ELECTRONIC SUPPLEMENTARY INFORMATION for:

Conformationally flexible arylethynyl bis-urea receptors bind disparate oxoanions with similar, high affinities

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Table of Contents

Experimental Procedures

General methods. ^{1}H, ^{13}C, and ^{19}F NMR spectra were obtained on a Varian Mercury 300 MHz (^{1}H: 300.09 MHz), Inova 500 MHz (^{1}H: 500.10 MHz, ^{13}C 125.75 MHz, ^{19}F: 470.56 MHz), or Bruker Avance III HD 600 MHz NMR spectrometer with Prodigy multinuclear broadband BBO CryoProbe (^{1}H: 600.02 MHz, ^{13}C: 150.89 MHz). Chemical shifts (δ) are expressed in ppm downfield from tetramethylsilane (TMS) using non-deutrated solvent present in the bulk deutrated solvent ($CDCl_3$: ^{1}H 7.26 ppm, ^{13}C 77.16 ppm; *d*$_6$-DMSO: ^{1}H 2.50 ppm, ^{13}C 39.52 ppm; *d*$_6$-acetone: ^{1}H 2.05 ppom, ^{13}C 206.7 and 29.9 ppm). Mixed solvent systems were referenced to the most abundant solvent. All NMR spectra were processed using MestReNova NMR processing software. All oxygen-sensitive reactions were performed under an inert atmosphere of nitrogen using Schlenk techniques. Unless otherwise specified, all materials were obtained from TCI-America, Sigma-Aldrich, or Acros and used as received. Tetrabutylammonium salts were dried at 60 °C in vacuo prior to use. Aniline **4** was synthesized and desilated following known procedures.[1] 2,6-Pyridine receptor **2** was synthesized via known procedures.[1] 2,2'-Bipyridyl-6,6'-bis-ethynylaniline was synthesized following published procedures.[2]

Dianiline 6. To a sealable flask, 3,5-dibromopyridine (0.505 g, 2.13 mmol), CuI (0.099 g, 0.524 mmol), and $Pd(PPh_3)_4$ (0.212 g, 0.184 mmol) was added under nitrogen. A mixture of degassed DIPA (30 mL) and THF (30 mL) was added to the flask via cannula. The solution was continuously purged with N_2 for an additional 30 min. An N_2-purged solution of 4-*tert*-butyl-2-ethynylaniline (1.11 g, 6.41 mmol) in degassed DIPA (15 mL) and THF (15 mL) was then transferred into the flask via cannula. The mixture was stirred overnight at 55 °C under an inert atmosphere. The cooled solution was filtered through a 10 cm silica gel plug eluting with CH_2Cl_2 and then concentrated *in vacuo*. Column chromatography (2:1 hexanes:Et_2O) of the crude material afforded **6** (0.368 g, 41%) as an brown-orange solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (s, 2H), 7.94 (s, 1H), 7.39 (d, *J* = 2.2 Hz, 2H), 7.23 (dd, *J* = 8.5, 2.2 Hz, 2H), 6.70 (d, *J* = 8.5 Hz, 2H), 4.18 (s, 4H), 1.30 (s, 18H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.48, 145.82, 141.17, 140.24, 128.99, 128.08, 120.47, 114.64, 106.53, 90.83, 90.15, 34.09, 31.51. HRMS (TOF-MS-ES^{+}) for $C_{29}H_{31}N_3$ $[M+H]^{+}$: calcd 422.2596, found 422.2587.

3,5-Pyridine receptor 1. In flame dried glassware under inert N_2 atmosphere, aniline **6** (0.240 g, 0.568 mmol) was dissolved in freshly distilled toluene (75 mL) and *p*-methoxyphenyl isocyanate (0.2 mL, 2.02 mmol) was added via syringe. The reaction mixture was stirred for 24 h at 55 °C. The reaction was cooled and the precipitate was isolated via vacuum filtration. The precipitate was washed with hexanes and dried to give **1** (0.209 g, 51%) as a yellow-white solid. ^{1}H NMR (500 MHz, d_6-acetone) δ 8.75 (s, 2H), 8.48 (s, 1H), 8.25 (d, J = 8.4 Hz, 2H), 8.18 (s, 1H), 7.91 (s, 1H), 7.57 (d, J = 2.5 Hz, 2H), 7.49 (dd, J = 8.9, 2.5 Hz, 2H), 7.43 (d, J = 8.4 Hz, 4H), 6.84 (d, J = 8.5 Hz, 4H), 3.74 (s, 6H), 1.34 (s, 18H). ^{13}C NMR (151 MHz, d_6-acetone/DMSO) δ 155.70, 153.23, 151.65, 144.99, 141.36, 139.59, 139.57, 133.66, 127.96, 120.90, 120.53, 120.24, 114.57, 110.89, 91.41, 90.57, 55.48, 34.52, 31.36. HRMS (TOF-MS-ES$^+$) for $C_{45}H_{45}N_5O_4$ [M+H] $^+$: calcd 720.3566, found 720.3559.

Bipyridine receptor 3. In flame dried glassware under inert N_2 atmosphere, 2,2'-bipyridyl-6,6'-bis-ethynylaniline (0.124 g, 0.248 mmol) was dissolved in freshly distilled toluene (50 mL) and *p*-methoxyphenyl isocyanate (0.150 mL, 1.52 mmol) was added via syringe. The reaction mixture was stirred at room temperature for 16 h. Hexanes was used to precipitate the crude product, which was then filtered and further washed with hexanes. A minimal amount of ethanol was then added to the crude product in a vial. The vial was sonicated and five drops of deionized water was added to re-precipitate the product. Receptor **3** was then isolated via vacuum filtration (0.104 g, 53%) as a cream-colored powder. ^{1}H NMR (500 MHz, d_6-acetone/DMSO) δ 9.28 (s, 2H), 8.55 (d, J = 7.9 Hz, 2H), 8.23 (s, 2H), 8.20 (d, J = 8.8 Hz, 2H), 8.07 (t, J = 7.8 Hz, 2H), 7.90 (d, J = 7.6 Hz, 2H), 7.60 (d, J = 2.4 Hz, 2H), 7.52–7.44 (m, 6H), 6.88 (d, J = 8.5 Hz, 4H), 3.75 (s, 6H), 1.35 (s, 18H). ^{13}C NMR (151 MHz, d_6-acetone/DMSO) δ 155.73, 155.26, 152.93, 144.77, 142.94, 139.33, 138.22, 133.31, 129.30, 128.72, 127.74, 120.88, 120.48, 120.09, 114.31, 110.55, 94.55, 85.76, 55.27, 34.25, 31.12. HRMS (TOF-MS-ES$^+$) for $C_{50}H_{48}N_6O_4$ [M+H] $^+$: calcd 797.3815, found 797.3799.

Titrations

General Titration Procedures. Concentration of receptor was kept constant by preparing a stock solution of the receptor and performing a serial dilution with the receptor stock solution to dissolve the guest. Receptor concentration was maintained constant throughout the titration. Tetrabutylammonium salts, purchased from TCI America or SigmaAldrich, were dried by heating to 60 °C *in vacuo* before use. Hamilton gas-tight syringes were used for all titrations. Titrations were performed in triplicate and the reported association constants represent the average fits across all titrations. Representative data are provided for each receptor and anion.

UV-Vis Titration Conditions. UV-Vis titrations were carried out on an Agilent Technologies Cary 60 UV-Vis spectrometer. Water-saturated 10% DMSO/90% $CHCl_3$ v/v% was prepared using HPLC-grade solvents purchased from SigmaAldrich or Fisher Scientific. Association constants were determined by non-linear regression models using Open Data Fit.[3] All host solutions in 10% DMSO/90% $CHCl_3$ started as deep, marigold-yellow solutions and transitioned to colorless over the course of the titrations. All host solutions in CHCN started as colorless and remained so over the course the titrations. The 10% DMSO/90% $CHCl_3$ spectra is more easily trackable when displayed as ε instead of absorbance. All data fit with change in absorbance values.

Tetrabutylammonium dihydrogenphosphate with 1. A concentrated solution of **1** (2.25 mg, [R] = 0.313 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 800 µL of 0.313 mM solution of **1** diluted to 10.00 mL to yield the stock solution of **1** ([R] = 25.0 µM). A 3.00 mL solution of $TBAH_2PO_4$ (2.14 mg, [G] = 2.10 mM) was prepared by solvation with the stock solution of **1**. A serial dilution was then performed with 1200 µL of the 2.10 mM solution of $TBAH_2PO_4$ diluted to 3.00 mL with the stock solution of **1** to yield guest solution ([G] = 8.41 mM). The starting volume in the cuvette was 2.0 mL.

Table S1. Representative titration data for $H_2PO_4^-$ with **1**.

	Guest (μL)	[**1**] (M)	[$H_2PO_4^-$] (M)	Equiv.
1	0	2.50E-05	0.00E+00	0.00
2	5	2.50E-05	2.39E-06	0.10
3	10	2.50E-05	4.78E-06	0.19
4	20	2.50E-05	9.50E-06	0.38
5	40	2.50E-05	1.88E-05	0.75
6	60	2.50E-05	2.79E-05	1.11
7	80	2.50E-05	3.67E-05	1.47
8	100	2.50E-05	4.54E-05	1.82
9	125	2.50E-05	5.60E-05	2.24
10	150	2.50E-05	6.64E-05	2.65
11	200	2.50E-05	8.62E-05	3.45
12	250	2.50E-05	1.05E-04	4.20
13	300	2.50E-05	1.23E-04	4.92
14	350	2.50E-05	1.40E-04	5.60
15	400	2.50E-05	1.56E-04	6.25
16	500	2.50E-05	1.87E-04	7.47
17	600	2.50E-05	2.15E-04	8.58
18	700	2.50E-05	2.40E-04	9.61
19	900	2.50E-05	2.85E-04	11.42
20	1100	2.50E-05	3.24E-04	12.98
21	1500	2.50E-05	3.88E-04	15.52

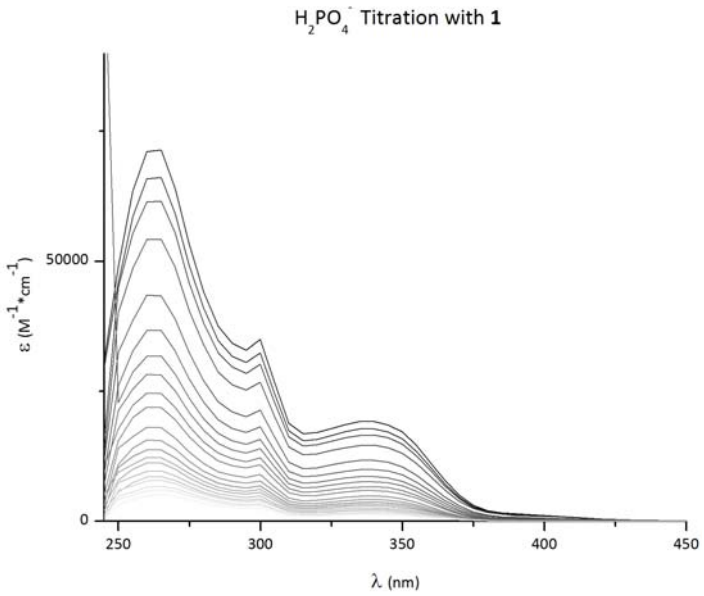

Figure S1. UV-Vis spectra of **1** titrated with $H_2PO_4^-$ in 10% DMSO/$CHCl_3$.

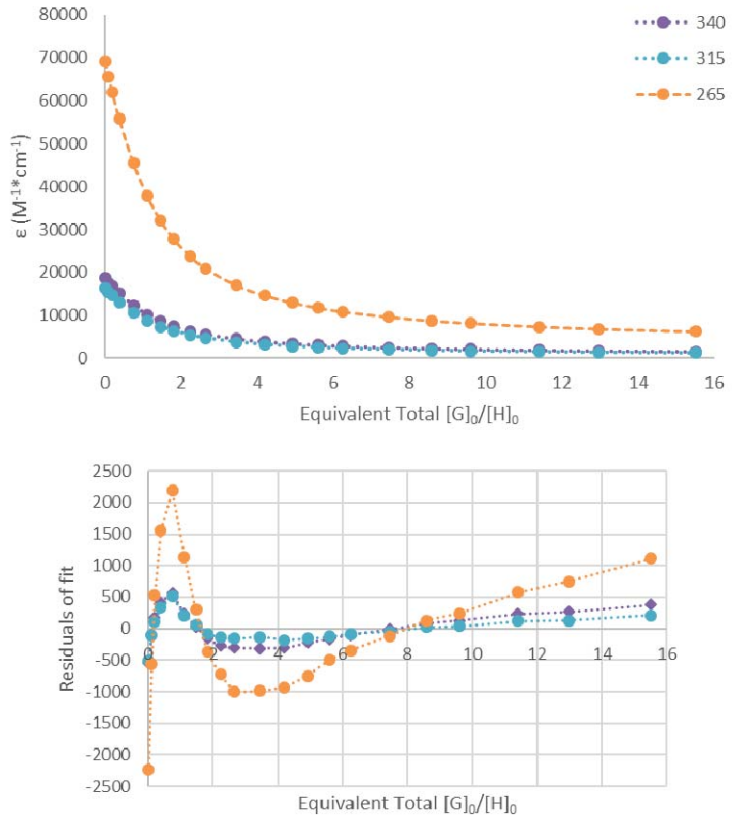

Figure S2. Binding isotherm and Bindfit output for $H_2PO_4^-$ titration with **1**.

Tetrabutylammonium hydrogensulfate with 1. A concentrated solution of **1** (2.25 mg, [R] = 0.313 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 800 µL of 0.313 mM solution of **1** diluted to 10.00 mL to yield the stock solution of **1** ([R] = 25.0 µM). A 3.00 mL solution of $TBAHSO_4$ (3.23 mg, [G] = 3.17 mM) was prepared by solvation with the stock solution of **1**. A serial dilution was then performed with 1200 µL of the 3.23 mM solution of $TBAHSO_4$ diluted to 3.00 mL with the stock solution of **1** to yield guest solution ([G] = 12.7 mM). The starting volume in the cuvette was 2.0 mL.

Table S2. Representative titration data for HSO_4^- with **1**.

	Guest (μL)	[**1**] (M)	[HSO_4^-] (M)	Equiv.
1	0	2.50E-05	0.00E+00	0.00
2	5	2.50E-05	3.61E-06	0.14
3	10	2.50E-05	7.21E-06	0.29
4	20	2.50E-05	1.43E-05	0.57
5	40	2.50E-05	2.84E-05	1.13
6	60	2.50E-05	4.21E-05	1.68
7	80	2.50E-05	5.55E-05	2.22
8	100	2.50E-05	6.86E-05	2.74
9	125	2.50E-05	8.46E-05	3.38
10	150	2.50E-05	1.00E-04	4.01
11	200	2.50E-05	1.30E-04	5.20
12	250	2.50E-05	1.59E-04	6.34
13	300	2.50E-05	1.86E-04	7.43
14	350	2.50E-05	2.11E-04	8.46
15	400	2.50E-05	2.36E-04	9.44
16	500	2.50E-05	2.82E-04	11.28
17	600	2.50E-05	3.24E-04	12.96
18	700	2.50E-05	3.62E-04	14.50
19	900	2.50E-05	4.31E-04	17.23
20	1100	2.50E-05	4.90E-04	19.58
21	1500	2.50E-05	5.86E-04	23.42

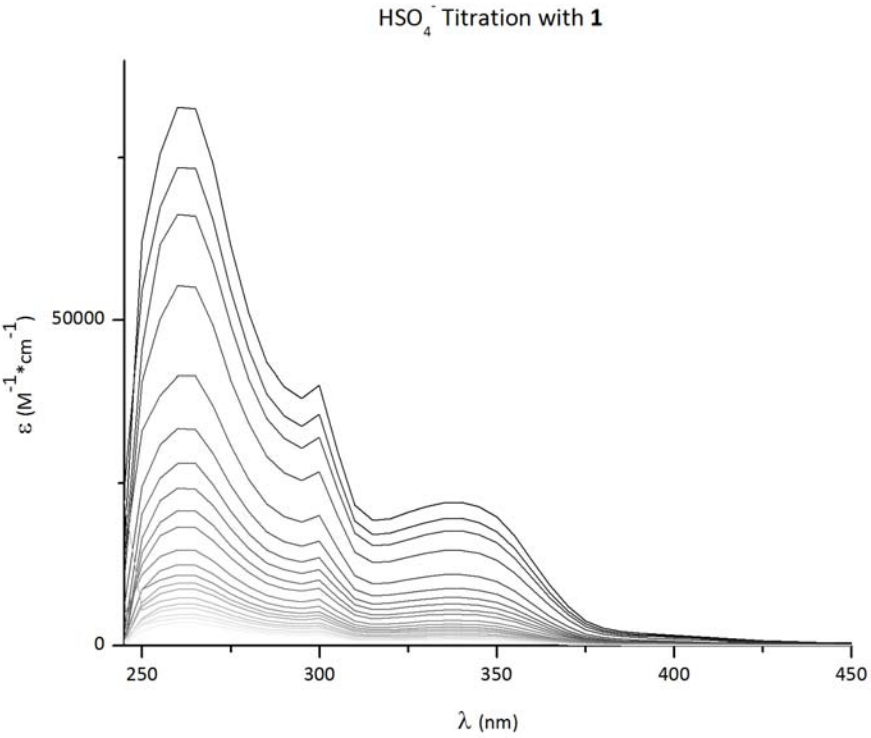

Figure S3. UV-Vis spectra of **1** titrated with HSO_4^- in 10% DMSO/$CHCl_3$.

