Supporting Information

Fluorescent calix[4]triazole for selective fluoride anion sensing

Jihee Cho and Sanghee Kim*

College of Pharmacy, Seoul National University, Seoul 08826, Republic of Korea

Contents

1. ^{1}H NMR spectrum

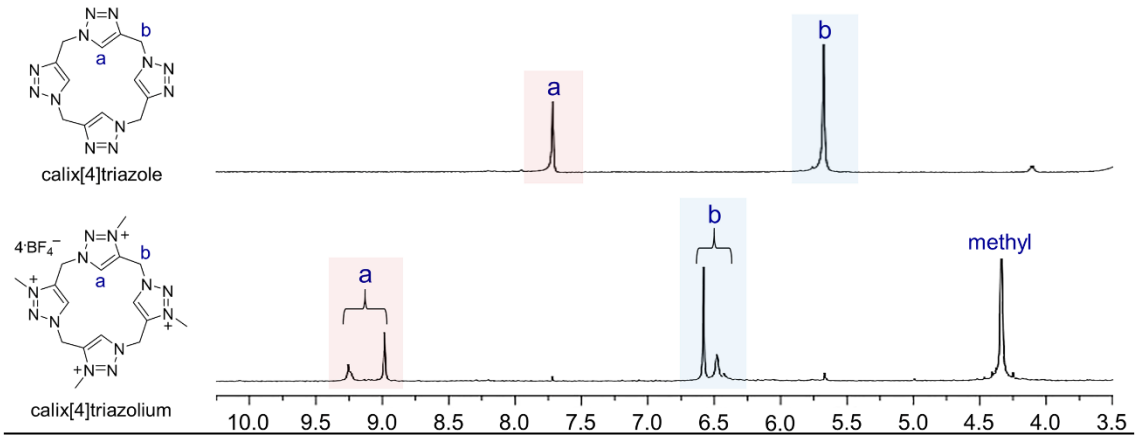

Fig. S1. ^{1}H NMR spectra of calix[4]triazole and calix[4]triazolium in DMSO-d_6.

2. Complexation studies between Py-CT4 and F^-

(1) Association constant calculated by bindfit

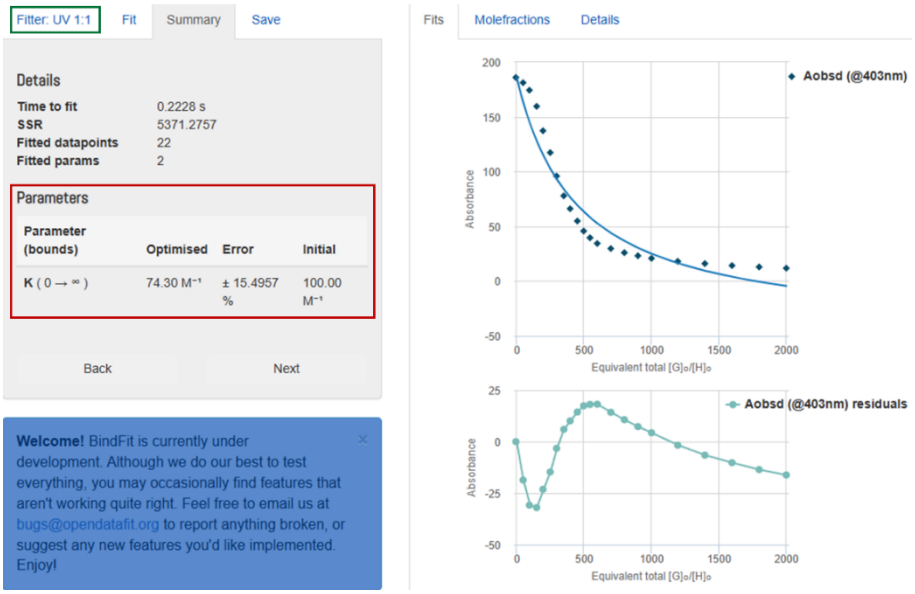

Fig. S2. Screenshot of the summary window of http://app.supramolecular.org/bindfit/. This screenshot shows the raw data for the fluorescence titration of **Py-CT4** with F^- with fluorescence emissions at 403 nm vs. the data fitted to a 1:1 UV binding model and the corresponding residual plot and association constants with the calculated asymptotic standard errors.

