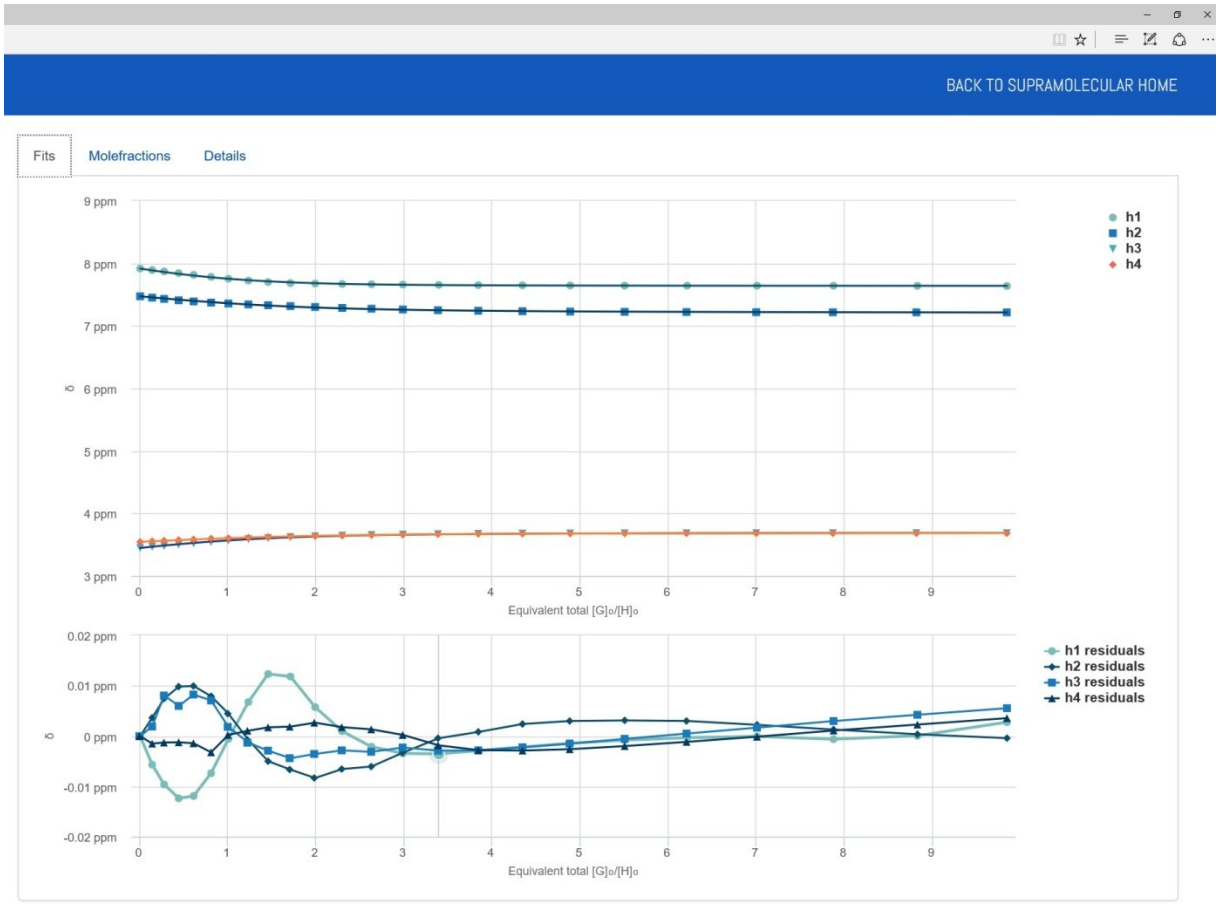

Fig. S2 Screenshot from the result window of *supramolecular.org*[1] from data archived at the unique url: http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be which was fitted to 1:2 NMR binding data. This screenshot shows the raw vs. fitted data (top) and the corresponding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

