Binding Studies

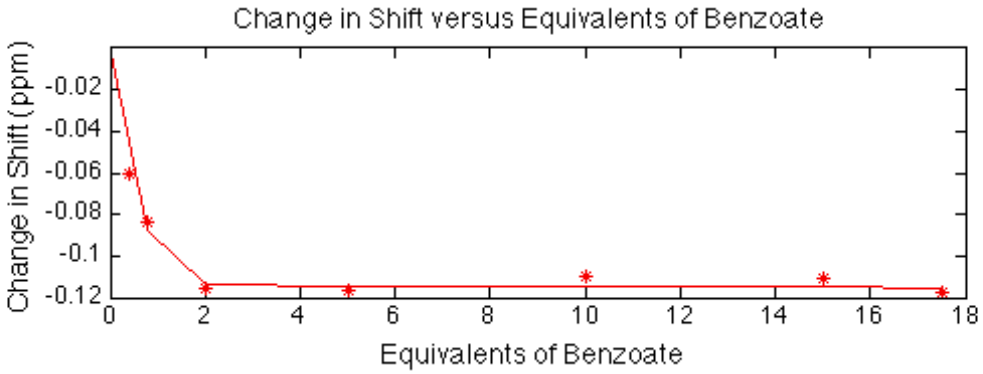
General Procedure for Association Constant Calculations:
Pall Thordarson's NMR titration fitting software for Matlab was used to calculate all association constants. Parameters were entered such that the lowest sum of squares was found for each trial. In cases where the parameters for finding the lowest sum of squares generated an error message, the parameters that yielded reasonable % conf. int. (from asymptotic error) and association constants were used.

Acylguanidinium Tetrafluoroborate (2) Bound to Potassium Benzoate (1) in 9:1 DMSO: D_2O

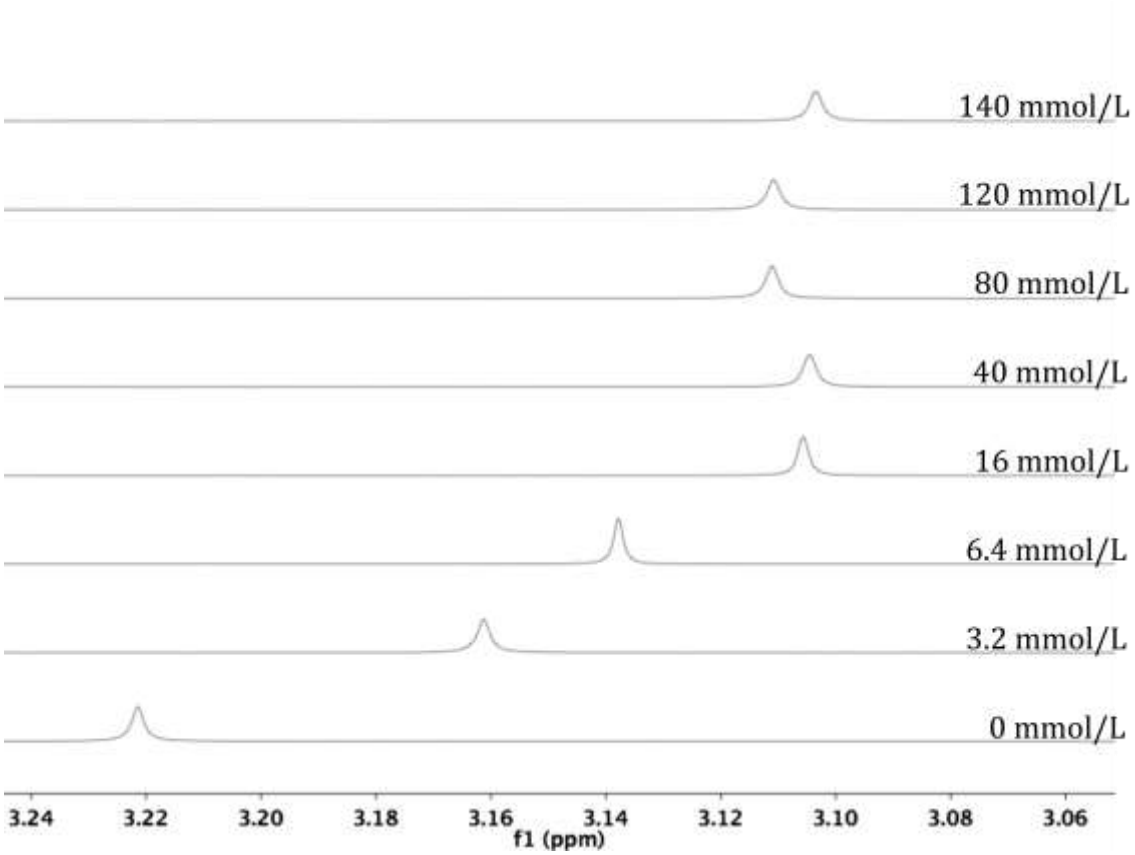
Procedure for NMR Titrations:
80 mmol/L and 160 mmol/L stock solutions of acylguanidinium tetrafluoroborate **2** (Host) and potassium benzoate **1** (Guest) were made, respectively. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 23°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

90% DMSO								
Host conc. (M)	Guest conc. (M)	Amt. Host Added (uL)	Amt. Guest Added (uL)	Equiv. of Guest	Final Vol. (mL)	δ (ppm) Acyl Trial 1	δ (ppm) Acyl Trial 2	δ (ppm) Acyl Trial 3
0.008	0.0000	100	0	0.00	1	3.221415	3.221415	3.221415
0.008	0.0032	100	20	0.40	1	3.161196	3.157562	3.160638
0.008	0.0064	100	40	0.80	1	3.137769	3.138596	3.138828
0.008	0.0160	100	100	2.00	1	3.105648	3.105749	3.104153
0.008	0.0400	100	250	5.00	1	3.104527	3.109005	3.108891
0.008	0.0800	100	500	10.00	1	3.111099	3.112506	3.107811
0.008	0.1200	100	750	12.50	1	3.110816	3.105730	3.110226
0.008	0.1400	100	875	18.75	1	3.103435	3.105862	3.105697

	Ka
Trial 1	1186.89
Trial 2	923.21
Trial 3	1160.18
Average	1090.09
Standard Deviation	145.14
% Error	13.31



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shift for acylguanidinium peak for Trial 1.