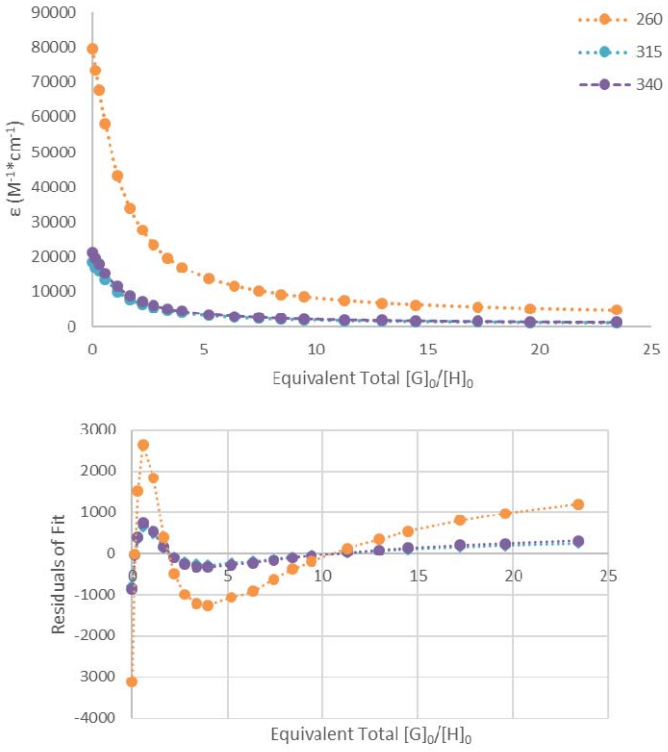

Figure S4. Binding isotherm and Bindfit output for HSO_4^- titration with **1**.

Tetrabutylammonium perchlorate with 1. A concentrated solution of **1** (2.27 mg, [R] = 0.285 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 900 μL of 0.285 mM solution of **1** diluted to 10.00 mL to yield the stock solution of **1** ([R] = 25.6 μM). A 3.00 mL solution of $TBAClO_4$ (3.53 mg, [G] = 3.44 mM) was prepared by solvation with the stock solution of **1**. A serial dilution was then performed with 1000 μL of the 3.53 mM solution of $TBAClO_4$ diluted to 3.00 mL with the stock solution of **1** to yield guest solution ([G] = 11.5 mM). The starting volume in the cuvette was 2.0 mL.

Table S3. Representative titration data for ClO_4^- with **1**.

	Guest (μL)	[**1**] (M)	[ClO_4^-] (M)	Equiv.
1	0	2.56E-05	0.00E+00	0.00
2	5	2.56E-05	3.27E-06	0.13
3	10	2.56E-05	6.52E-06	0.25
4	20	2.56E-05	1.30E-05	0.51
5	40	2.56E-05	2.56E-05	1.00
6	60	2.56E-05	3.80E-05	1.48
7	80	2.56E-05	5.01E-05	1.96
8	105	2.56E-05	6.49E-05	2.53
9	125	2.56E-05	7.65E-05	2.98
10	150	2.56E-05	9.06E-05	3.53
11	200	2.56E-05	1.18E-04	4.59
12	250	2.56E-05	1.43E-04	5.59
13	300	2.56E-05	1.68E-04	6.55
14	350	2.56E-05	1.91E-04	7.46
15	400	2.56E-05	2.13E-04	8.33
16	500	2.56E-05	2.55E-04	9.94
17	600	2.56E-05	2.93E-04	11.43
18	700	2.56E-05	3.28E-04	12.79
19	900	2.56E-05	3.90E-04	15.20
20	1100	2.56E-05	4.43E-04	17.27
21	1500	2.56E-05	5.29E-04	20.65

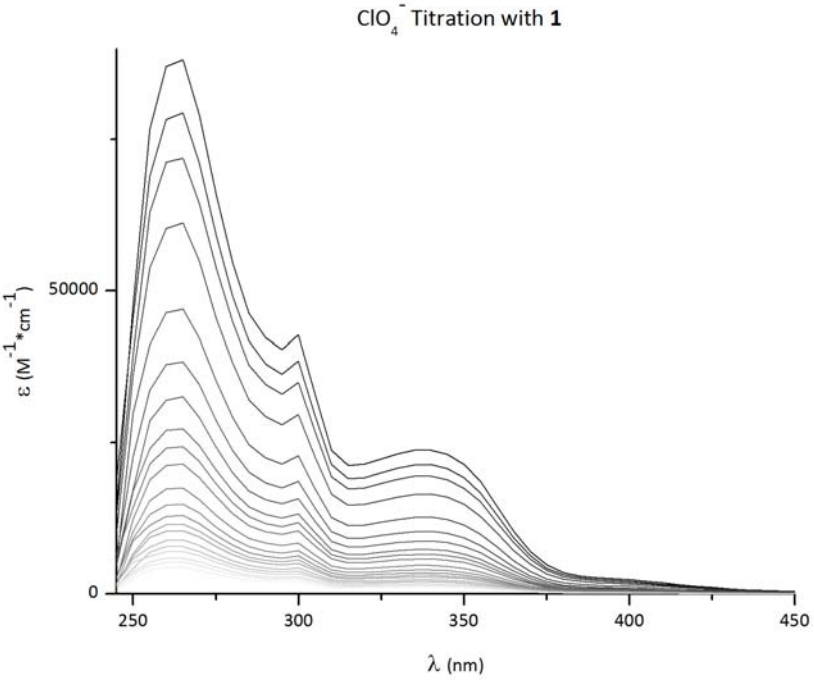

Figure S5. UV-Vis spectra of **1** titrated with ClO_4^- in 10% DMSO/$CHCl_3$.

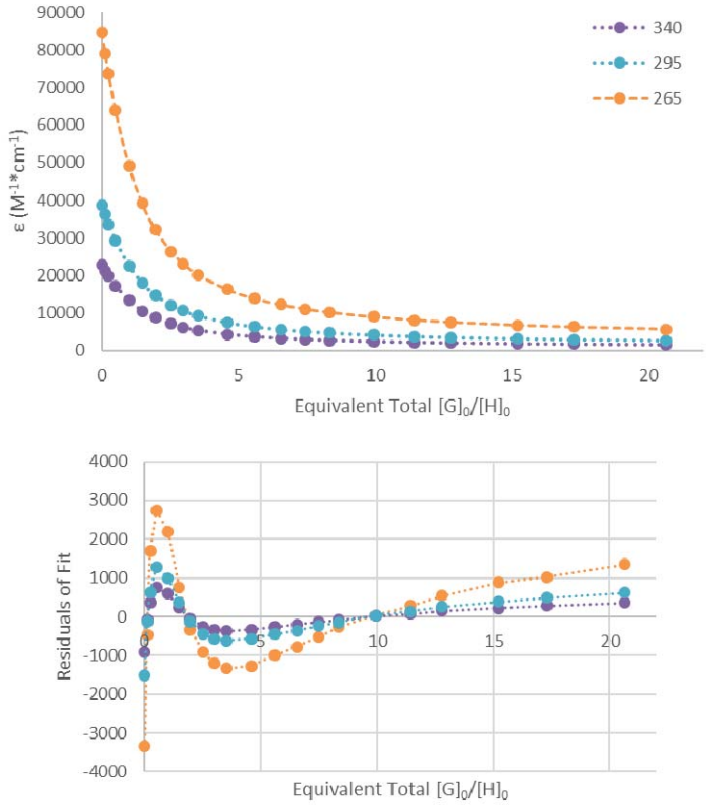

Figure S6. Binding isotherm and Bindfit output for ClO_4^- titration with **1**.

Tetrabutylammonium dihydrogenphosphate with 2. A concentrated solution of **2** (2.23 mg, [R] = 0.310 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 800 μL of 0.310 mM solution of **2** diluted to 10.00 mL to yield the stock solution of **2** ([R] = 24.7 μM). A 3.00 mL solution of $TBAH_2PO_4$ (2.02 mg, [G] = 1.97 mM) was prepared by solvation with the stock solution of **2** to prepare guest solution. The starting volume in the cuvette was 2.0 mL.

Table S4. Representative titration data for $H_2PO_4^-$ with **2**.

	Guest (μL)	[**2**] (M)	[$H_2PO_4^-$] (M)	Equiv.
1	0	2.48E-05	0.00E+00	0.00
2	5	2.48E-05	5.61E-06	0.23
3	10	2.48E-05	1.12E-05	0.45
4	20	2.48E-05	2.23E-05	0.90
5	40	2.48E-05	4.40E-05	1.78
6	60	2.48E-05	6.53E-05	2.64
7	80	2.48E-05	8.62E-05	3.48
8	100	2.48E-05	1.07E-04	4.30
9	125	2.48E-05	1.31E-04	5.30
10	150	2.48E-05	1.56E-04	6.28
11	200	2.48E-05	2.02E-04	8.16
12	250	2.48E-05	2.46E-04	9.94
13	300	2.48E-05	2.88E-04	11.64
14	350	2.48E-05	3.28E-04	13.25
15	400	2.48E-05	3.67E-04	14.80
16	500	2.48E-05	4.38E-04	17.67
17	600	2.48E-05	5.03E-04	20.30
18	700	2.48E-05	5.63E-04	22.72
19	900	2.48E-05	6.69E-04	27.01
20	1100	2.48E-05	7.61E-04	30.69
21	1500	2.48E-05	9.10E-04	36.70

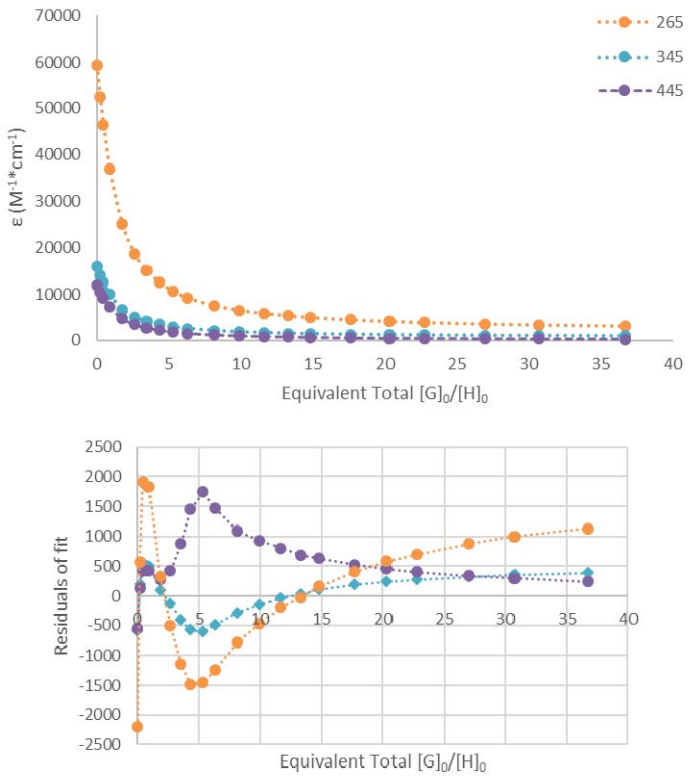

Figure S7. Binding isotherm and Bindfit output for $H_2PO_4^-$ titration with **2**.

Tetrabutylammonium hydrogensulfate with 2. A concentrated solution of **2** (2.58 mg, [R] = 0.358 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 700 µL of 0.358 mM solution of **2** diluted to 10.00 mL to yield the stock solution of **2** ([R] = 25.1 µM). A 3.00 mL solution of $TBAHSO_4$ (2.27 mg, [G] = 1.34 mM) was prepared by solvation with the stock solution of **2** to yield the guest solution. The starting volume in the cuvette was 2.0 mL.

Table S5. Representative titration data for HSO_4^- with **2**.

	Guest (μL)	[**2**] (M)	[HSO_4^-] (M)	Equiv.
1	0	2.51E-05	0.00E+00	0.00
2	5	2.51E-05	3.81E-06	0.15
3	10	2.51E-05	7.60E-06	0.30
4	15	2.51E-05	1.14E-05	0.45
5	35	2.51E-05	2.62E-05	1.05
6	55	2.51E-05	4.07E-05	1.62
7	75	2.51E-05	5.50E-05	2.19
8	95	2.51E-05	6.89E-05	2.74
9	115	2.51E-05	8.25E-05	3.29
10	140	2.51E-05	9.90E-05	3.95
11	165	2.51E-05	1.15E-04	4.59
12	215	2.51E-05	1.46E-04	5.83
13	265	2.51E-05	1.76E-04	7.01
14	315	2.51E-05	2.04E-04	8.13
15	365	2.51E-05	2.31E-04	9.20
16	415	2.51E-05	2.56E-04	10.22
17	515	2.51E-05	3.04E-04	12.12
18	615	2.51E-05	3.48E-04	13.86
19	715	2.51E-05	3.88E-04	15.46
20	915	2.51E-05	4.59E-04	18.30
21	1115	2.51E-05	5.20E-04	20.74

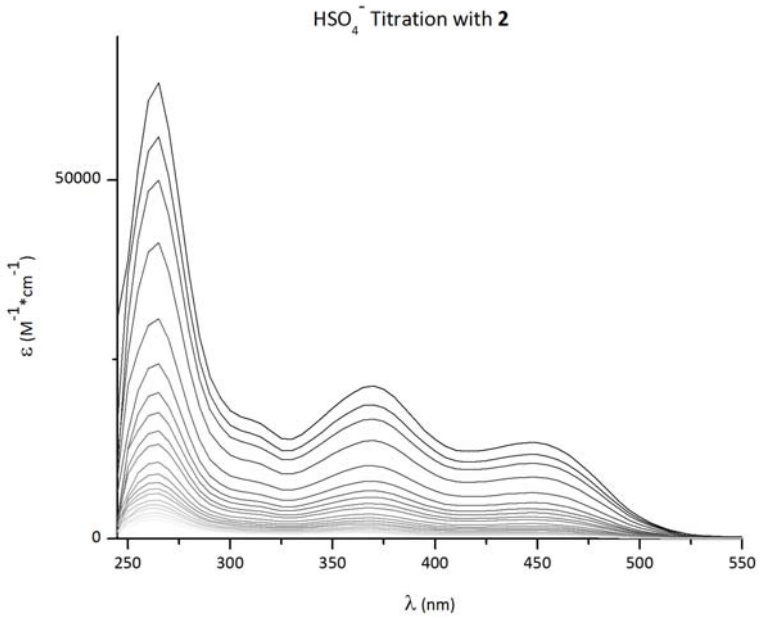

Figure S8. UV-Vis spectra of **2** titrated with HSO_4^- in 10% DMSO/$CHCl_3$.