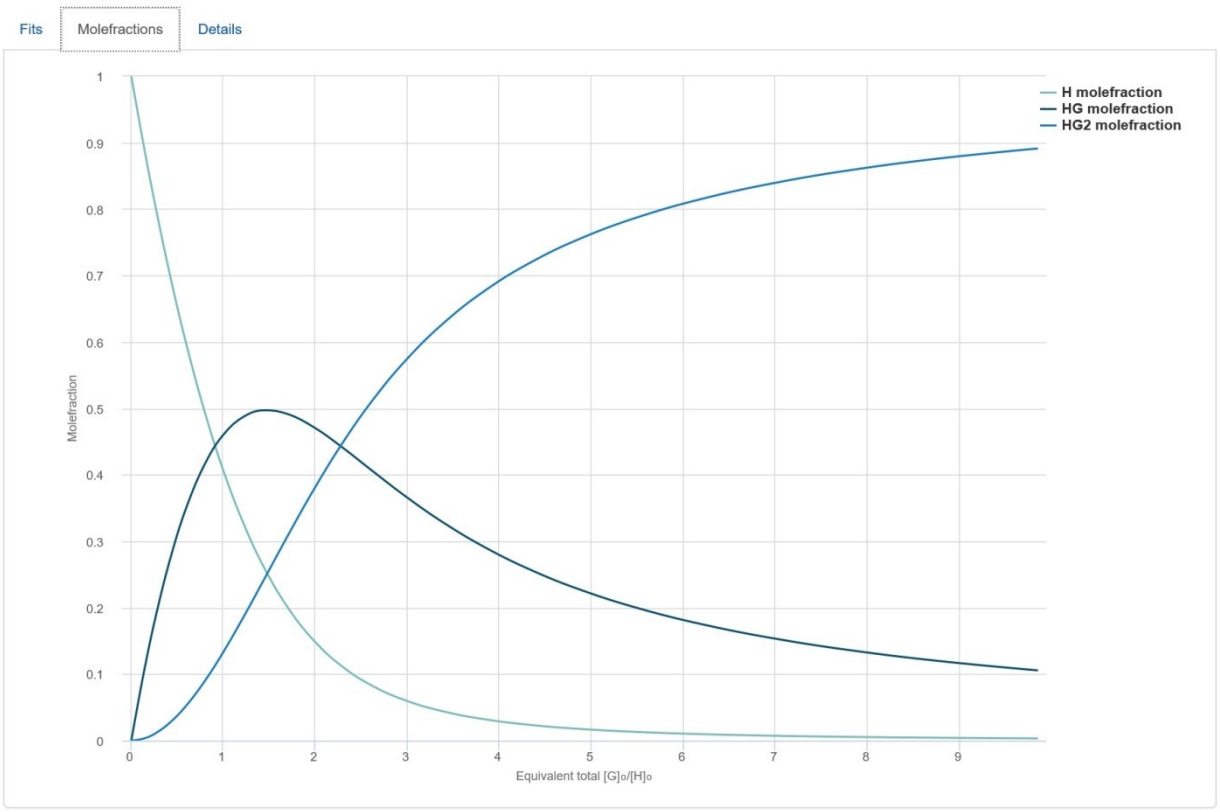

Fig. S3 Screenshot from the result window of *supramolecular.org*[1] from data archived at the unique url: http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be which was fitted to 1:2 NMR binding data. This screenshot shows the calculated molefractions.

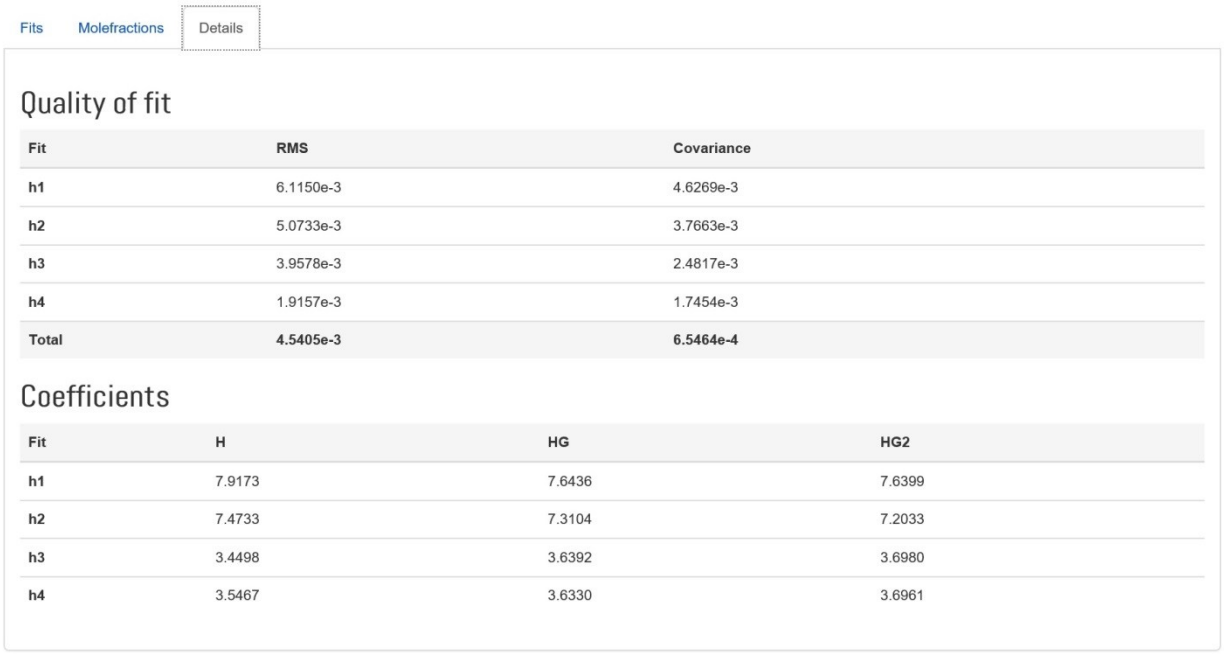

Fig. S4 Screenshot from the result window of *supramolecular.org*[1] from data archived at the unique url: http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be which was fitted to 1:2 NMR binding data. This screenshot shows some the additional calculated parameters from the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