Job's Method for Stoichiometry Determination in 9:1 DMSO: D_2O

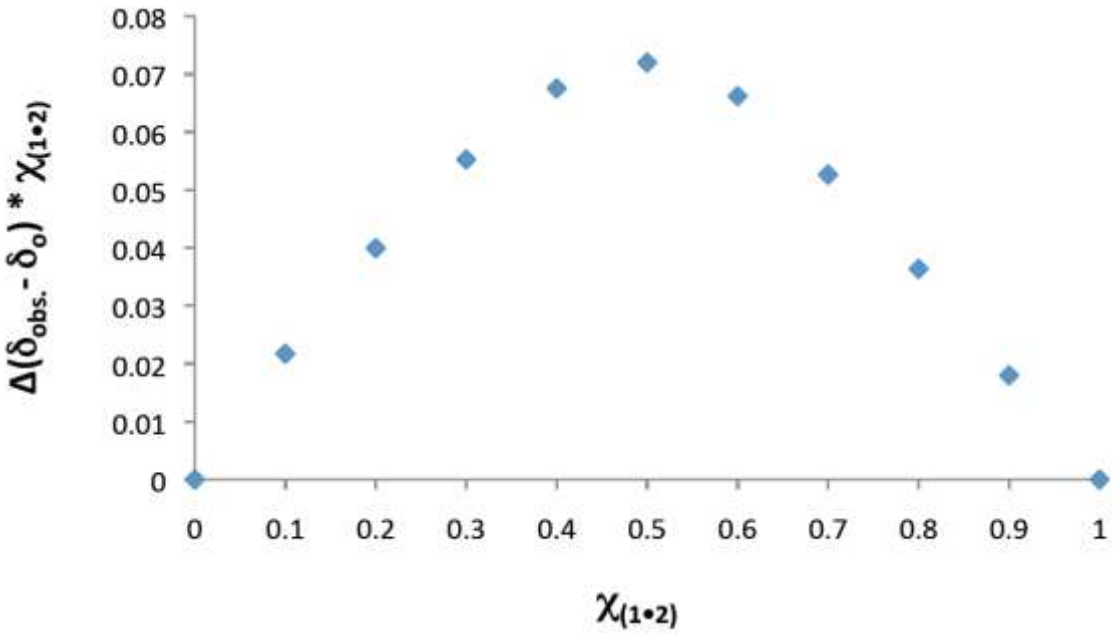
General Procedure: 8 mmol/ L stock solutions were made of acylguanidinium tetrafluoroborate **2** (Host) and of potassium benzoate **1** (Guest). Contents were bound for two hours at 22˚C. The acyl peak of the host and five of the benzoate peaks of the guest were monitored. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

Sample	δ (ppm) Acyl Trial 1	δ (ppm) Benzoate 1 Trial 1	δ (ppm) Benzoate 2 Trial 1	δ (ppm) Benzoate 3 Trial 1	δ (ppm) Benzoate 4 Trial 1	δ (ppm) Benzoate 5 Trial 1	$\chi_{(1•2)}$	Amt. 2 (mL)	Amt. 1 mL)
1	3.2361739						0	1	0
2	3.2066877	8.5574104	8.5759823	8.5952125	9.0102323	9.0367601	0.1	0.9	0.1
3	3.1787721	8.5399206	8.5582248	8.5777249	9.0121851	9.0293789	0.2	0.8	0.2
4	3.1492055	8.5244397	8.5429080	8.5623816	9.0055900	9.0227827	0.3	0.7	0.3
5	3.1187170	8.5090678	8.5268550	8.5462553	8.9985571	9.0167039	0.4	0.6	0.4
6	3.0883041	8.4842134	8.5019015	8.5210240	8.9863522	9.0034648	0.5	0.5	0.5
7	3.0657571	8.4505627	8.4679489	8.4866170	8.9699445	8.9870534	0.6	0.4	0.6
8	3.0448004	8.4154339	8.4325066	8.4509554	8.9521835	8.9691616	0.7	0.3	0.7
9	3.0208814	8.3856757	8.4026733	8.4203858	8.9373094	8.9538263	0.8	0.2	0.8
10	2.9855634	8.3602190	8.3763823	8.3941767	8.9253890	8.9419320	0.9	0.1	0.9
11		8.3402374	8.3543683	8.3742584	8.9163798	8.9315440	1	0	1

Sample	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\chi_{(1•2)}$	χ_2	χ_1
1	0						0	1	0
2	0.0294862	0.2171730	0.2216140	0.2209541	0.0938525	0.1052161	0.1	0.9	0.1
3	0.0574018	0.1996832	0.2038565	0.2034665	0.0958053	0.0978349	0.2	0.8	0.2
4	0.0869684	0.1842023	0.1885397	0.1881232	0.0892102	0.0912387	0.3	0.7	0.3
5	0.1174569	0.1688304	0.1724867	0.1719969	0.0821773	0.0851599	0.4	0.6	0.4
6	0.1478698	0.1439760	0.1475332	0.1467656	0.0699724	0.0719208	0.5	0.5	0.5
7	0.1704168	0.1103253	0.1135806	0.1123586	0.0535647	0.0555094	0.6	0.4	0.6
8	0.1913735	0.0751965	0.0781383	0.0766970	0.0358037	0.0376176	0.7	0.3	0.7
9	0.2152925	0.0454383	0.0483050	0.0461274	0.0209296	0.0222823	0.8	0.2	0.8
10	0.2506105	0.0199816	0.0220140	0.0199183	0.0090092	0.0103880	0.9	0.1	0.9
11		0	0	0	0	0	1	0	1

Sample	$\Delta(\delta_o - \delta_{obs.}) * \chi_1$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\chi_{(1•2)}$	χ_2	χ_1
1	0						0	1	0
2	0.0265375	0.0217173	0.0221614	0.0220954	0.0093852	0.0105216	0.1	0.9	0.1
3	0.0459214	0.0399366	0.0407713	0.0406933	0.0191610	0.0195669	0.2	0.8	0.2
4	0.0608778	0.0552606	0.0565619	0.0564369	0.0267630	0.0273716	0.3	0.7	0.3
5	0.0704741	0.0675321	0.0689946	0.0687987	0.0328709	0.0340639	0.4	0.6	0.4
6	0.0739349	0.0719880	0.0737666	0.0733828	0.0349862	0.0359604	0.5	0.5	0.5
7	0.0681667	0.0661951	0.0681483	0.0674151	0.0321388	0.0333056	0.6	0.4	0.6
8	0.0574120	0.0526375	0.0546968	0.0536879	0.0250625	0.0263323	0.7	0.3	0.7
9	0.0430585	0.0363506	0.0386440	0.0369019	0.0167436	0.0178258	0.8	0.2	0.8
10	0.0250610	0.0179834	0.0198126	0.0179264	0.0081082	0.0093492	0.9	0.1	0.9
11		0	0	0	0	0	1	0	1