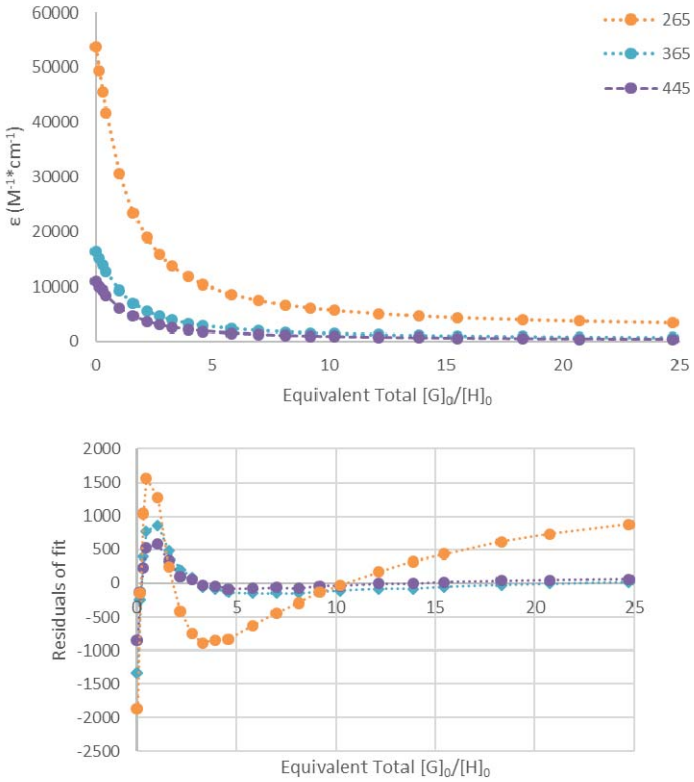

Figure S9. Binding isotherm and Bindfit output for HSO_4^- titration with **2**.

Tetrabutylammonium perchlorate with 2. A concentrated solution of **2** (2.58 mg, [R] = 0.358 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 6500 μL of 0.358 mM solution of **2** diluted to 10.00 mL to yield the stock solution of **2** ([R] = 23.3 μM). A 3.00 mL solution of $TBAClO_4$ (2.79 mg, [G] = 1.63 mM) was prepared by solvation with the stock solution of **2** to yield the guest solution. The starting volume in the cuvette was 2.0 mL.

Table S6. Representative titration data for ClO_4^- with **2**.

	Guest (μL)	[**2**] (M)	[ClO_4^-] (M)	Equiv.
1	0	2.33E-05	0.00E+00	0.00
2	5	2.33E-05	4.65E-06	0.20
3	10	2.33E-05	9.27E-06	0.40
4	20	2.33E-05	1.84E-05	0.79
5	40	2.33E-05	3.65E-05	1.57
6	60	2.33E-05	5.41E-05	2.32
7	85	2.33E-05	7.56E-05	3.25
8	100	2.33E-05	8.82E-05	3.79
9	125	2.33E-05	1.09E-04	4.67
10	150	2.33E-05	1.29E-04	5.53
11	200	2.33E-05	1.67E-04	7.19
12	250	2.33E-05	2.04E-04	8.76
13	300	2.33E-05	2.39E-04	10.25
14	350	2.33E-05	2.72E-04	11.68
15	450	2.33E-05	3.34E-04	14.33
16	550	2.33E-05	3.90E-04	16.75
17	700	2.33E-05	4.66E-04	20.02
18	900	2.33E-05	5.54E-04	23.79
19	1100	2.33E-05	6.30E-04	27.04
20	1400	2.33E-05	7.25E-04	31.14
21	1800	2.33E-05	8.27E-04	35.52

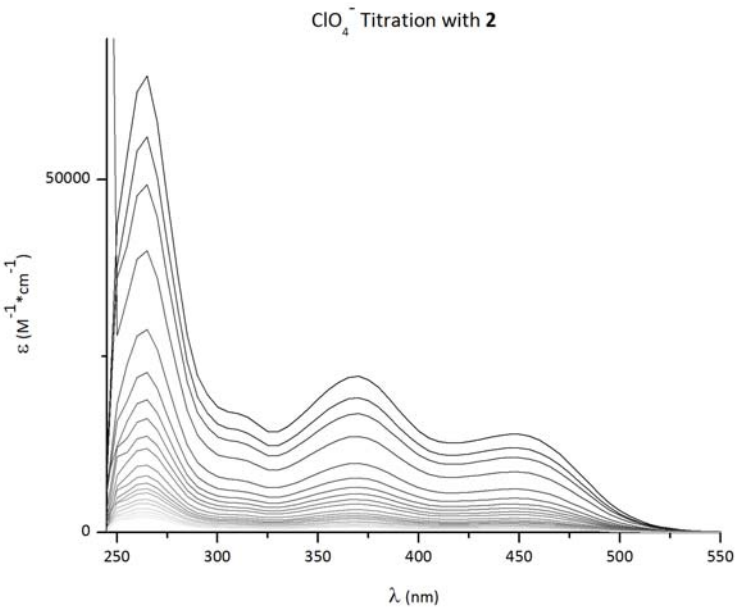

Figure S10. UV-Vis spectra of **2** titrated with ClO_4^- in 10% DMSO/$CHCl_3$.

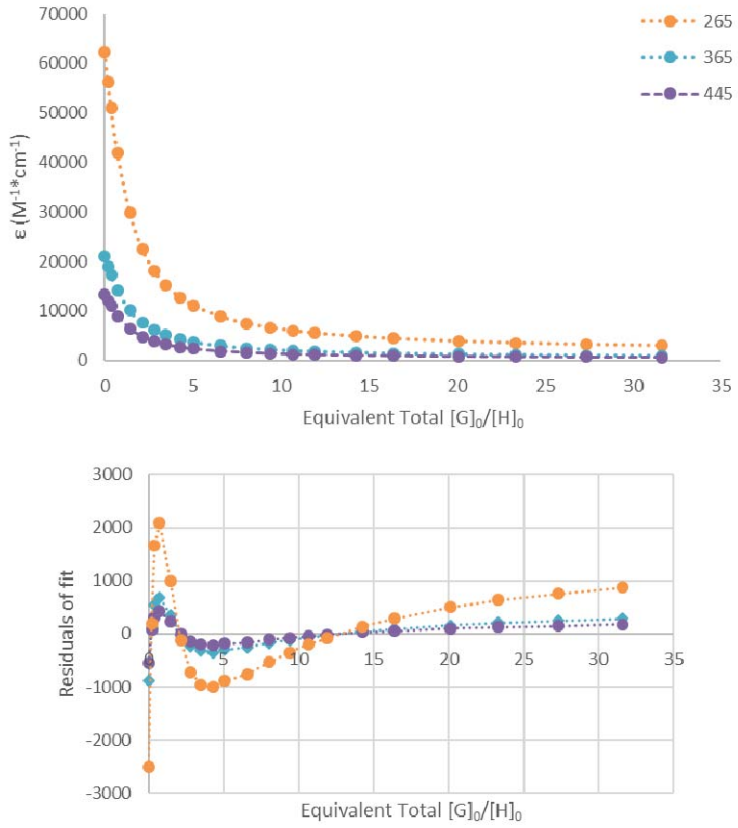

Figure S11. Binding isotherm and Bindfit output for ClO_4^- titration with **2**.

Tetrabutylammonium dihydrogenphosphate with 3. A concentrated solution of **3** (2.05 mg, [R] = 0.257 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 975 µL of 0.257 mM solution of **3** diluted to 10.00 mL to yield the stock solution of **3** ([R] = 25.1 µM). A 3.00 mL solution of $TBAH_2PO_4$ (2.46 mg, [G] = 2.42 mM) was prepared by solvation with the stock solution of **3**. A serial dilution was then performed with 500 µL of the 2.42 mM solution of $TBAH_2PO_4$ diluted to 3.00 mL with the stock solution of **3** to yield guest solution ([G] = 4.03 mM). The starting volume in the cuvette was 2.0 mL.

Table S7. Representative titration data for $H_2PO_4^-$ with **3**.

	Guest (µL)	[**3**] (M)	[$H_2PO_4^-$] (M)	Equiv.
1	0	2.51E-05	0.00E+00	0.00
2	5	2.51E-05	1.15E-06	0.05
3	10	2.51E-05	2.29E-06	0.09
4	20	2.51E-05	4.55E-06	0.18
5	40	2.51E-05	9.00E-06	0.36
6	60	2.51E-05	1.33E-05	0.53
7	80	2.51E-05	1.76E-05	0.70
8	100	2.51E-05	2.18E-05	0.87
9	125	2.51E-05	2.68E-05	1.07
10	150	2.51E-05	3.18E-05	1.27
11	200	2.51E-05	4.13E-05	1.65
12	250	2.51E-05	5.03E-05	2.01
13	300	2.51E-05	5.89E-05	2.35
14	350	2.51E-05	6.71E-05	2.68
15	400	2.51E-05	7.49E-05	2.99
16	500	2.51E-05	8.95E-05	3.57
17	600	2.51E-05	1.03E-04	4.10
18	700	2.51E-05	1.15E-04	4.59
19	900	2.51E-05	1.37E-04	5.45
20	1100	2.51E-05	1.55E-04	6.20
21	1500	2.51E-05	1.86E-04	7.41

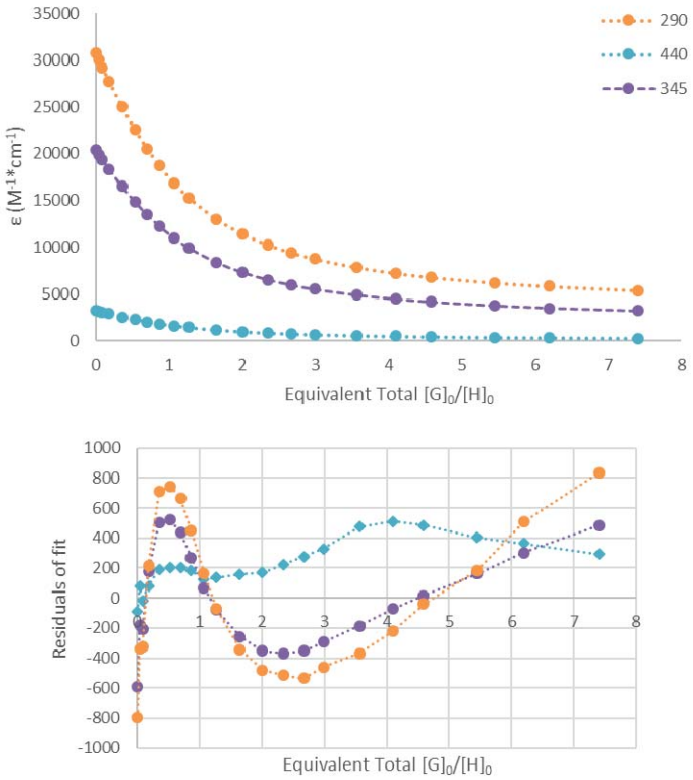

Figure S12. Binding isotherm and Bindfit output for $H_2PO_4^-$ titration with **3**.

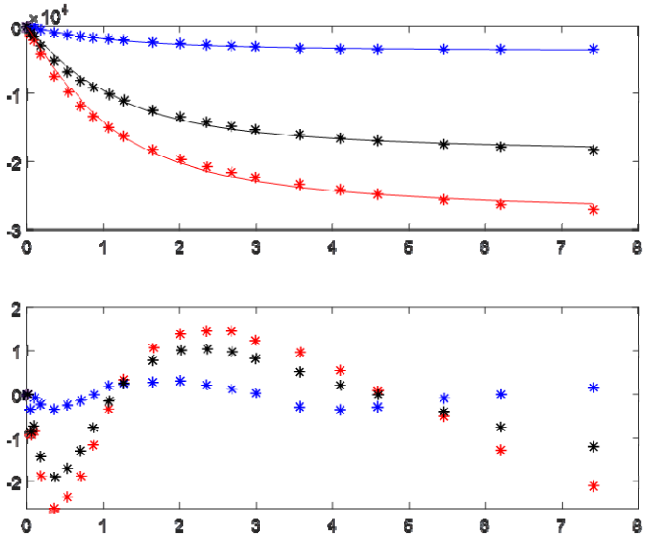

Figure S13. MatLab fit of binding isotherm for $H_2PO_4^-$ titration with **3**.

Tetrabutylammonium hydrogensulfate with 3. A concentrated solution of **3** (2.27 mg, [R] = 0.285 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 800 μL of 0.285 mM solution of **3** diluted to 10.00 mL to yield the stock solution of **3** ([R] = 22.8 μM). A 3.00 mL solution of $TBAHSO_4$ (2.87 mg, [G] = 2.82 mM) was prepared by solvation with the stock solution of **3**. A serial dilution was then performed with 1000 μL of the 2.82 mM solution of $TBAHSO_4$ diluted to 3.00 mL with the stock solution of **3** to yield guest solution ([G] = 9.39 mM). The starting volume in the cuvette was 2.0 mL.

Table S8. Representative titration data for HSO_4^- with **3**.

	Guest (μL)	[**3**] (M)	[HSO_4^-] (M)	Equiv.
1	0	2.28E-05	0.00E+00	0.00
2	5	2.28E-05	2.68E-06	0.12
3	10	2.28E-05	5.34E-06	0.23
4	20	2.28E-05	1.06E-05	0.47
5	40	2.28E-05	2.10E-05	0.92
6	60	2.28E-05	3.11E-05	1.37
7	80	2.28E-05	4.11E-05	1.80
8	105	2.28E-05	5.32E-05	2.33
9	125	2.28E-05	6.26E-05	2.75
10	150	2.28E-05	7.41E-05	3.25
11	200	2.28E-05	9.63E-05	4.23
12	250	2.28E-05	1.17E-04	5.15
13	300	2.28E-05	1.37E-04	6.03
14	350	2.28E-05	1.57E-04	6.87
15	400	2.28E-05	1.75E-04	7.67
16	500	2.28E-05	2.09E-04	9.16
17	600	2.28E-05	2.40E-04	10.52
18	700	2.28E-05	2.68E-04	11.78
19	900	2.28E-05	3.19E-04	14.00
20	1100	2.28E-05	3.63E-04	15.91
21	1500	2.28E-05	4.33E-04	19.02

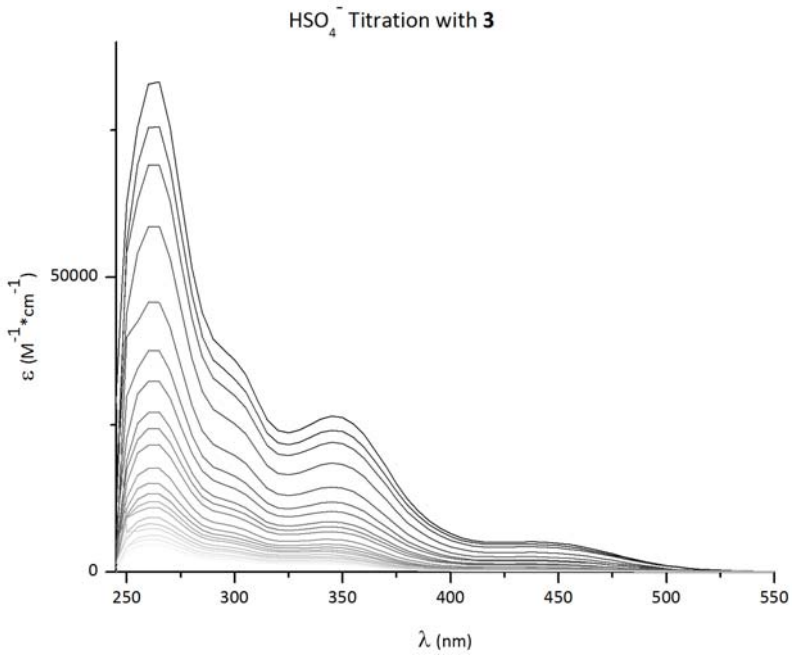

Figure S14. UV-Vis spectra of **3** titrated with HSO_4^- in 10% DMSO/$CHCl_3$.

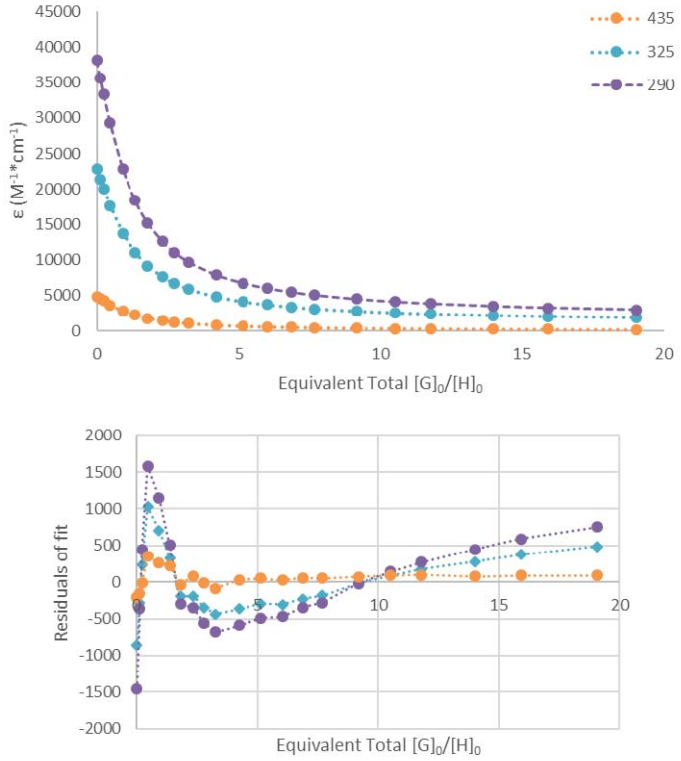

Figure S15. Binding isotherm and Bindfit output for HSO_4^- titration with **3**.