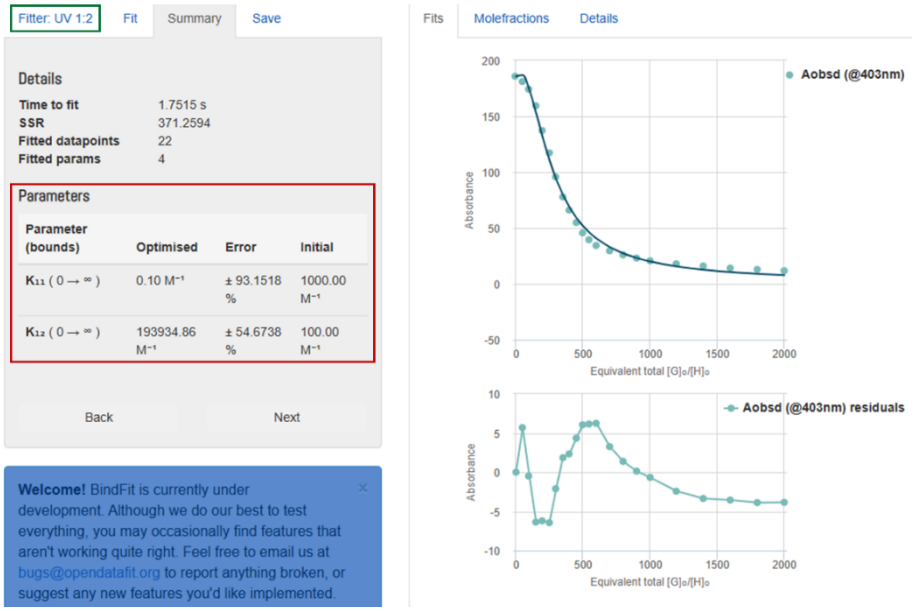

Fig. S3. Screenshot of the summary window of http://app.supramolecular.org/bindfit/. This screenshot shows the raw data for the fluorescence titration of **Py-CT4** with F^- with fluorescence emissions at 403 nm vs. the data fitted to a 1:2 UV binding model and the corresponding residual plot and association constants with the calculated asymptotic standard errors.

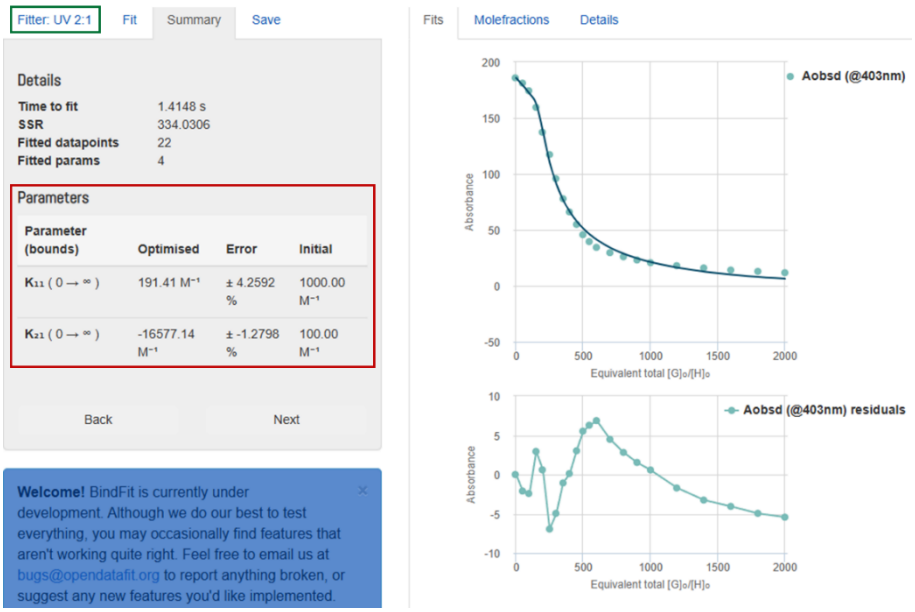

Fig. S4. Screenshot of the summary window of http://app.supramolecular.org/bindfit/. This screenshot shows the raw data for the fluorescence titration of **Py-CT4** with F^- with fluorescence emissions at 403 nm vs. the data fitted to a 2:1 UV binding model and the corresponding residual plot and association constants with the calculated asymptotic standard errors.

Table S1. Summary of association constants between **Py-CT4** and F^- according to different binding models.[a]

Binding models		
1:1	1:2	2:1
74.30 (±15.50%)	K_{11} 0.10 (±93.15%) K_{12} 193934.86 (±54.67%)	K_{11} 191.41 (±4.26%) K_{21} -16577.14 (±-1.28%)

[a] Bindfit software from *supramolecular.org* was used for data analysis.

(2) Job's plot for determining binding stoichiometric ratio

Experiment details. Stock solutions with equal concentrations of **Py-CT4** (10 μM) and F^- (10 μM) in DMSO were prepared. Ten vials were each filled with a 10 mL solution of **Py-CT4** and F^- in the following ratios (**Py-CT4**:F^-): 10:0, 9:1, 8:2, 7:3, 6:4, 5:5, 4:6, 3:7, 2:8, 1:9. Job's plot was constructed by plotting the change in the fluorescence at 403 nm of **Py-CT4** against the molar fraction of the host.

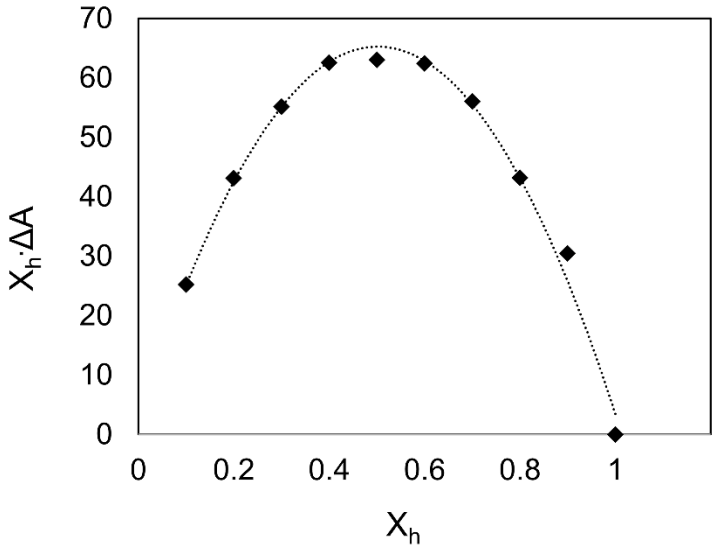

Fig. S5. Job's plot generated from the fluorescence titration data of **Py-CT4** with F^- in a DMSO solution.