Sample	δ (ppm) Acyl Trial 2	δ (ppm) Benzoate 1 Trial 2	δ (ppm) Benzoate 2 Trial 2	δ (ppm) Benzoate 3 Trial 2	δ (ppm) Benzoate 4 Trial 2	δ (ppm) Benzoate 5 Trial 2	$\chi_{(1•2)}$	Amt. 2 (mL)	Amt. 1 mL)
1	3.2185120						0	1	0
2	3.1884134	8.5388782	8.5575312	8.5769509	9.0031140	9.0203238	0.1	0.9	0.1
3	3.1611428	8.5211116	8.5397357	8.5591029	8.9956519	9.0130832	0.2	0.8	0.2
4	3.1338423	8.5074249	8.5255142	8.5450493	8.9896080	9.0070596	0.3	0.7	0.3
5	3.1045568	8.4914094	8.5091422	8.5282302	8.9824731	8.9997172	0.4	0.6	0.4
6	3.0766003	8.4667163	8.4844244	8.5030453	8.9703380	8.9878671	0.5	0.5	0.5
7	3.0556283	8.4331696	8.4506832	8.4696327	8.9540061	8.9711270	0.6	0.4	0.6
8	3.0366637	8.4009591	8.4180862	8.4365248	8.9383175	8.9554446	0.7	0.3	0.7
9	3.0134314	8.3725935	8.3896520	8.4076039	8.9238910	8.9403230	0.8	0.2	0.8
10	2.9781264	8.3483793	8.3644240	8.3821740	8.9118291	8.9276353	0.9	0.1	0.9
11		8.3276583	8.3419521	8.3611416	8.9018381	8.9170365	1	0	1
Sample	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\chi_{(1•2)}$	χ_2	χ_1
1	0						0	1	0
2	0.0300986	0.2112199	0.2155791	0.2158093	0.1012759	0.1032873	0.1	0.9	0.1
3	0.0573692	0.1934533	0.1977836	0.1979613	0.0938138	0.0960467	0.2	0.8	0.2
4	0.0846697	0.1797666	0.1835621	0.1839077	0.0877699	0.0900231	0.3	0.7	0.3
5	0.1139552	0.1637511	0.1671901	0.1670886	0.080635	0.0826807	0.4	0.6	0.4
6	0.1419117	0.1390580	0.1424723	0.1419037	0.0684999	0.0708306	0.5	0.5	0.5
7	0.1628837	0.1055113	0.1087311	0.1084911	0.0521680	0.0540905	0.6	0.4	0.6
8	0.1818483	0.0733008	0.0761341	0.0753832	0.0364794	0.0384081	0.7	0.3	0.7
9	0.2050806	0.0449352	0.0476999	0.0464623	0.0220529	0.0232865	0.8	0.2	0.8
10	0.2403856	0.0207210	0.0224719	0.0210324	0.0099910	0.0105988	0.9	0.1	0.9
11		0	0	0	0	0	1	0	1
Sample	$\Delta(\delta_o - \delta_{obs.}) * \chi_1$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\Delta(\delta_{obs.} - \delta_o) * \chi_{(1•2)}$	$\delta\chi_{(1•2)}$	χ_2	χ_1
1	0						0	1	0
2	0.0270887	0.0211219	0.0215579	0.0215809	0.0101275	0.0103287	0.1	0.9	0.1
3	0.0458953	0.0386906	0.0395567	0.0395922	0.0187627	0.0192093	0.2	0.8	0.2
4	0.0592687	0.0539299	0.0550686	0.0551723	0.0263309	0.0270069	0.3	0.7	0.3
5	0.0683731	0.0655004	0.0668760	0.0668354	0.0322540	0.0330722	0.4	0.6	0.4
6	0.0709558	0.0695290	0.0712361	0.0709518	0.0342499	0.0354153	0.5	0.5	0.5
7	0.0651534	0.0633067	0.0652386	0.0650946	0.0313008	0.0324543	0.6	0.4	0.6
8	0.0545544	0.0513105	0.0532938	0.0527682	0.0255355	0.0268856	0.7	0.3	0.7
9	0.0410161	0.0359481	0.0381599	0.0371698	0.0176423	0.0186292	0.8	0.2	0.8
10	0.0240385	0.0186489	0.0202247	0.0189291	0.0089919	0.0095389	0.9	0.1	0.9
11		0	0	0	0	0	1	0	1



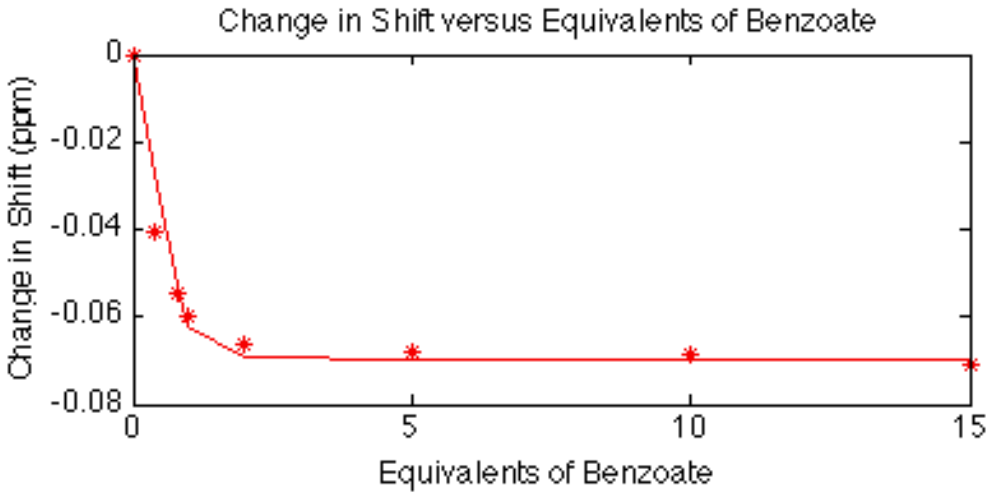
Job Plot for Benzoate 1 Trial 1 depicting a maximum at mole fraction equal to 0.5, indicating a 1:1 stoichiometry between host and guest.