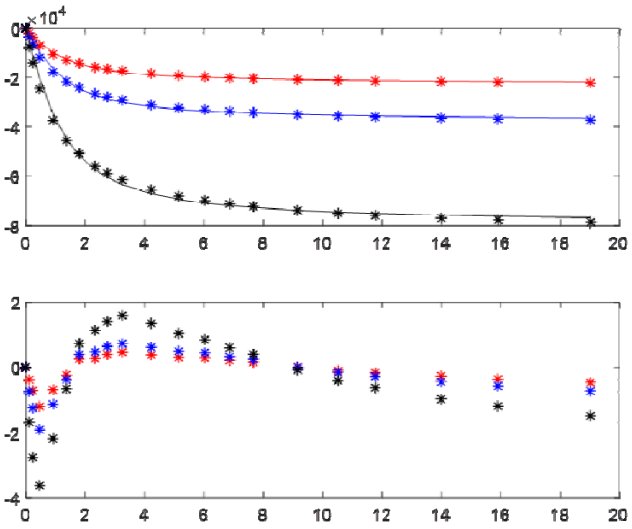

Figure S16. MatLab fit of binding isotherm for HSO_4^- titration with **3**.

Tetrabutylammonium perchlorate with 3. A concentrated solution of **3** (2.27 mg, [R] = 0.285 mM) in 10% DMSO/$CHCl_3$ (10.00 mL) was prepared. A serial dilution was then performed with 900 µL of 0.285 mM solution of **3** diluted to 10.00 mL to yield the stock solution of **3** ([R] = 25.6 µM). A 2.00 mL solution of $TBAClO_4$ (3.50 mg, [G] = 5.12 mM) was prepared by solvation with the stock solution of **3**. A serial dilution was then performed with 700 µL of the 5.12 mM solution of $TBAClO_4$ diluted to 3.00 mL with the stock solution of **3** to yield guest solution ([G] = 11.9 mM). The starting volume in the cuvette was 2.0 mL.

Table S9. Representative titration data for ClO_4^- with **3**.

	Guest (μL)	[**3**] (M)	[ClO_4^-] (M)	Equiv.
1	0	2.56E-05	0.00E+00	0.00
2	5	2.56E-05	3.40E-06	0.13
3	10	2.56E-05	6.79E-06	0.26
4	20	2.56E-05	1.35E-05	0.53
5	40	2.56E-05	2.67E-05	1.04
6	60	2.56E-05	3.96E-05	1.54
7	80	2.56E-05	5.22E-05	2.04
8	105	2.56E-05	6.76E-05	2.64
9	125	2.56E-05	7.96E-05	3.11
10	150	2.56E-05	9.43E-05	3.68
11	200	2.56E-05	1.22E-04	4.78
12	250	2.56E-05	1.49E-04	5.82
13	300	2.56E-05	1.75E-04	6.82
14	350	2.56E-05	1.99E-04	7.76
15	400	2.56E-05	2.22E-04	8.67
16	500	2.56E-05	2.65E-04	10.35
17	600	2.56E-05	3.05E-04	11.89
18	700	2.56E-05	3.41E-04	13.31
19	900	2.56E-05	4.06E-04	15.82
20	1100	2.56E-05	4.61E-04	17.98
21	1500	2.56E-05	5.51E-04	21.50

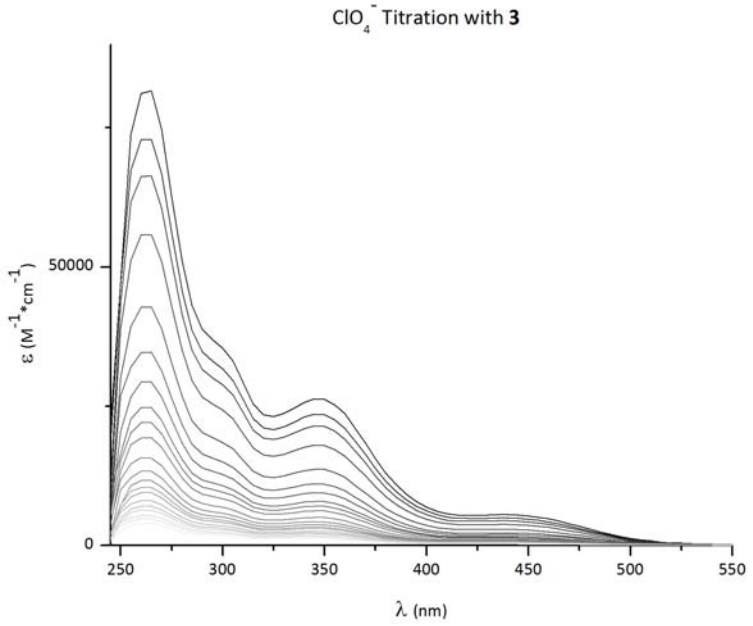

Figure S17. UV-Vis spectra of **3** titrated with ClO_4^- in 10% DMSO/$CHCl_3$.

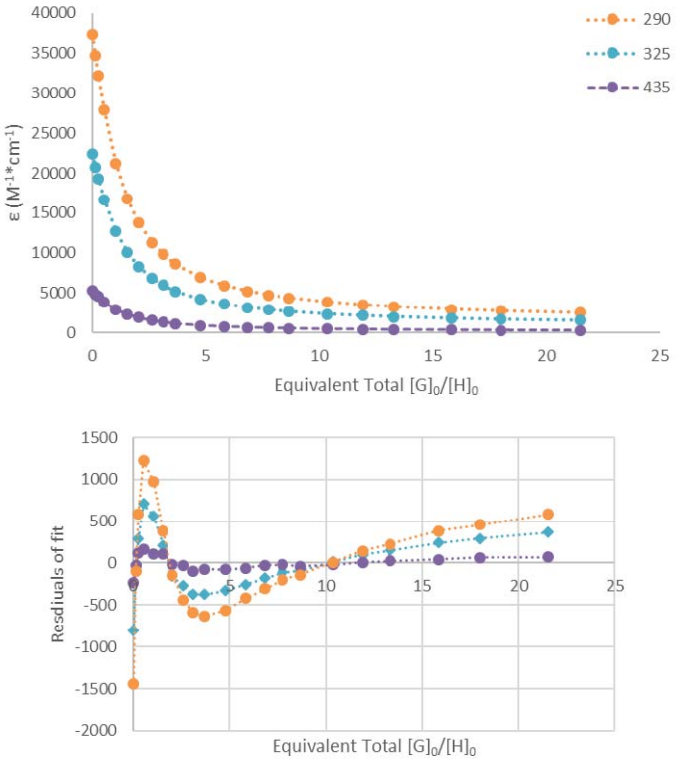

Figure S18. Binding isotherm and Bindfit output for ClO_4^- titration with **3**.

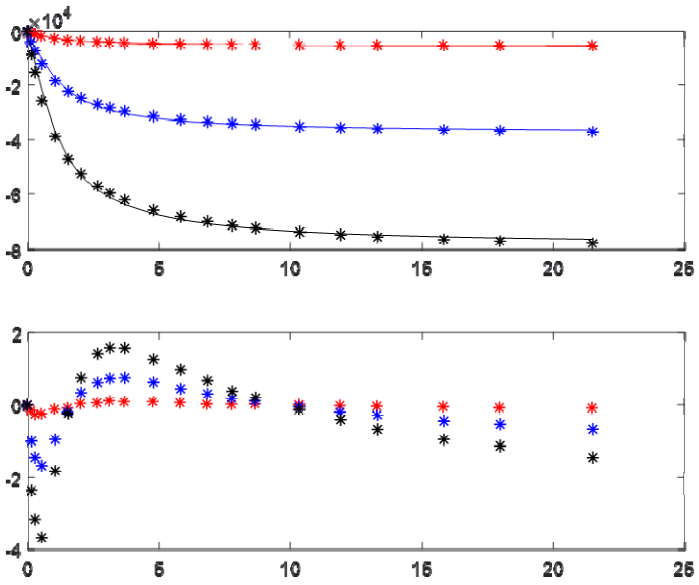

Figure S19. MatLab fit of binding isotherm for ClO_4^- titration with **3**.

Acetonitrile titrations:

Tetrabutylammonium dihydrogenphosphate with 1. A concentrated solution of **1** (2.43 mg, [R] = 0.338 mM) in CHCN (10.00 mL) was prepared. A serial dilution was then performed with 600 μL of 0.338 mM solution of **1** diluted to 10.00 mL to yield the stock solution of **1** ([R] = 20.3 μM). A 3.00 mL solution of $TBAH_2PO_4$ (2.80 mg, [G] = 2.75 mM) was prepared by solvation with the stock solution of **1**. A serial dilution was then performed with 350 μL of the 2.75 mM solution of $TBAH_2PO_4$ diluted to 2.00 mL with the stock solution of **1** to yield guest solution ([G] = 0.481 mM). The starting volume in the cuvette was 2.0 mL.

Table S10. Representative titration data for $H_2PO_4^-$ with **1**.

	Guest (μL)	[**1**] (M)	[$H_2PO_4^-$] (M)	Equiv.
1	0	2.03E-05	0.00E+00	0.00
2	5	2.03E-05	1.37E-06	0.07
3	10	2.03E-05	2.73E-06	0.13
4	20	2.03E-05	5.44E-06	0.27
5	40	2.03E-05	1.08E-05	0.53
6	60	2.03E-05	1.60E-05	0.79
7	80	2.03E-05	2.10E-05	1.04
8	100	2.03E-05	2.60E-05	1.28
9	125	2.03E-05	3.21E-05	1.58
10	150	2.03E-05	3.80E-05	1.88
11	200	2.03E-05	4.94E-05	2.44
12	250	2.03E-05	6.01E-05	2.97
13	300	2.03E-05	7.04E-05	3.48
14	350	2.03E-05	8.02E-05	3.96
15	400	2.03E-05	8.95E-05	4.42
16	500	2.03E-05	1.07E-04	5.28
17	600	2.03E-05	1.23E-04	6.07
18	700	2.03E-05	1.37E-04	6.79
19	900	2.03E-05	1.63E-04	8.07
20	1100	2.03E-05	1.86E-04	9.17
21	1500	2.03E-05	2.22E-04	10.97

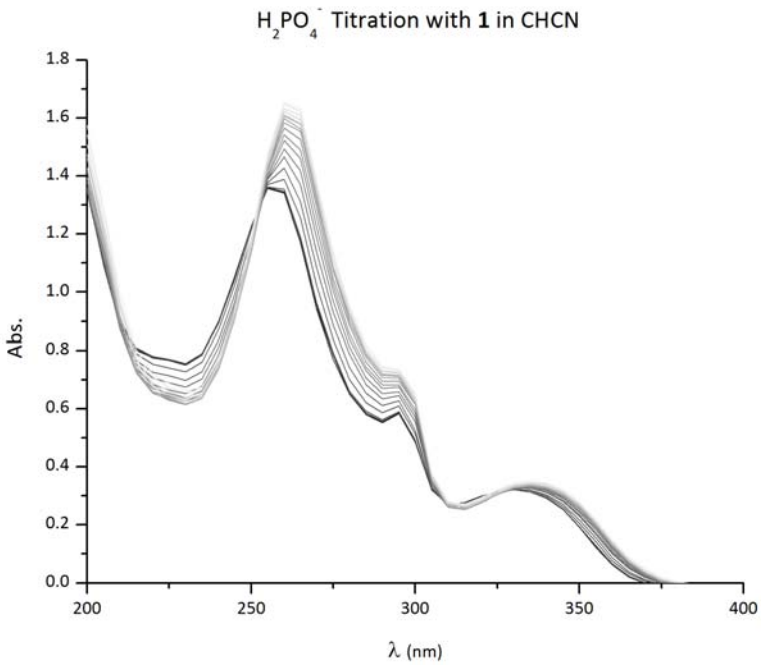

Figure S20. UV-Vis spectra of **1** titrated with $H_2PO_4^-$ in CHCN.

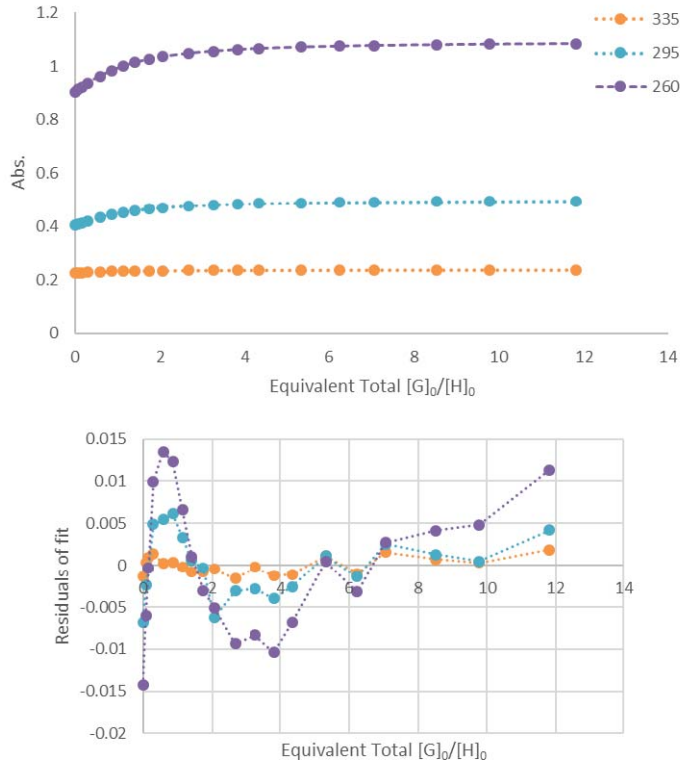

Figure S21. Binding isotherm and Bindfit output for $H_2PO_4^-$ titration with **1**.

Tetrabutylammonium hydrogensulfate with 1. A concentrated solution of **1** (2.43 mg, [R] = 0.338 mM) in CHCN (10.00 mL) was prepared. A serial dilution was then performed with 500 μL of 0.338 mM solution of **1** diluted to 10.00 mL to yield the stock solution of **1** ([R] = 16.9 μM). A 2.015 mL solution of $TBAHSO_4$ (6.54 mg, [G] = 9.56 mM) was prepared by solvation with the stock solution of **1**. A serial dilution was then performed with 1400 μL of the 9.56 mM solution of $TBAHSO_4$ diluted to 3.046 mL with the stock solution of **1** to yield guest solution ([G] = 4.39 mM). The starting volume in the cuvette was 2.0 mL.

Table S11. Representative titration data for HSO_4^- with **1**.