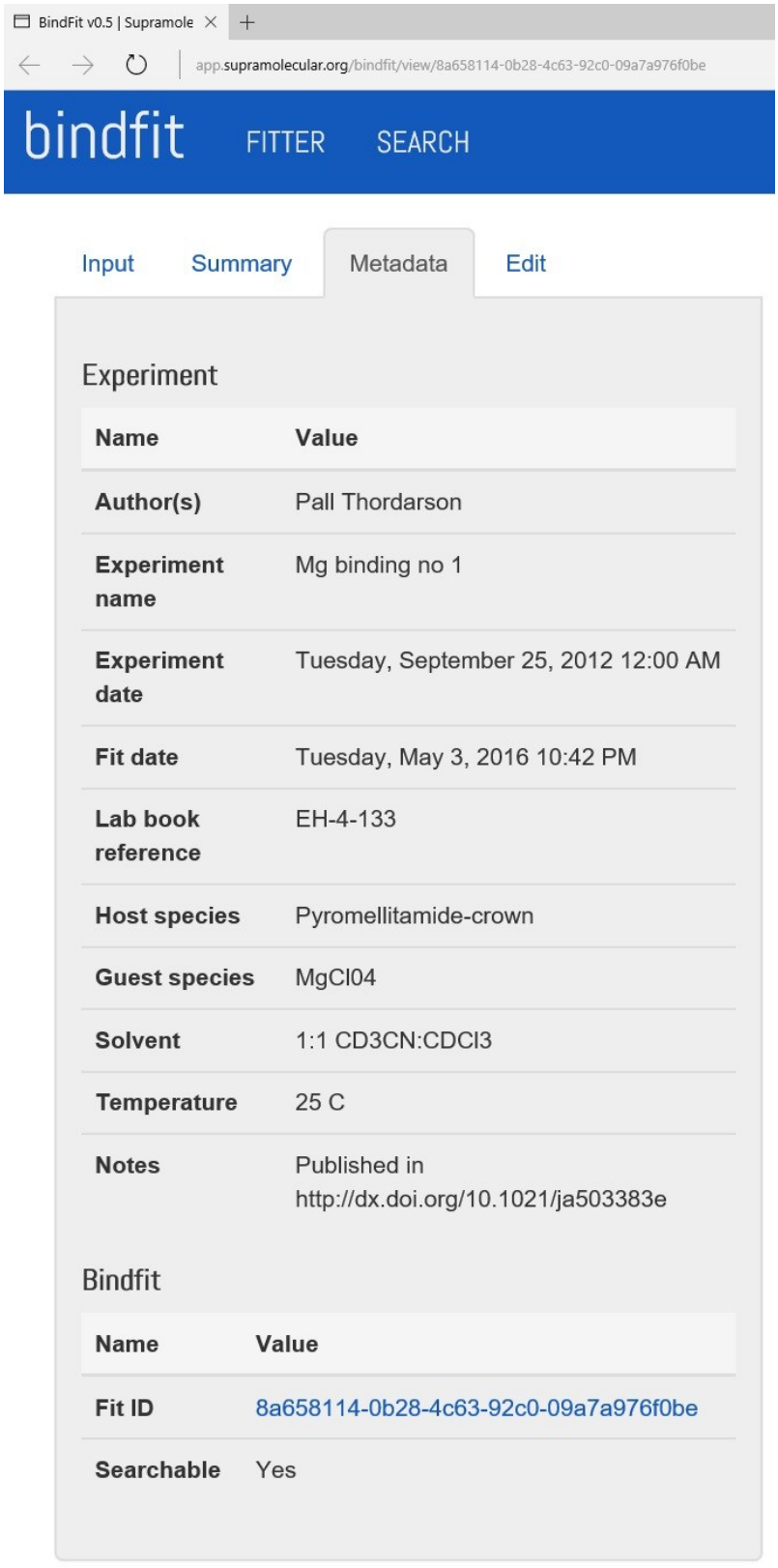

Fig. S5 Screenshot from the result window of *supramolecular.org*[1] from data archived at the unique url: http://app.supramolecular.org/bindfit/view/8a658114-0b28-4c63-92c0-09a7a976f0be which was fitted to 1:2 NMR binding data. This screenshot shows some of the metadata (labels) that can be added to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

References.

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