Acylguanidinium Tetrafluoroborate (2) Bound to Potassium Benzoate (1) in 8:2 DMSO: D_2O

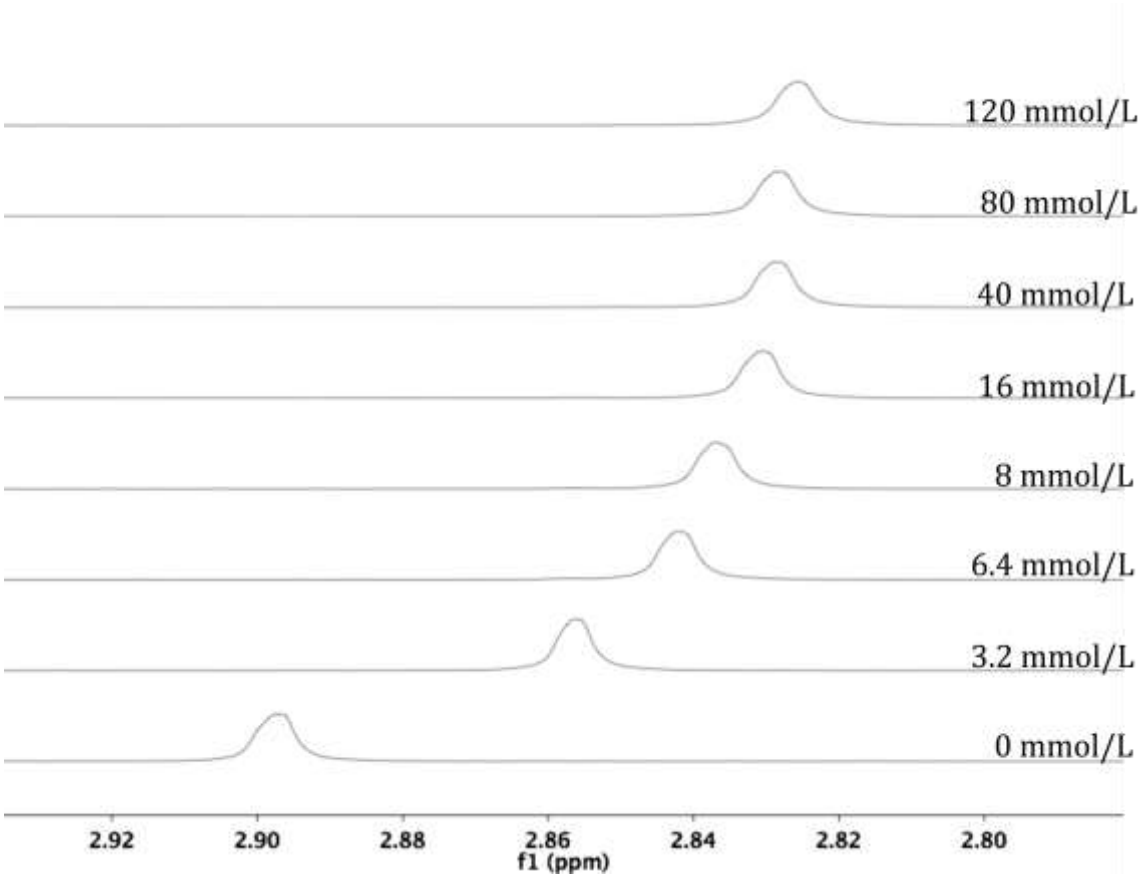
General Procedure for NMR Titrations:
80 mmol/L and 160 mmol/L stock solutions of acylguanidinium tetrafluoroborate **2** (Host) and potassium benzoate **1** (Guest) were made, respectively. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 22°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

80% DMSO								
Host conc. (M)	Guest conc. (M)	Amt. Host Added (uL)	Amt. Guest Added (uL)	Equiv. of Guest	Final Vol. (mL)	δ (ppm) Acyl Trial 1	δ (ppm) Acyl Trial 2	δ (ppm) Acyl Trial 3
0.008	0.0000	100	0	0.0	1	2.896699	2.896699	2.896699
0.008	0.0032	100	20	0.4	1	2.856205	2.856603	2.855392
0.008	0.0064	100	40	0.8	1	2.842047	2.841206	2.842884
0.008	0.0080	100	50	1.0	1	2.836976	2.838085	2.838023
0.008	0.0160	100	100	2.0	1	2.830618	2.830458	2.830949
0.008	0.0400	100	250	5.0	1	2.828588	2.827951	2.828603
0.008	0.0800	100	500	10.0	1	2.828342	2.828356	2.827512
0.008	0.1200	100	750	12.5	1	2.825602	2.826318	2.825715

	Ka
Trial 1	991.98
Trial 2	982.71
Trial 3	733.02
Average	902.57
Standard Deviation	146.91
% Error	16.28



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



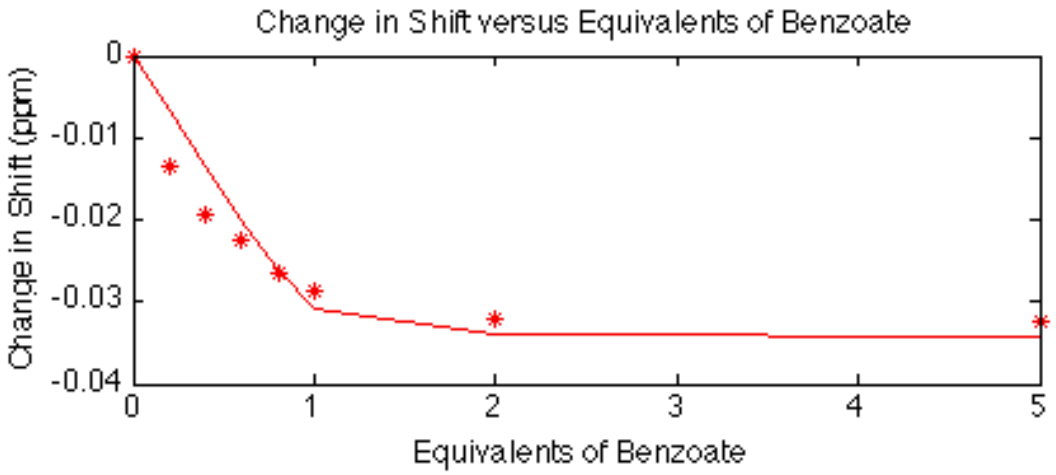
Stacked NMR spectra depicting NMR shift for acylguanidinium peak for Trial 1.