	Guest (μL)	[**1**] (M)	[HSO_4^-] (M)	Equiv.
1	0	1.69E-05	0.00E+00	0.00
2	5	1.69E-05	1.25E-05	0.74
3	10	1.69E-05	2.50E-05	1.48
4	20	1.69E-05	4.97E-05	2.94
5	40	1.69E-05	9.82E-05	5.82
6	60	1.69E-05	1.46E-04	8.63
7	80	1.69E-05	1.92E-04	11.38
8	100	1.69E-05	2.38E-04	14.07
9	125	1.69E-05	2.93E-04	17.36
10	150	1.69E-05	3.47E-04	20.56
11	200	1.69E-05	4.51E-04	26.71
12	250	1.69E-05	5.49E-04	32.55
13	300	1.69E-05	6.43E-04	38.11
14	350	1.69E-05	7.32E-04	43.40
15	400	1.69E-05	8.18E-04	48.44
16	500	1.69E-05	9.77E-04	57.86
17	600	1.69E-05	1.12E-03	66.48
18	700	1.69E-05	1.26E-03	74.40
19	900	1.69E-05	1.49E-03	88.43
20	1100	1.69E-05	1.70E-03	100.50
21	1500	1.69E-05	2.03E-03	120.18
22	1900	1.69E-05	2.29E-03	135.54
23	2300	1.69E-05	2.50E-03	147.87

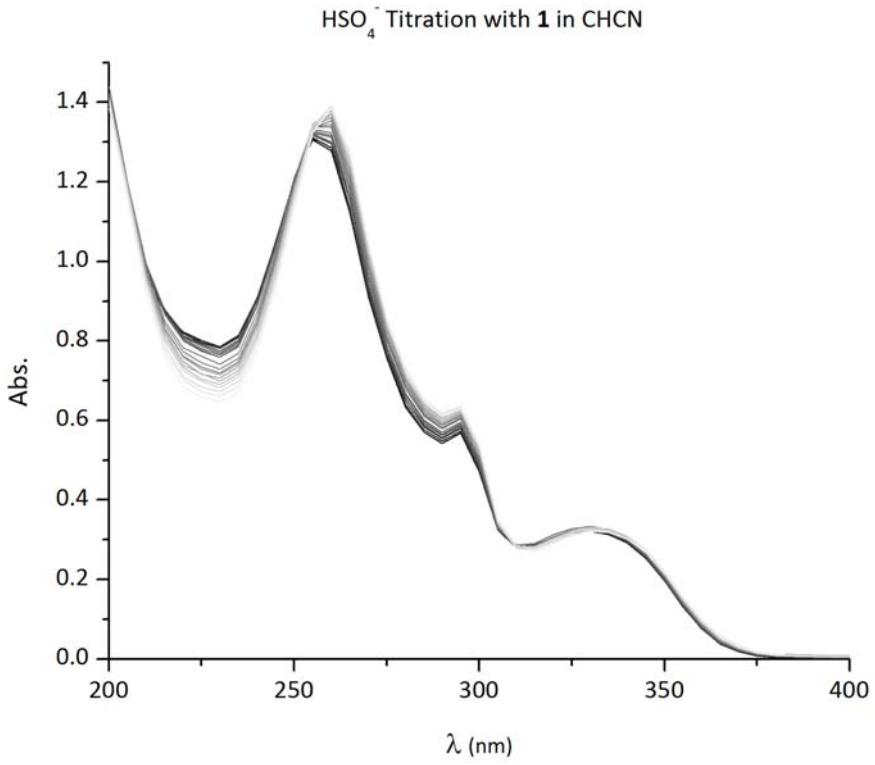

Figure S22. UV-Vis spectra of **1** titrated with HSO_4^- in CHCN.

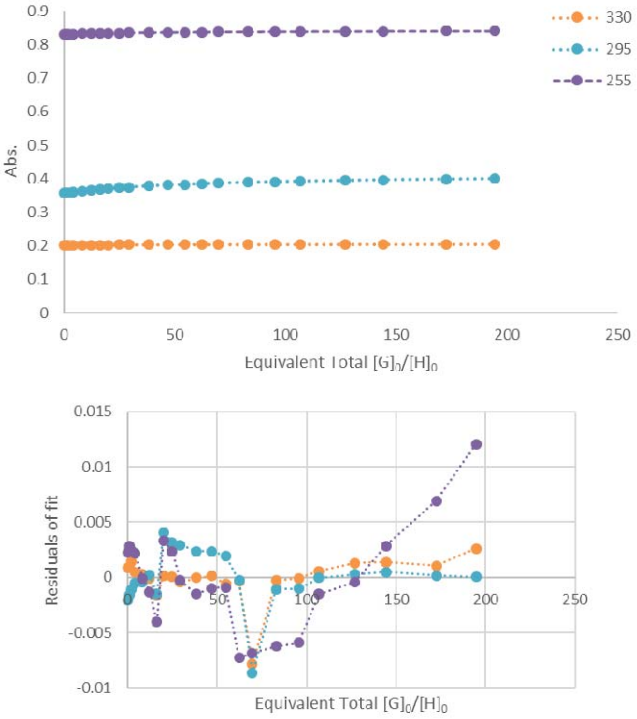

Figure S23. Binding isotherm and Bindfit output for HSO_4^- titration with **1**.

Tetrabutylammonium perchlorate with 1. A concentrated solution of **1** (2.43 mg, [R] = 0.338 mM) in CHCN (10.00 mL) was prepared. A serial dilution was then performed with 300 μL of 0.338 mM solution of **1** diluted to 10.00 mL to yield the stock solution of **1** ([R] = 10.1 μM). A 2.00 mL solution of $TBAClO_4$ (6.53 mg, [G] = 9.55 mM) was prepared by solvation with the stock solution of **1**. A serial dilution was then performed with 1300 μL of the 9.55 mM solution of $TBAClO_4$ diluted to 3.00 mL with the stock solution of **1** to yield guest solution ([G] = 4.14 mM). The starting volume in the cuvette was 2.0 mL.

Table S12. Representative titration data for ClO_4^- with **1**.

	Guest (μL)	[**1**] (M)	[ClO_4^-] (M)	Equiv.
1	0	1.01E-05	0.00E+00	0.00
2	5	1.01E-05	1.18E-05	1.16
3	10	1.01E-05	2.35E-05	2.32
4	20	1.01E-05	4.68E-05	4.62
5	40	1.01E-05	9.25E-05	9.13
6	60	1.01E-05	1.37E-04	13.55
7	80	1.01E-05	1.81E-04	17.86
8	100	1.01E-05	2.24E-04	22.09
9	125	1.01E-05	2.76E-04	27.24
10	150	1.01E-05	3.27E-04	32.26
11	200	1.01E-05	4.24E-04	41.91
12	250	1.01E-05	5.17E-04	51.08
13	300	1.01E-05	6.06E-04	59.80
14	350	1.01E-05	6.90E-04	68.11
15	400	1.01E-05	7.70E-04	76.02
16	500	1.01E-05	9.20E-04	90.81
17	600	1.01E-05	1.06E-03	104.33
18	700	1.01E-05	1.18E-03	116.75
19	900	1.01E-05	1.41E-03	138.78
20	1100	1.01E-05	1.60E-03	157.72
21	1500	1.01E-05	1.91E-03	188.60

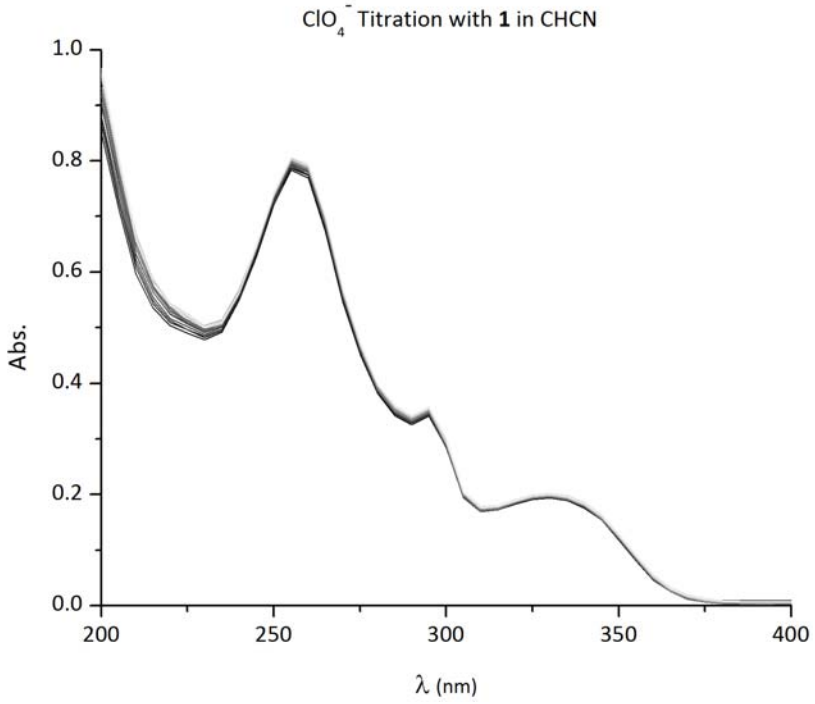

Figure S24. UV-Vis spectra of **1** titrated with ClO_4^- in CHCN.

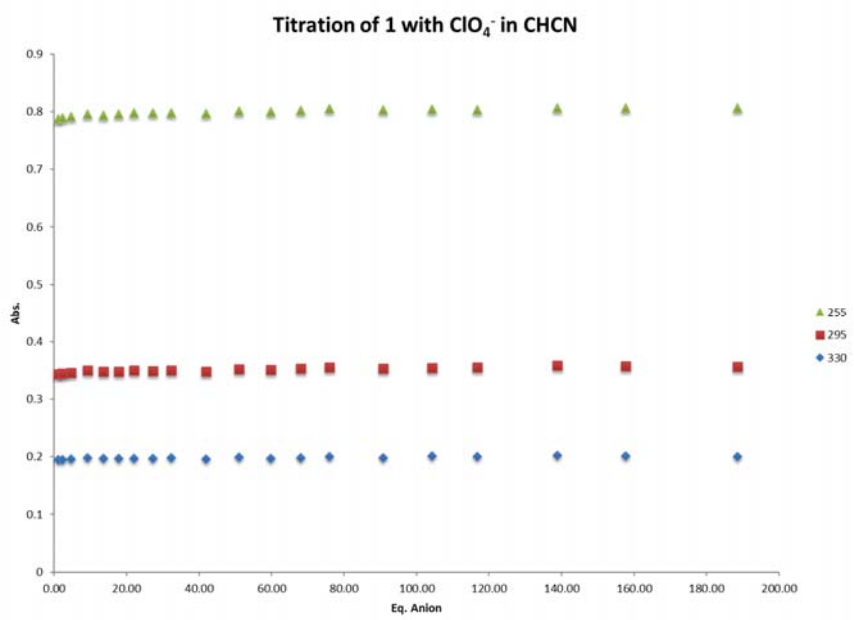

Figure S25. Binding isotherm ClO_4^- titration with **1**. The change in absorbance is negligible.

Fitting the data across a series of titrations with ClO_4^- in CHCN resulted in an error for K_a value.

^{1}H NMR Titration Conditions. ^{1}H NMR titrations were carried out on an Inova 500 MHz NMR spectrometer (^{1}H: 500.10 MHz). Chemical shifts (δ) are expressed in ppm downfield from tetramethylsilane (TMS) using non-deutrated solvent present in the bulk deutrated solvent ($CDCl_3$, ^{1}H 7.26 ppm; *d*$_6$-DMSO: ^{1}H 2.50 ppm). Mixed solvent systems were referenced to the most abundant solvent. All NMR spectra were processed using MestReNova NMR processing software. Association constants were determined using step-wise non-linear regression fitting in MatLab.[4]

Tetrabutylammonium dihydrogenphosphate with 1. A concentrated solution of 1 (2.09 mg, [R] = 0.968 mM) in 10% *d*$_6$-DMSO/$CDCl_3$ (3.00 mL) was prepared to yield the stock solution of **1**. This solution (2.34 mL) was used in the dilution of $TBAH_2PO_4$ guest solution (12.84 mg, [G] = 16.2 mM). The remaining stock solution (0.600 mL) was used as the starting volume in the NMR tube.

Table S13. Representative titration data for $H_2PO_4^-$ with **1**.

	Guest (μL)	[**1**] (M)	[$H_2PO_4^-$] (M)	Equiv.	H^c δ (ppm)	H^d δ (ppm)	H^a δ (ppm)	H^b δ (ppm)
1	0	9.68E-04	0.00E+00	0.00	8.635	8.592	8.024	7.714
2	5	9.68E-04	1.34E-04	0.14	8.829	8.575	8.125	7.819
3	10	9.68E-04	2.65E-04	0.27	9.140	8.551	8.274	7.993
4	15	9.68E-04	3.94E-04	0.41	9.444	8.529	8.409	8.152
5	20	9.68E-04	5.21E-04	0.54	9.705	8.510	8.484	8.307
6	25	9.68E-04	6.47E-04	0.67	9.927	8.496	8.626	8.419
7	30	9.68E-04	7.70E-04	0.80	10.099	8.483	8.693	8.517
8	35	9.68E-04	8.91E-04	0.92	10.215	8.472	8.733	8.581
9	40	9.68E-04	1.01E-03	1.04	10.317	8.464	8.773	8.642
10	50	9.68E-04	1.24E-03	1.28	10.455	8.453	8.824	8.708
11	60	9.68E-04	1.47E-03	1.52	10.558	8.446	8.851	8.774
12	80	9.68E-04	1.90E-03	1.97	10.639	8.436	8.877	8.811
13	100	9.68E-04	2.31E-03	2.39	10.688	8.430	8.890	8.838
14	150	9.68E-04	3.23E-03	3.34	10.801	8.442	8.902	8.902
15	200	9.68E-04	4.04E-03	4.18	10.847	8.418	8.905	8.905
16	300	9.68E-04	5.39E-03	5.57	10.831	8.415	8.904	8.904
17	400	9.68E-04	6.47E-03	6.68	10.852	8.412	8.904	8.904
18	600	9.68E-04	8.08E-03	8.35	10.925	8.411	8.906	8.906

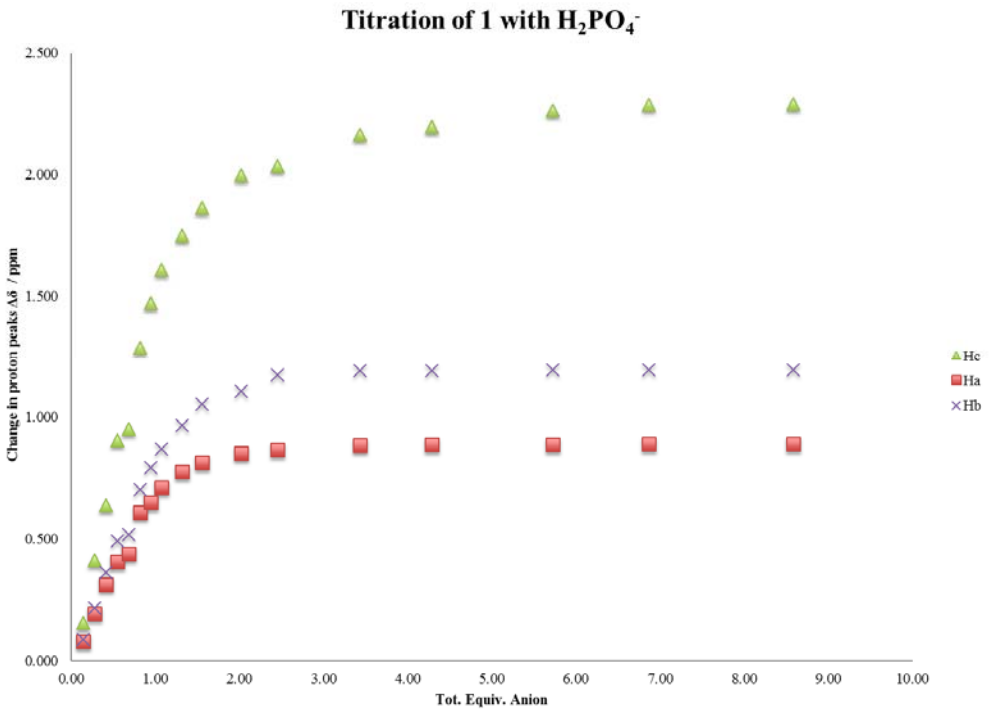

Figure S26. Binding isotherm for $H_2PO_4^-$ titration with **1** in 10% d_6-DMSO/$CDCl_3$ by ^1H NMR.

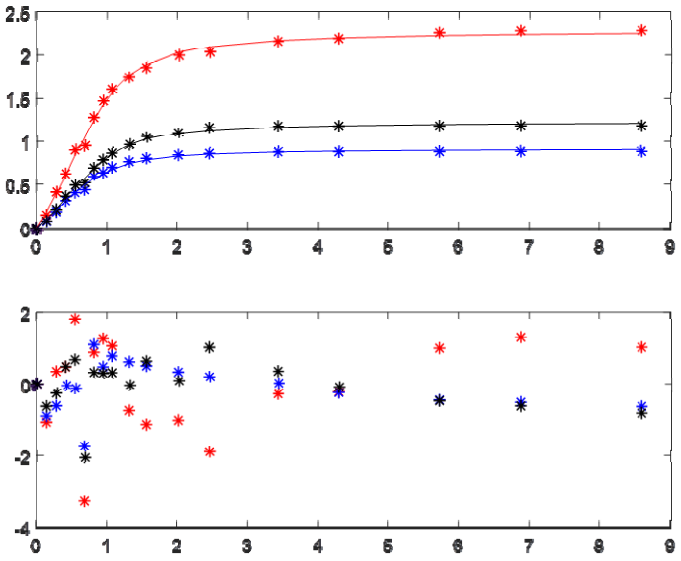

Figure S27. MatLab fit to a 2:1 model of the binding isotherm for $H_2PO_4^-$ titration with **1**.

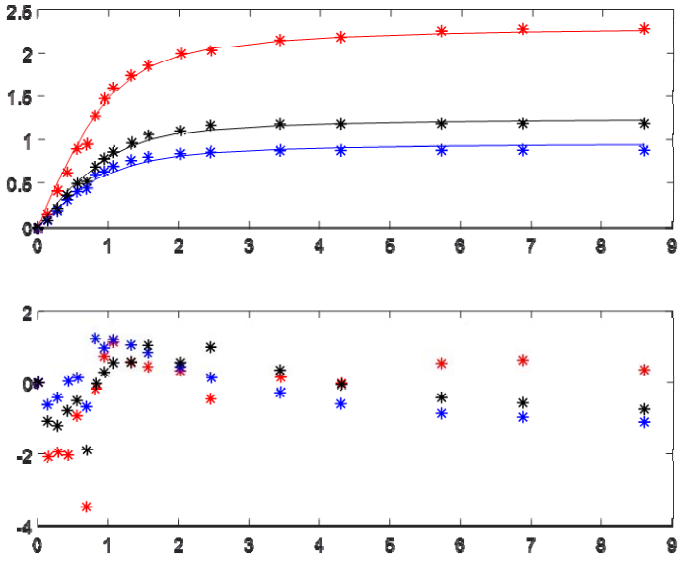

Figure S28. MatLab fit to a 1:1 model of the binding isotherm for $H_2PO_4^-$ titration with **1**. Improper fitting model due to lack of randomness of residuals.

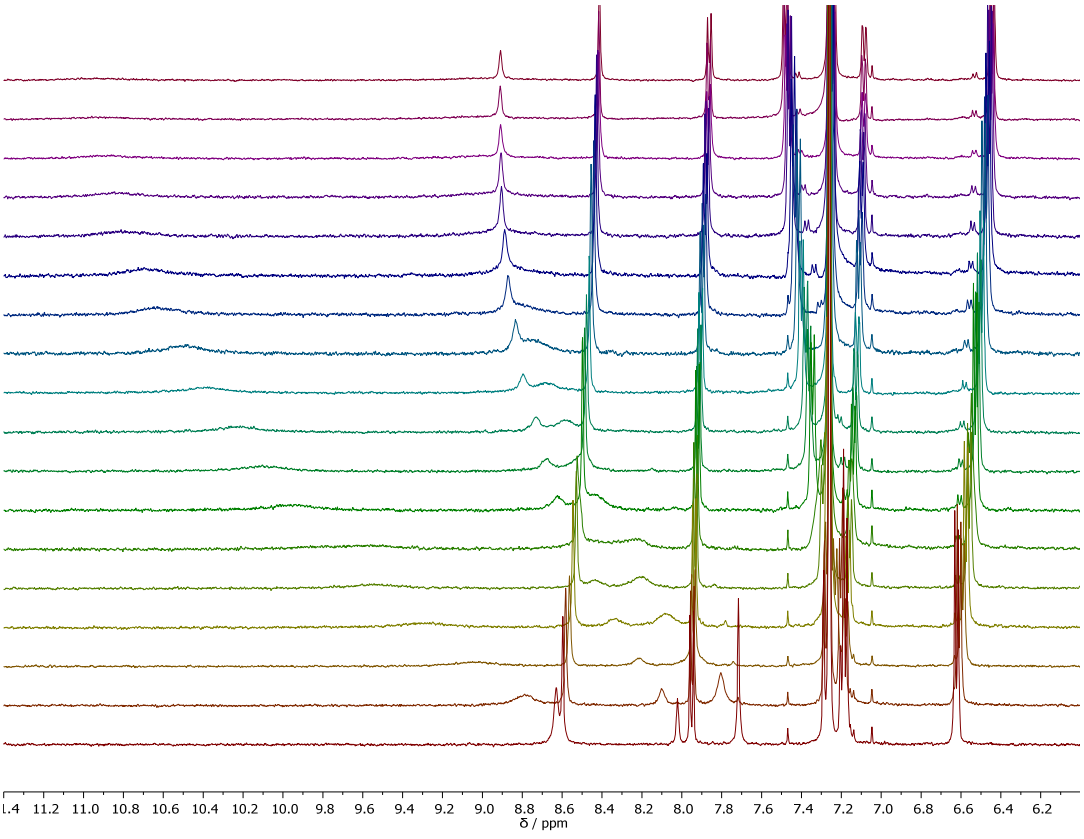

Figure S29. ^{1}H NMR spectra of $H_2PO_4^-$ titration with **1**.

Tetrabutylamamonium bromide with 1. A stock solution of **1** (2.19 mg, [R] = 1.01 mM) in 10% d_6-DMSO/$CDCl_3$ (3.00 mL) was prepared. This solution (2.34 mL) was used in the dilution of TBABr guest solution (28.1 mg, [G] = 37.3 mM). The remaining stock solution (0.600 mL) was used as the starting volume in the NMR tube.

Table S14. Representative titration data for Br^- with **1**.

	Guest (μL)	[**1**] (M)	[Br^-] (M)	Equiv.	H^c δ (ppm)	H^d δ (ppm)	H^b δ (ppm)	H^a δ (ppm)
1	0	1.01E-03	0.00E+00	0.00	8.628	8.596	8.018	7.714
2	5	1.01E-03	3.08E-04	0.30	8.657	8.592	8.056	7.717
3	10	1.01E-03	6.12E-04	0.60	8.681	8.589	8.089	7.717
4	15	1.01E-03	9.10E-04	0.90	8.701	8.584	8.116	7.718
5	20	1.01E-03	1.20E-03	1.19	8.723	8.583	8.145	7.719
6	25	1.01E-03	1.49E-03	1.47	8.744	8.580	8.174	7.720
7	30	1.01E-03	1.78E-03	1.75	8.763	8.578	8.198	7.721
8	35	1.01E-03	2.06E-03	2.03	8.780	8.575	8.220	7.722
9	40	1.01E-03	2.33E-03	2.30	8.795	8.573	8.240	7.223
10	50	1.01E-03	2.87E-03	2.83	8.821	8.569	8.276	7.726
11	60	1.01E-03	3.39E-03	3.34	8.845	8.566	8.308	7.728
12	80	1.01E-03	4.39E-03	4.33	8.885	8.561	8.363	7.731
13	100	1.01E-03	5.33E-03	5.26	8.920	8.559	8.411	7.733
14	150	1.01E-03	7.46E-03	7.36	8.985	8.550	8.506	7.739
15	200	1.01E-03	9.33E-03	9.20	9.031	8.546	8.565	7.743
16	300	1.01E-03	1.24E-02	12.26	9.094	8.538	8.655	7.747
17	400	1.01E-03	1.49E-02	14.71	9.123	8.535	8.682	7.751
18	600	1.01E-03	1.87E-02	18.39	9.160	8.532	8.722	7.756

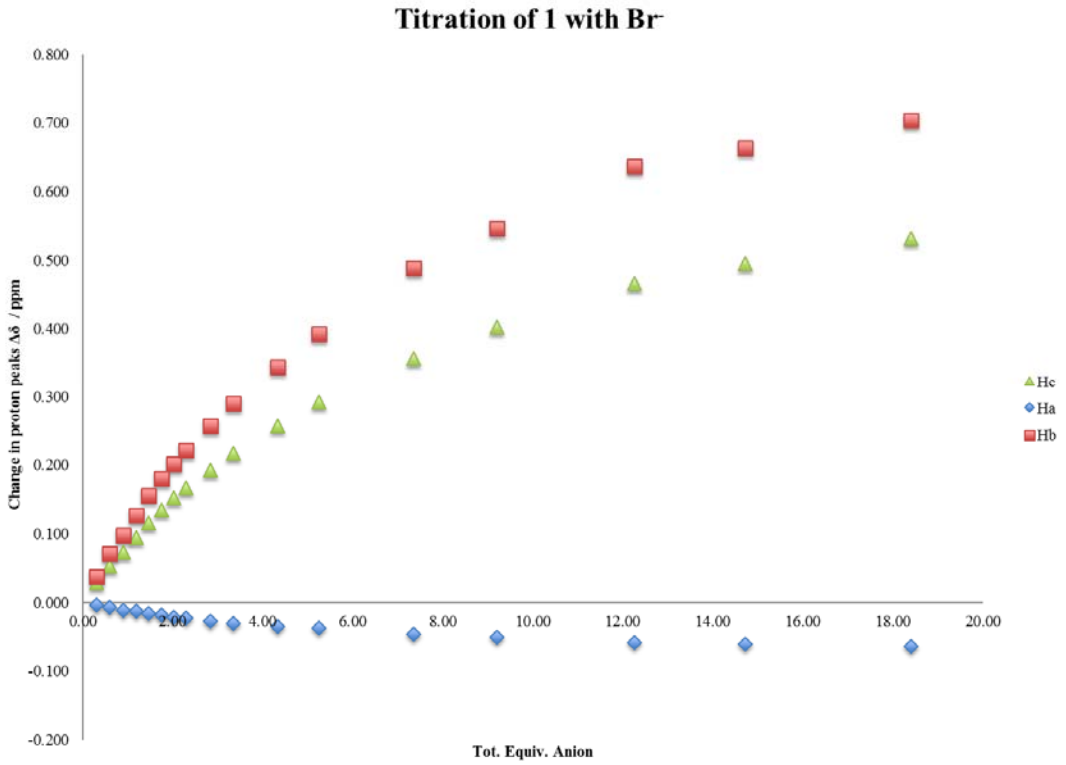

Figure S30. Binding isotherm for Br^- titration with **1** in 10% d_6-DMSO/$CDCl_3$ by ^1H NMR.

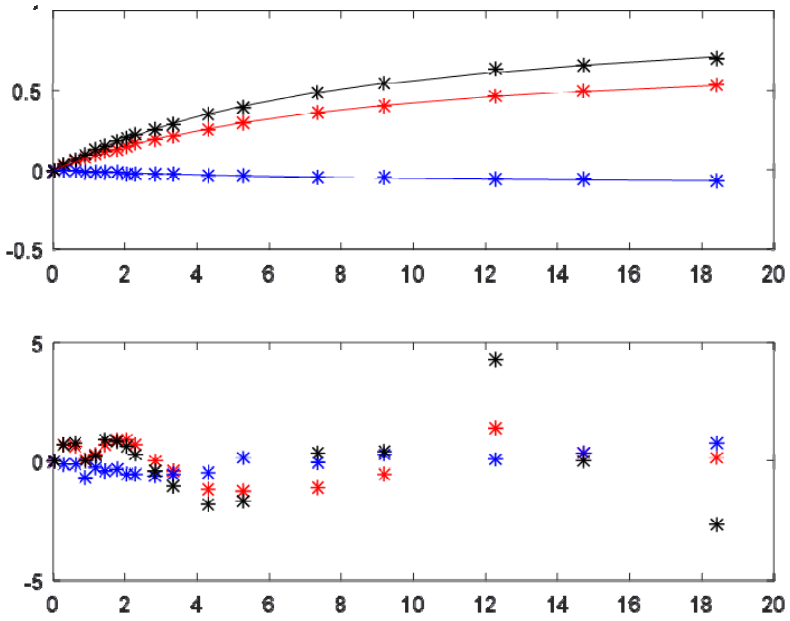

Figure S31. MatLab fit of binding isotherm for Br^- titration with **1**.

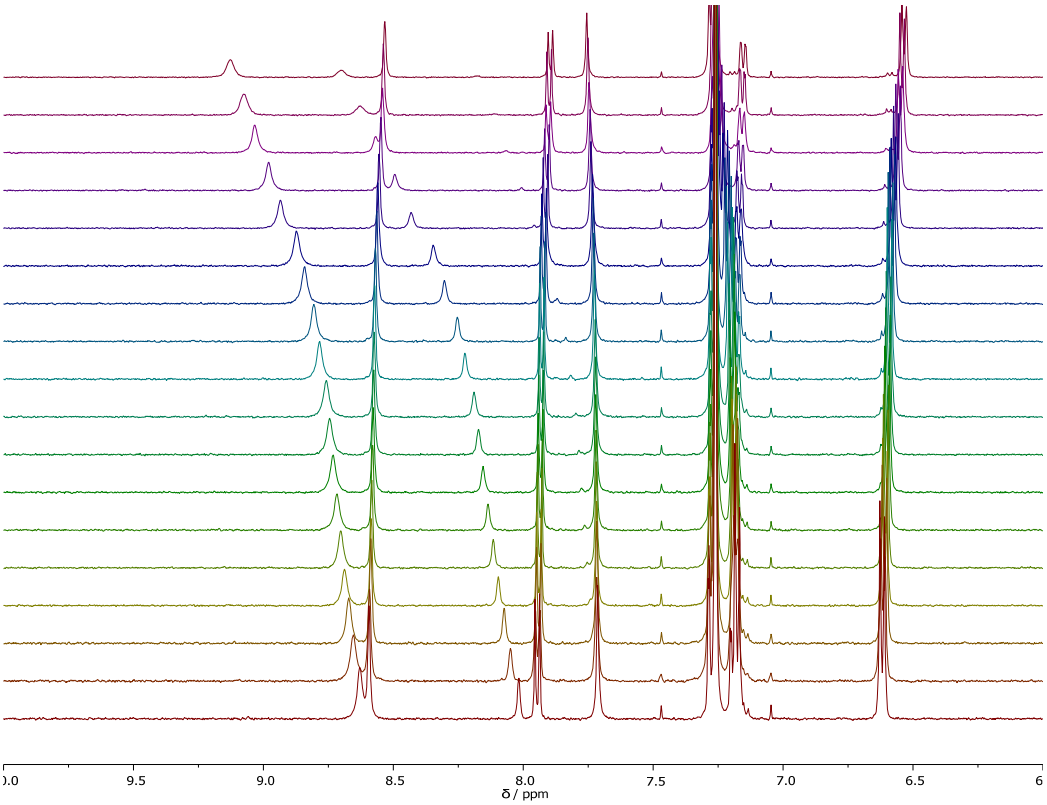

Figure S32. ^{1}H NMR spectra of Br^{-} titration with **1**.

Job's Plot Analysis

Figure S33. Binding isotherm for $H_2PO_4^-$ titration with **2** in 10% DMSO/$CHCl_3$ by UV-Vis.

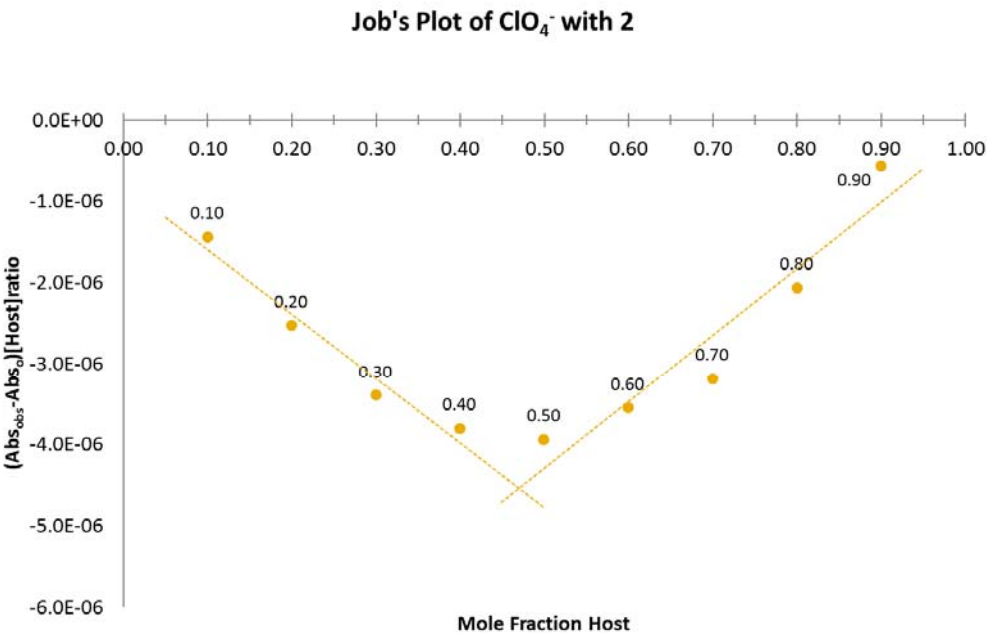

Figure S34. Binding isotherm for ClO_4^- titration with **2** in 10% DMSO/$CHCl_3$ by UV-Vis.