Acylguanidinium Tetrafluoroborate (2) Bound to Potassium Benzoate (1) in 7:3 DMSO: D_2O

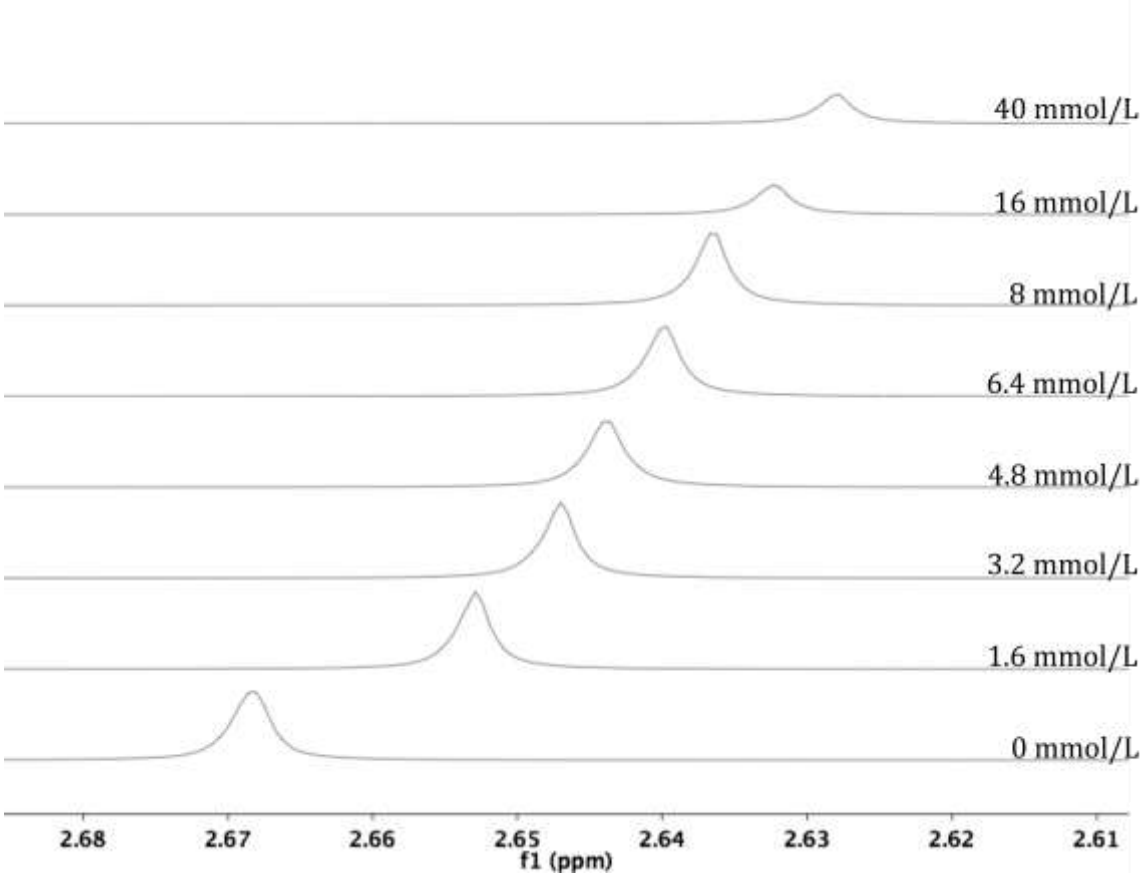
General Procedure for NMR Titrations:
80 mmol/L and 160 mmol/L stock solutions of acylguanidinium tetrafluoroborate **2** (Host) and potassium benzoate **1** (Guest) were made, respectively. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 22°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400**.** Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

70% DMSO								
Host conc. (M)	Guest conc. (M)	Amt. Host Added (uL)	Amt. Guest Added (uL)	Equiv. of Guest	Final Vol. (mL)	δ (ppm) Acyl Trial 1	δ (ppm) Acyl Trial 2	δ (ppm) Acyl Trial 3
0.008	0.0000	100	0	0.0	1	2.6474786	2.6462408	2.6488258
0.008	0.0016	100	10	0.2	1	2.6339328	2.6358634	2.6351768
0.008	0.0032	100	20	0.4	1	2.6280614	2.6286052	2.6290467
0.008	0.0048	100	30	0.6	1	2.6248967	2.6250567	2.6248944
0.008	0.0064	100	40	0.8	1	2.6210186	2.6217102	2.6225548
0.008	0.0080	100	50	1.0	1	2.6186515	2.6201926	2.6199830
0.008	0.0160	100	100	2.0	1	2.6152982	2.6143169	2.6159387
0.008	0.0400	100	250	5.0	1	2.6150388	2.6138418	2.6142134

	Ka
Trial 1	610.49
Trial 2	558.68
Trial 3	454.25
Average	541.14
Standard Deviation	79.59
% Error	14.71



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



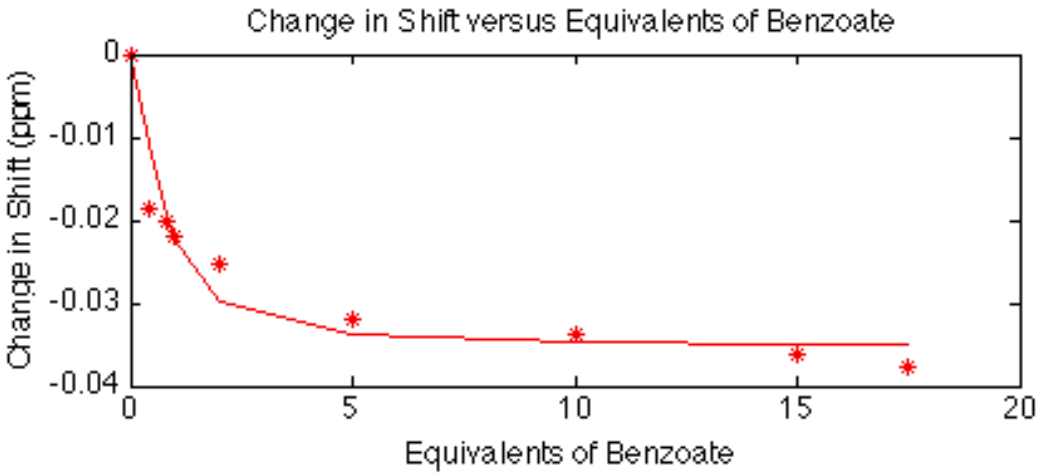
Stacked NMR spectra depicting NMR shift for acylguanidinium peak for Trial 1.