Figure S35. Binding isotherm for $H_2PO_4^-$ titration with **3** in 10% DMSO/$CHCl_3$ by UV-Vis.

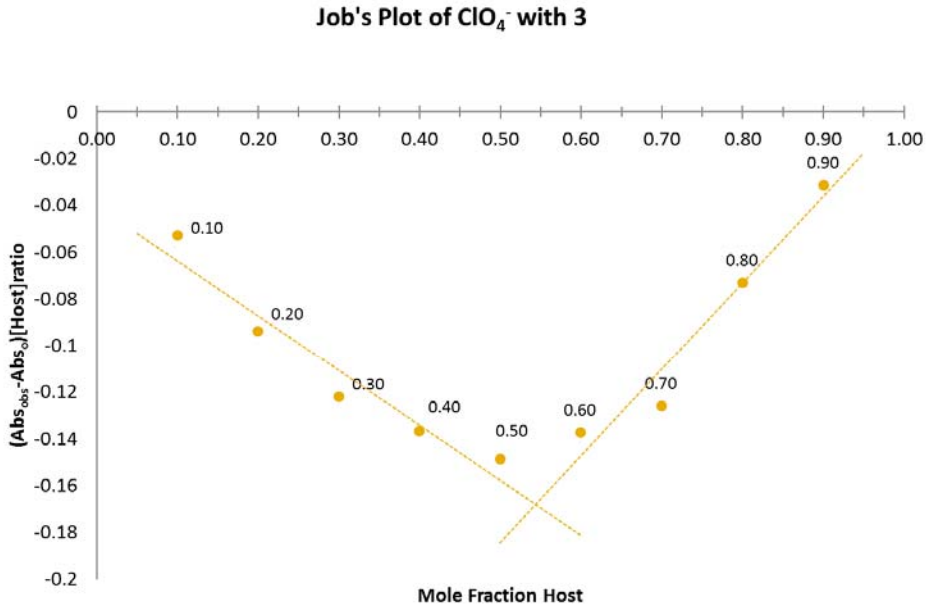

Figure S36. Binding isotherm for ClO_4^- titration with **3** in 10% DMSO/$CHCl_3$ by UV-Vis.

Complete Authorship of Gaussian 09

Gaussian 09, Revision **D.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.[5]

General Computational Procedure

Manual, exhaustive conformation searches were performed to locate all relevant structures. All conformers were optimized using the Gaussian 09 computational package (see above reference) using PBE[5] with the 6-31G(d)[6] basis set for all atoms. Minima were confirmed with vibrational frequency computations, with all structures having zero imaginary vibrational frequencies. Frequencies were computed at 1 atm and 298.15 K (25 ºC) in order to match experimental reaction conditions as close as possible. All images were generated with PyMOL[7] with distances in Ångströms (Å).

Computed Geometries

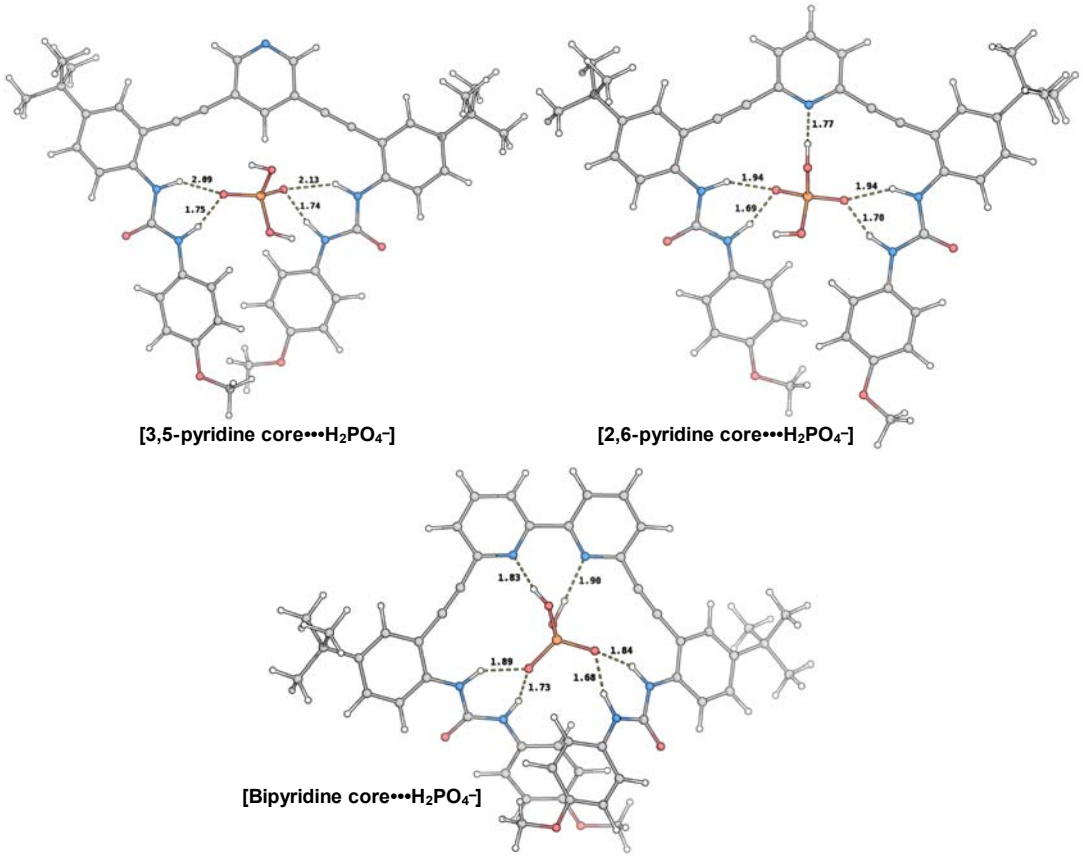

Figure S37. Optimized hosts with $H_2PO_4^-$.

[3,5-pyridine core•••$H_2PO_4^-$]

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

pbepbe/6-31G*/auto gfprint gfinput scf=(direct,tight,maxcycle=300,xqc) opt=(maxcycle=250) freq=noraman iop(1/8=18) Temperature=298.15
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---

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Charge = -1 Multiplicity = 1

SCF Energy= -2956.88311529 Predicted Change= -4.813685D-08

==========

Optimization completed. {Found 1 times}

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P	-0.258074	-0.029645	1.314522
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Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

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Zero-point correction (ZPE)=	-2956.0544	0.82871
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Gibbs Free Energy (G)=	-2956.1557	0.72740

Frequencies -- 7.1336 11.5027 14.1963

[2,6-pyridine core•••$H_2PO_4^-$]

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

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Pointgroup= C1 Stoichiometry= C45H47N5O8P(1-) C1[X(C45H47N5O8P)] #Atoms= 106
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H	-8.047049	-3.622618	-3.106262
H	-8.984755	-4.999126	-2.448776
C	-6.152898	-2.890398	-0.354789
H	-5.945787	-3.965938	-0.326458
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O	2.642118	7.335197	-1.072028
C	3.754795	8.210062	-0.985519
H	4.490267	8.025772	-1.794668
H	4.276189	8.123401	-0.010529
H	3.350270	9.229020	-1.090597
C	1.791594	5.128164	-1.045727

H	0.801013	5.563961	-1.208143
C	1.942135	3.748995	-0.918650
H	1.066019	3.095753	-1.001693
C	-3.608752	4.571234	0.881263
H	-4.660956	4.355477	0.694114
C	-3.172046	5.880130	1.097750
H	-3.885573	6.710788	1.083156
C	-1.814437	6.166501	1.331828
O	-1.499495	7.497845	1.523111
C	-0.123557	7.809797	1.709307
H	0.294678	7.309477	2.605661
H	-0.081835	8.900824	1.855201
H	0.492165	7.537117	0.829623
C	-0.888465	5.108767	1.356664
H	0.176813	5.287094	1.520752
C	-1.323214	3.795170	1.139950
H	-0.590837	2.980450	1.154389
P	-0.134276	-0.034376	-0.390360
O	-1.337900	0.024849	0.568570
O	-0.273110	1.175560	-1.523338
H	-1.211914	1.235258	-1.795239
O	-0.252913	-1.350661	-1.342679
H	-0.323174	-2.142592	-0.719852
O	1.266350	0.120867	0.207207

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy= -2956.88200469 Predicted Change= -1.501878D-08
Zero-point correction (ZPE)= -2956.0539 0.82808
Internal Energy (U)= -2955.9944 0.88754
Enthalpy (H)= -2955.9935 0.88849
Gibbs Free Energy (G)= -2956.1544 0.72752

Frequencies -- 6.4289 9.4121 15.7228

[Bipyridine core•••$H_2PO_4^-$]

Using Gaussian 09: AM64L-G09RevD.01 24-Apr-2013

==========

# pbepbe/6-31G*/auto gfprint gfinput scf=(direct,tight,maxcycle=300,xqc)
opt=(maxcycle=250) freq=noraman iop(1/8=18) Temperature=298.15
#N Geom=AllCheck Guess=TCheck SCRF=Check Test GenChk RPBEPBE/6-31G(d)/Auto
Freq

Pointgroup= C1 Stoichiometry= C50H50N6O8P(1-) C1[X(C50H50N6O8P)] #Atoms= 115
Charge = -1 Multiplicity = 1

SCF Energy= -3203.67970897 Predicted Change= -7.545578D-09

==========

Optimization completed. {Found 1 times}

Item	Max Val.	Criteria	Pass?	RMS Val.	Criteria	Pass?
Force	0.00001	0.00045	[YES]	0.00000	0.00030	[YES]
Displ	0.00372	0.00180	[NO]	0.00372	0.00180	[YES]

Atomic Type	Coordinates (Angstroms) X	Y	Z
C	-3.700700	-5.349797	0.721841
H	-4.744192	-5.268573	1.038436
C	-2.997836	-6.548607	0.813905
H	-3.484075	-7.445823	1.212061
C	-1.654051	-6.588267	0.417491
H	-1.064554	-7.503406	0.523296
C	-1.061885	-5.413176	-0.087699
N	-1.736095	-4.249319	-0.186800
C	-3.031037	-4.197984	0.229646
C	-3.717651	-2.955350	0.178060
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C	-5.282912	-0.833413	0.408433
C	-4.830782	0.472192	0.806147
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H	-1.175895	1.219549	0.710620
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C	-5.826691	1.446887	1.060457
H	-5.503342	2.430601	1.400576
C	-7.181334	1.163471	0.888355
H	-7.894560	1.969732	1.086884
C	-7.647279	-0.100299	0.459206
C	-9.138316	-0.425342	0.238890
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H	-9.823051	1.645217	-0.079457
H	-9.949840	1.092320	1.616115
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C	-9.556587	-1.605930	1.150263
H	-8.958352	-2.510267	0.945558
H	-10.620661	-1.861962	0.990081
H	-9.420030	-1.347875	2.214914
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C	0.903378	-6.576879	-1.141413
H	0.266104	-7.443678	-1.338514
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H	9.469730	0.416988	1.963406
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H	10.721321	-0.782579	1.547293
C	7.129961	0.523643	0.317177
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N	3.579330	0.609072	-0.839988
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P	-0.170249	-0.988826	-0.911894

O	1.138982	-0.551726	-1.590245
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H	0.498858	-2.636016	0.347560
O	-0.802265	-2.168706	-1.854658
H	-1.224280	-2.853254	-1.261102
O	-1.198578	0.122918	-0.632044

Statistical Thermodynamic Analysis
Temperature= 298.150 Kelvin Pressure= 1.00000 Atm

==========

SCF Energy=	-3203.67970897	Predicted Change= -7.545578D-09
Zero-point correction (ZPE)=	-3202.7835	0.89616
Internal Energy (U)=	-3202.7200	0.95961
Enthalpy (H)=	-3202.7191	0.96055
Gibbs Free Energy (G)=	-3202.8889	0.79077

Frequencies --	4.7093	10.1799	13.3351

References

1. (*a*) C. N. Carroll, B. A. Coombs, S. P. McClintock, C. A. Johnson, O. B. Berryman, D. W. Johnson and M. M. Haley, *Chem. Commun.* 2011, **47**, 5539–5541; (*b*) C. N. Carroll, O. B. Berryman, C. A. Johnson, L. N. Zakharov, M. M. Haley and D. W. Johnson, *Chem. Commun.* 2009, 2520–2522.

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3. http://supramolecular.org

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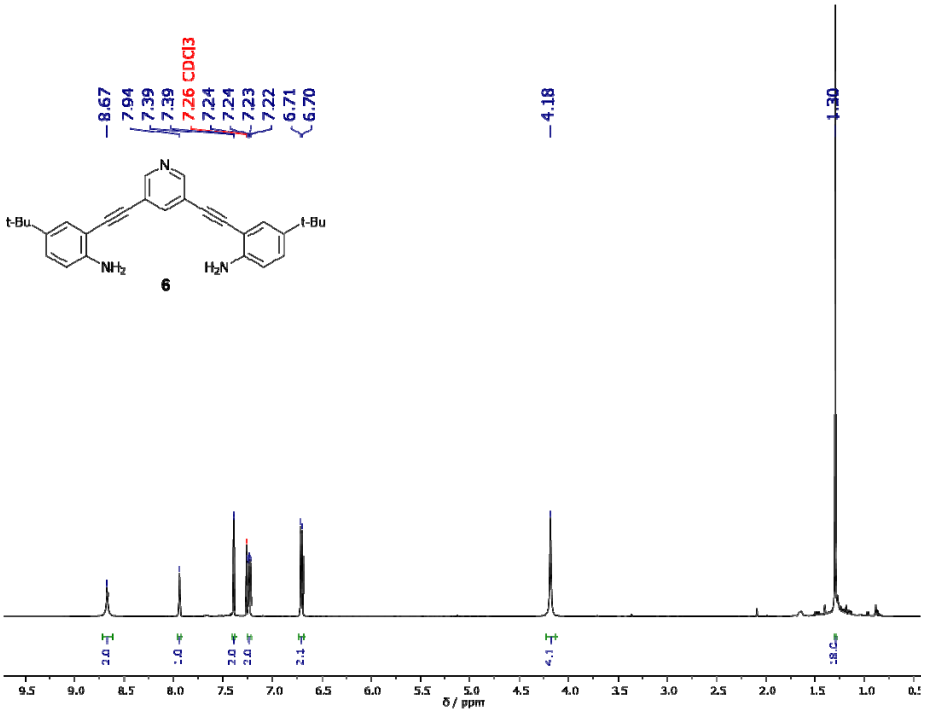
5. (a) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 1996, **77**, 3865–6868. (b) J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* 1997, **78**, 1396.