Acylguanidinium Tetrafluoroborate (2) Bound to Potassium Benzoate (1) in 6:4 DMSO: D_2O

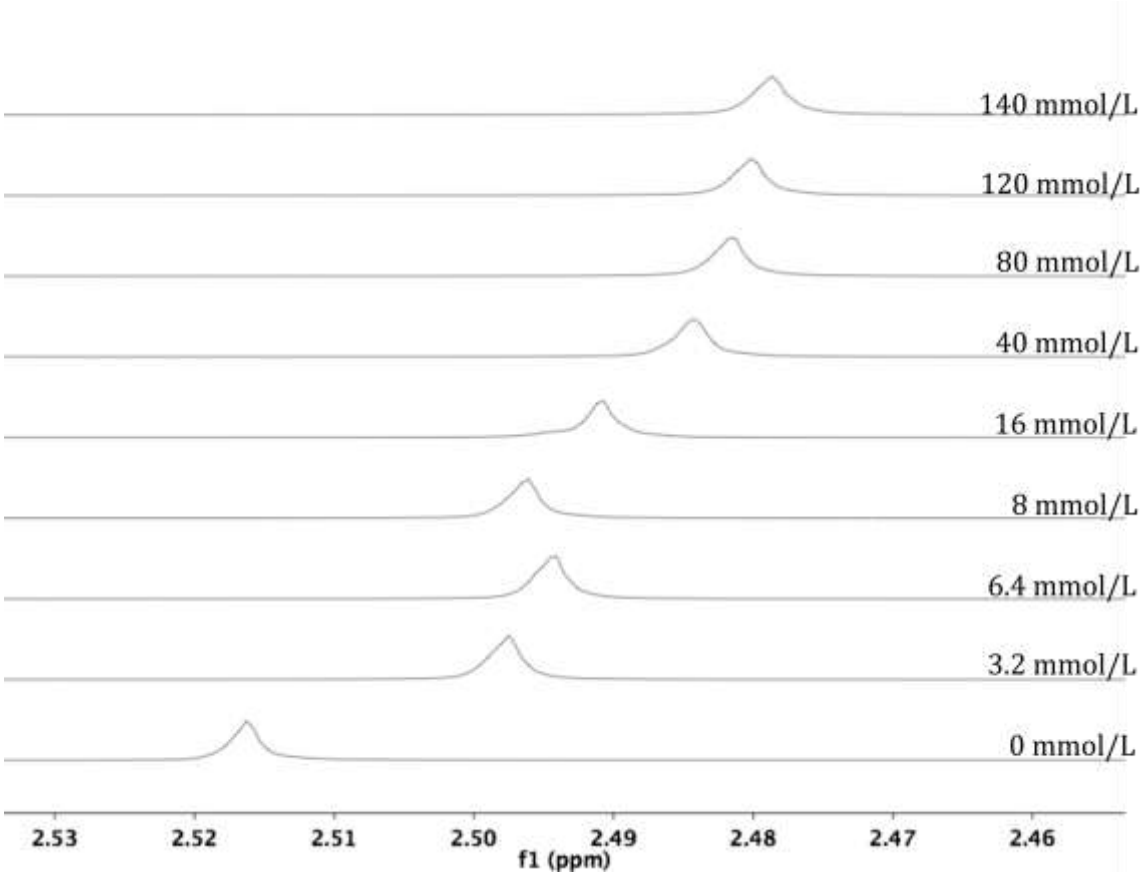
General Procedure for NMR Titrations:
80 mmol/L and 160 mmol/L stock solutions of acylguanidinium tetrafluoroborate **2** (Host) and potassium benzoate **1** (Guest) were made, respectively. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 22°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

60% DMSO								
Host conc. (M)	Guest conc. (M)	Amt. Host Added (uL)	Amt. Guest Added (uL)	Equiv. of Guest	Final Vol. (mL)	δ (ppm) Acyl Trial 1	δ (ppm) Acyl Trial 2	δ (ppm) Acyl Trial 3
0.008	0.0000	100	0	0.00	1	2.516245	2.516245	2.516245
0.008	0.0032	100	20	0.40	1	2.497536	2.498463	2.498477
0.008	0.0064	100	40	0.80	1	2.496205	2.496454	2.496504
0.008	0.0080	100	50	1.00	1	2.494264	2.498566	2.493125
0.008	0.0160	100	100	2.00	1	2.490850	2.490783	2.490710
0.008	0.0400	100	250	5.00	1	2.484280	2.484879	2.484372
0.008	0.0800	100	500	10.00	1	2.482497	2.480279	2.483848
0.008	0.1200	100	750	12.50	1	2.480138	2.478628	2.478354
0.008	0.1400	100	875	18.75	1	2.478667	2.478831	2.477507

	Ka
Trial 1	211.03
Trial 2	155.87
Trial 3	198.07
Average	188.32
Standard Deviation	28.84
% Error	15.32



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



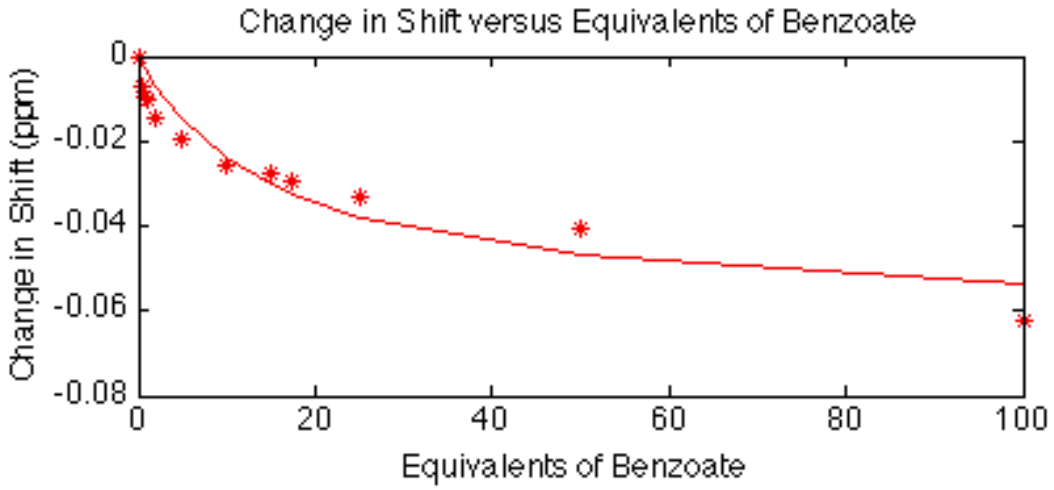
Stacked NMR spectra depicting NMR shift for acylguanidinium peak for Trial 1.