6. S. Grimme, S. Ehrlich, L. Goerigk. *J. Comput. Chem.* 2011, **32**, 1456–1465.

7. The PyMOL Molecular Graphics System, Version 1.7.4.2 Schrödinger, LLC.

NMR Spectra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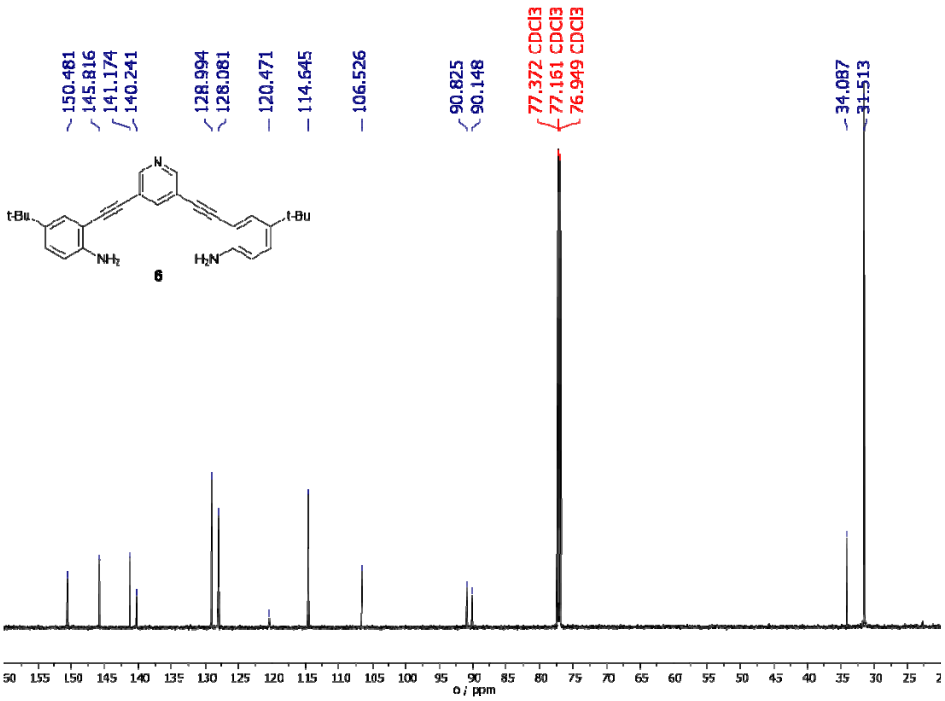
4.18
1.30
t-Bu
t-Bu
NH2
H2N
6
δ / ppm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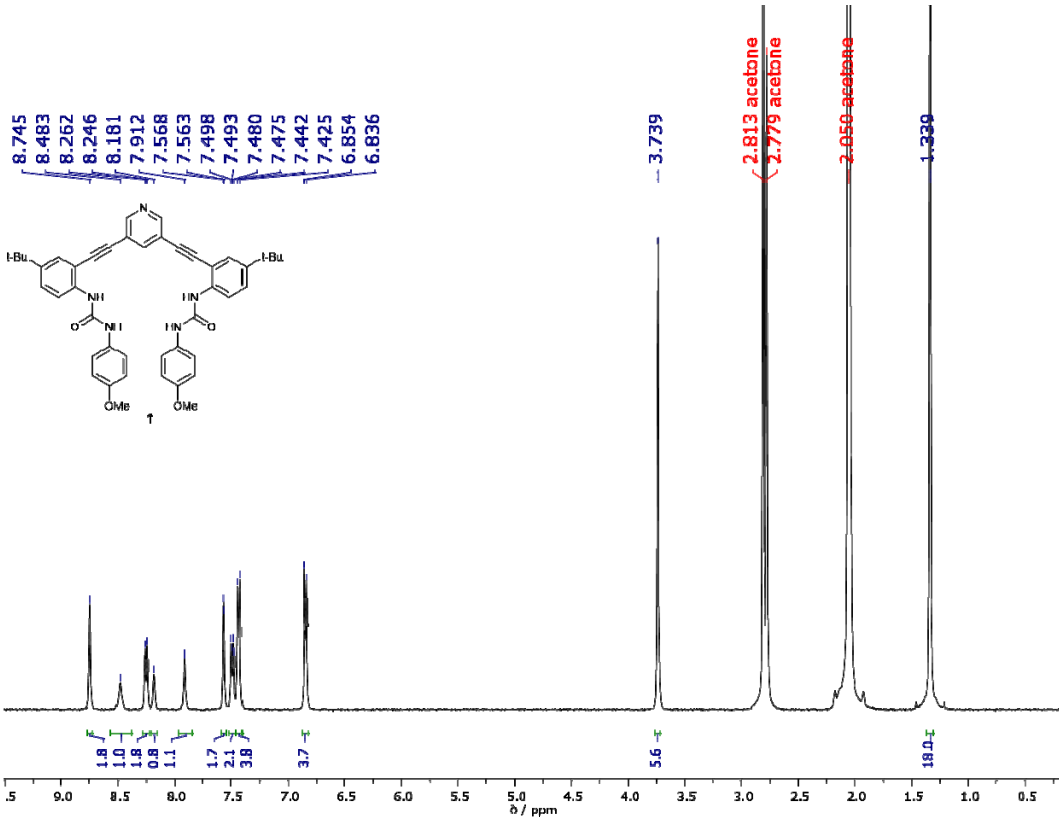
6
δ / ppm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3.739
2.813 acetone
2.779 acetone
2.050 acetone
1.339
t-Bu
t-Bu
NH
HN
NH
HN
OMe
OMe
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1.8
0.8
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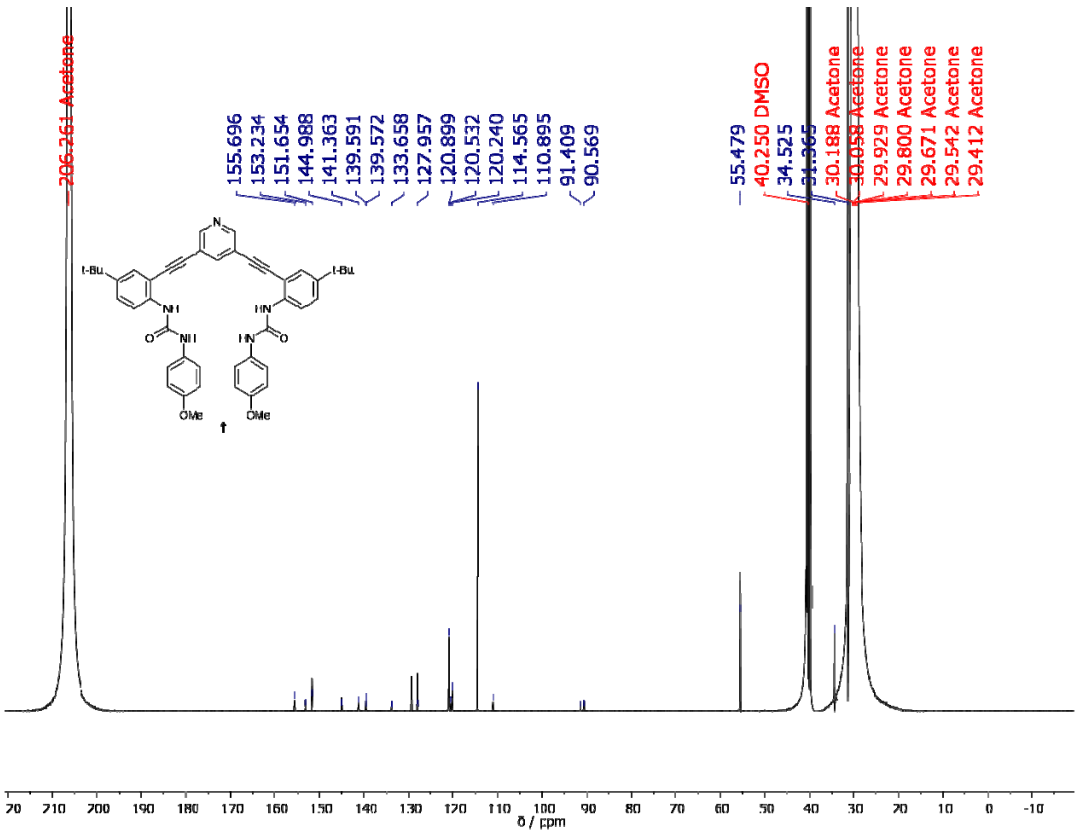
1.7
2.1
3.8
3.7
5.6
18.0
δ / ppm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90.569
55.479
40.250 DMSO
34.525
31.365
30.188 Acetone
30.038 Acetone
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29.800 Acetone
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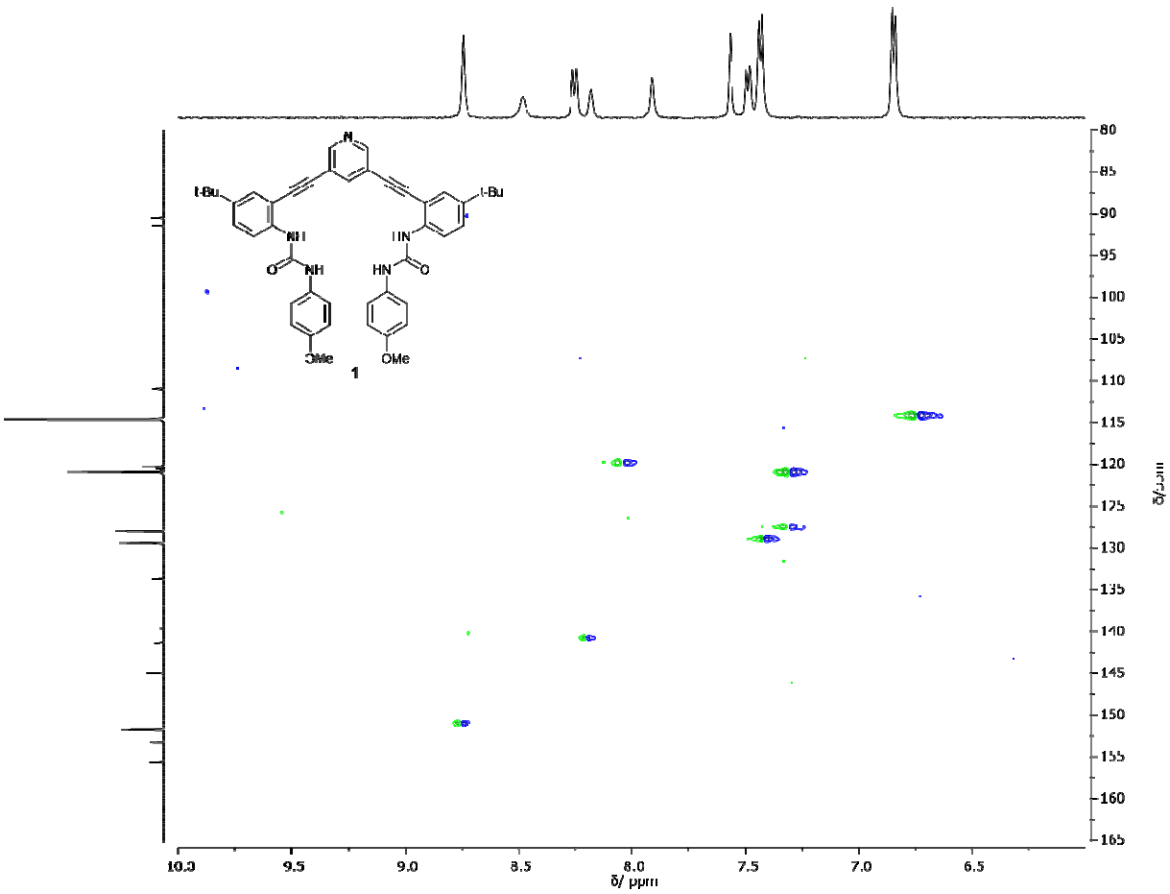
t-Bu
t-Bu
NH
HN
NH
HN
OMe
OMe
δ / ppm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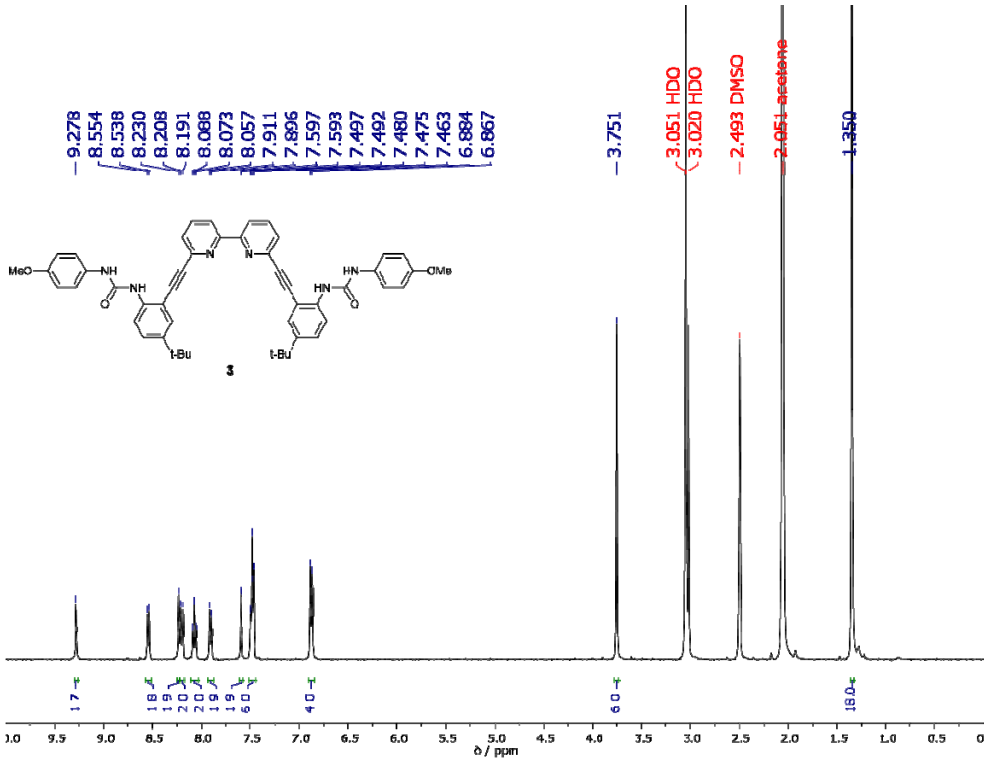
δ/ ppm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7.463
6.884
6.867
3.751
3.051 HDO
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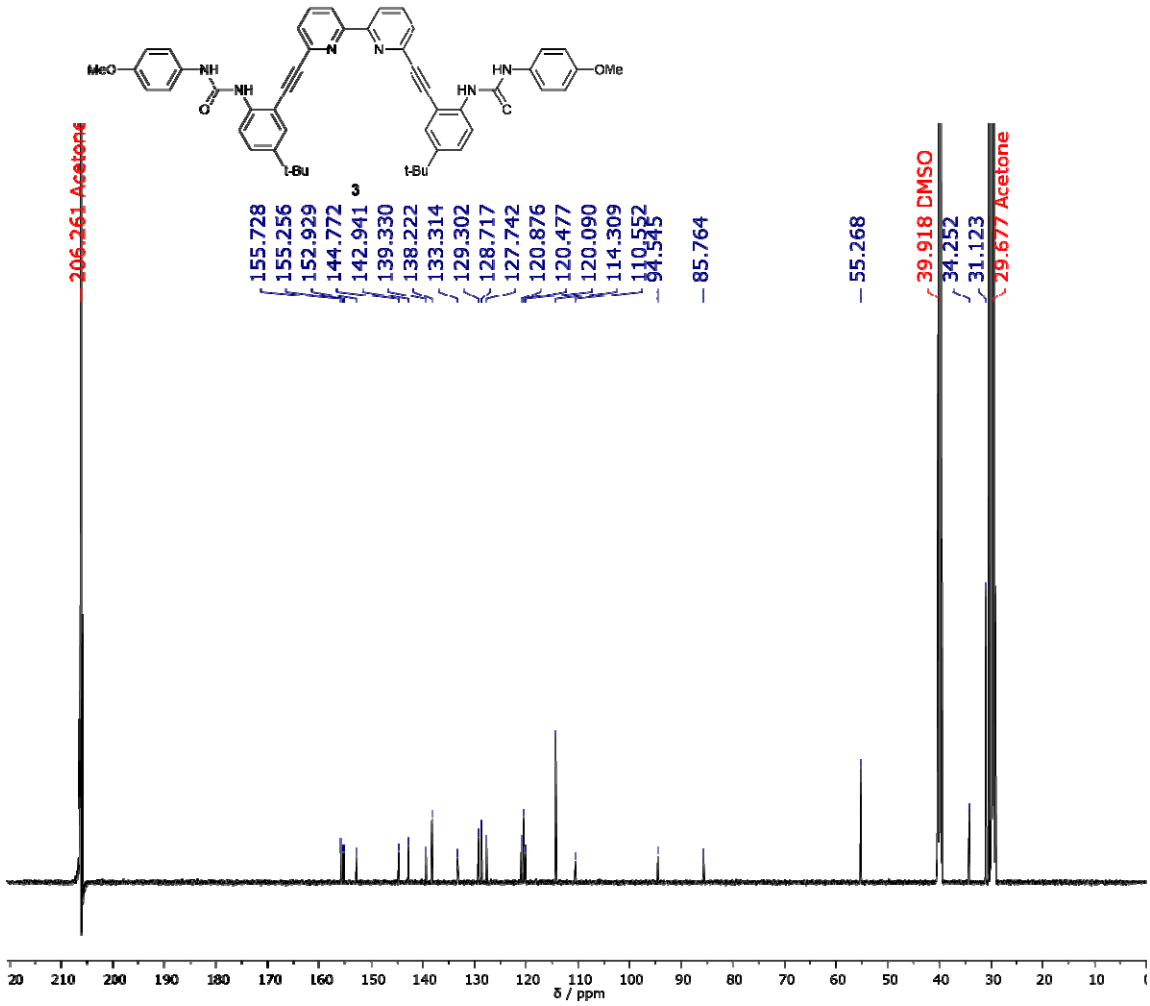
2.493 DMSO
2.051 acetone
1.350
MeO
NH
NH
HN
OMe
t-Bu
t-Bu
3
δ / ppm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138.222
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55.268
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31.123
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δ / ppm