Acylguanidinium Tetrafluoroborate Bound (2) to Potassium Benzoate (1) in 1:1 DMSO: D_2O

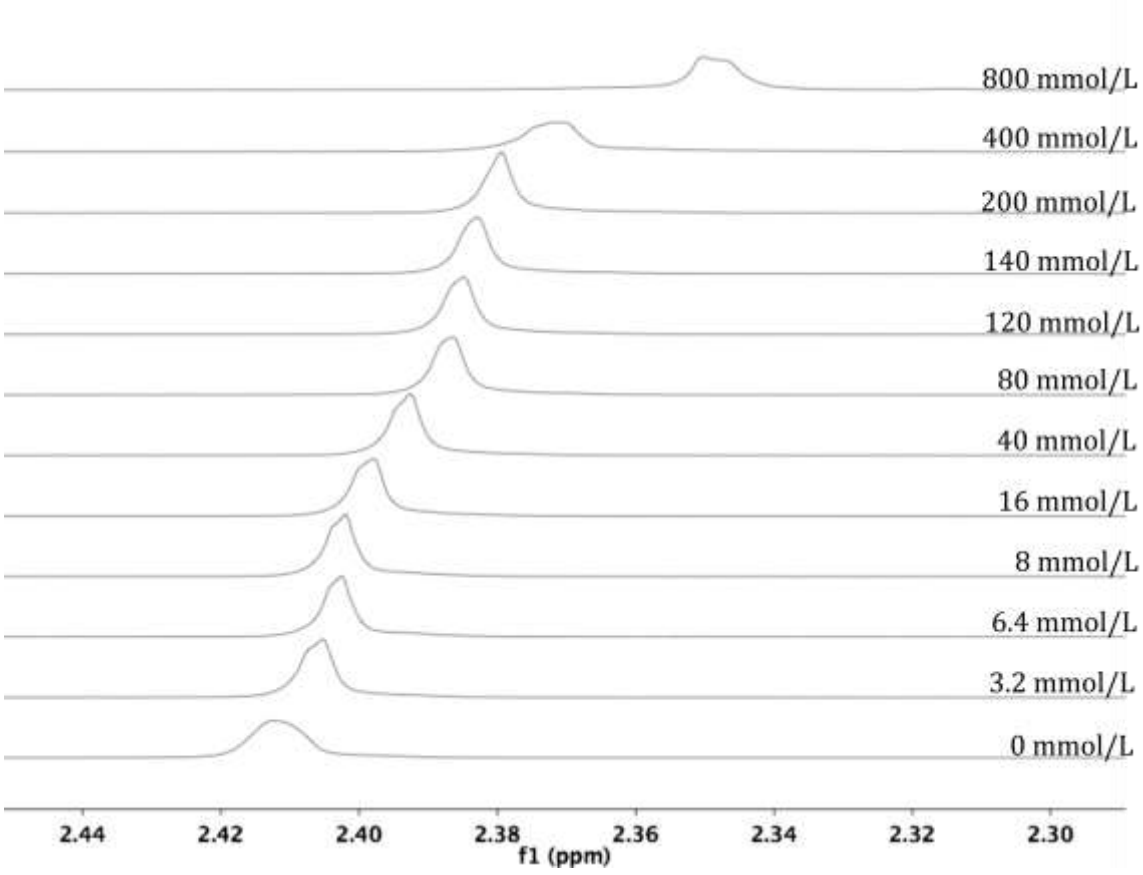
General Procedure for NMR Titrations:
An 80 mmol/L stock solution of acylguanidinium tetrafluoroborate **2** (Host) was made. Two stock solutions of potassium benzoate **1** (guest) were made, 160 mmol/L and 1 M. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. For samples 2-9, the 160 mmol/L stock solution of potassium benzoate was used. For samples 10-12, the 1 M stock solution of potassium benzoate was used. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 22°C. All ^1H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

50% DMSO								
Host conc. (M)	Guest conc. (M)	Amt. Host Added (uL)	Amt. Guest Added (uL)	Equiv. of Guest	Final Vol. (mL)	δ (ppm) Acyl Trial 1	δ (ppm) Acyl Trial 2	δ (ppm) Acyl Trial 3
0.008	0.0000	100	0	0.00	1	2.412439	2.412439	2.412439
0.008	0.0032	100	20	0.40	1	2.405301	2.405749	2.405447
0.008	0.0064	100	40	0.80	1	2.402615	2.402542	2.402754
0.008	0.0080	100	50	1.00	1	2.402070	2.401838	2.401753
0.008	0.0160	100	100	2.00	1	2.397957	2.398714	2.392427
0.008	0.0400	100	250	5.00	1	2.392642	2.392505	2.392574
0.008	0.0800	100	500	10.00	1	2.386451	2.386830	2.386407
0.008	0.1200	100	750	12.50	1	2.384900	2.383860	2.383949
0.008	0.1400	100	875	18.75	1	2.382908	2.383459	2.382273
0.008	0.2000	100	200	25.00	1	2.379424	2.379467	2.380674
0.008	0.4000	100	400	50.00	1	2.371856	2.370623	2.369814
0.008	0.8000	100	800	100.0	1	2.350417	2.349492	2.350075

	Ka
Trial 1	8.25
Trial 2	7.53
Trial 3	6.86
Average	7.55
Standard Deviation	0.69
% Error	9.19



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shift for acylguanidinium peak for Trial 1.

Aminomethylferrocenium Hydrochloride (3) Bound to Potassium Benzoate (1) in 9:1 DMSO: D_2O

General Procedure for NMR Titrations:
An 80 mmol/L stock solution of aminomethylferrocenium hydrochloride **3** (Host) was made. Two stock solutions of potassium benzoate **1** (guest) were made; 4 mmol/L and 160 mmol/L. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. For samples 2-8, the 4 mmol/L stock solution of potassium benzoate was used. For samples 9-14, the 160 mmol/L stock solution of potassium benzoate was used. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790). Blank spaces in the table below are due to peaks overlapping with the D_2O solvent residual peak or with other peaks.

90% DMSO Ferrocene 1								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 1	δ (ppm) Ferrocene 1 Trial 2	δ (ppm) Ferrocene 1 Trial 3
0.008	100	1	0	0	0	5.2837403	5.2854740	5.2860700
0.008	100	1	0.00008	20	0.01	5.2849531	5.2850100	5.2838920
0.008	100	1	0.00024	60	0.03	5.2859998	5.2846192	5.2901602
0.008	100	1	0.0004	100	0.05	5.2856802	5.2867221	5.2867472
0.008	100	1	0.00056	140	0.07	5.2859273	5.2857793	5.2856254
0.008	100	1	0.00072	180	0.09	5.2846765	5.2837407	5.2839577
0.008	100	1	0.0016	400	0.2	5.2752841	5.2762492	5.2756903
0.008	100	1	0.0032	800	0.4	5.2677262	5.2676696	5.2675296
0.008	100	1	0.0064	40	0.8	5.2537112	5.2546084	5.2544452
0.008	100	1	0.008	50	1			
0.008	100	1	0.016	100	2	5.2288971	5.2302341	5.2301737
0.008	100	1	0.04	250	5	5.1995349	5.1996762	5.1998182
0.008	100	1	0.08	500	10	5.1779843	5.1781120	5.1775803
0.008	100	1	0.14	875	18.75	5.1487891	5.1488002	5.1494670

Ferrocene 1	Ka
Trial 1	29.93
Trial 2	31.08
Trial 3	32.31
Average	31.11
Standard Deviation	1.19
% Error	3.82

90% DMSO Ferrocene 2								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 1	δ (ppm) Ferrocene 2 Trial 2	δ (ppm) Ferrocene 2 Trial 3
0.008	100	1	0	0	0	5.4080531	5.4098199	5.4100738
0.008	100	1	0.00008	20	0.01	5.4092991	5.4093894	5.4081005
0.008	100	1	0.00024	60	0.03	5.4103481	5.4089869	5.4143811
0.008	100	1	0.0004	100	0.05	5.4101117	5.4113960	5.4113789
0.008	100	1	0.00056	140	0.07	5.4105094	5.4104629	5.4103859
0.008	100	1	0.00072	180	0.09	5.4095239	5.4085922	5.4088694
0.008	100	1	0.0016	400	0.2	5.4015235	5.4024368	5.4019754
0.008	100	1	0.0032	800	0.4	5.3935599	5.3963160	5.3963770
0.008	100	1	0.0064	40	0.8	5.3876368	5.3883699	5.3882121
0.008	100	1	0.008	50	1	5.3857559	5.3837559	5.3860115
0.008	100	1	0.016	100	2	5.3729108	5.3743721	5.3743032
0.008	100	1	0.04	250	5	5.3570514	5.3570416	5.3573610
0.008	100	1	0.08	500	10	5.3470881	5.3476277	5.3469969
0.008	100	1	0.14	875	18.75	5.3289249	5.3289461	5.3296094

Ferrocene 2	Ka
Trial 1	41.29
Trial 2	45.21
Trial 3	44.12
Average	43.54
Standard Deviation	2.02
% Error	4.64

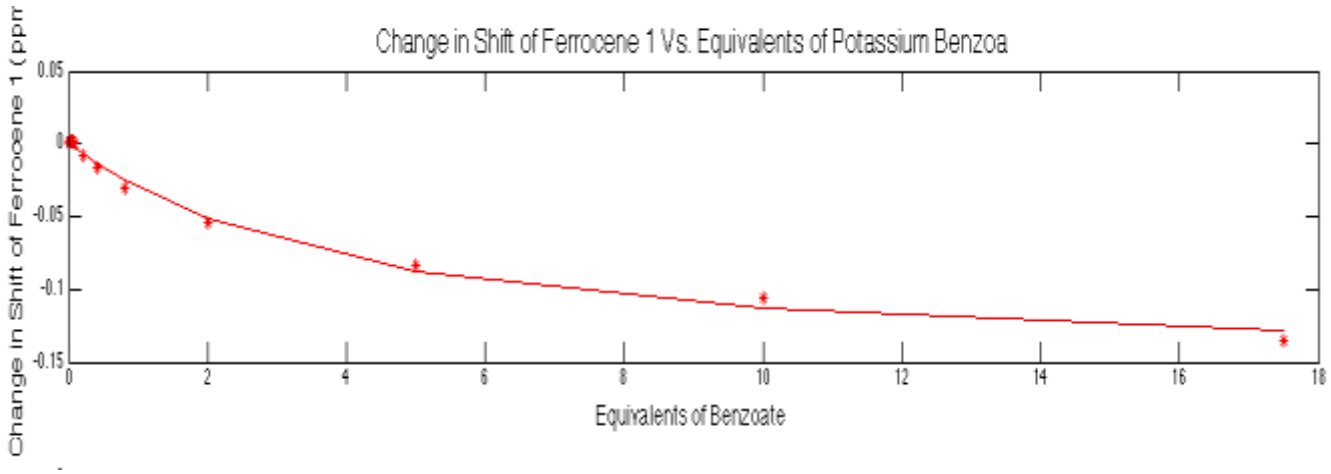
90% DMSO Methylene								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Methylene Trial 1	δ (ppm) Methylene Trial 2	δ (ppm) Methylene Trial 3
0.008	100	1	0	0	0	4.8368756	4.8387831	4.8391239
0.008	100	1	0.00008	20	0.01	4.8379200	4.8381217	4.8369422
0.008	100	1	0.00024	60	0.03	4.8387831	4.8378462	4.8427698
0.008	100	1	0.0004	100	0.05	4.8382621	4.8393135	4.8392468
0.008	100	1	0.00056	140	0.07	4.8373566	4.8372119	4.8368376
0.008	100	1	0.00072	180	0.09	4.8343524	4.8342424	4.8343843
0.008	100	1	0.0016	400	0.2	4.8201881	4.8209419	4.8193158
0.008	100	1	0.0032	800	0.4	4.7986383	4.8073886	4.8073565
0.008	100	1	0.0064	40	0.8			
0.008	100	1	0.008	50	1			
0.008	100	1	0.016	100	2	4.7640648	4.7655146	4.7649177
0.008	100	1	0.04	250	5	4.7397286	4.7396145	4.7401753
0.008	100	1	0.08	500	10	4.7279735	4.7291668	4.7278315
0.008	100	1	0.14	875	18.75	4.7123810	4.7124307	4.7127307

Methylene	Ka
Trial1	86.75
Trial2	79.29
Trial3	81.66
Average	82.57
Standard Deviation	3.81
% Error	4.61

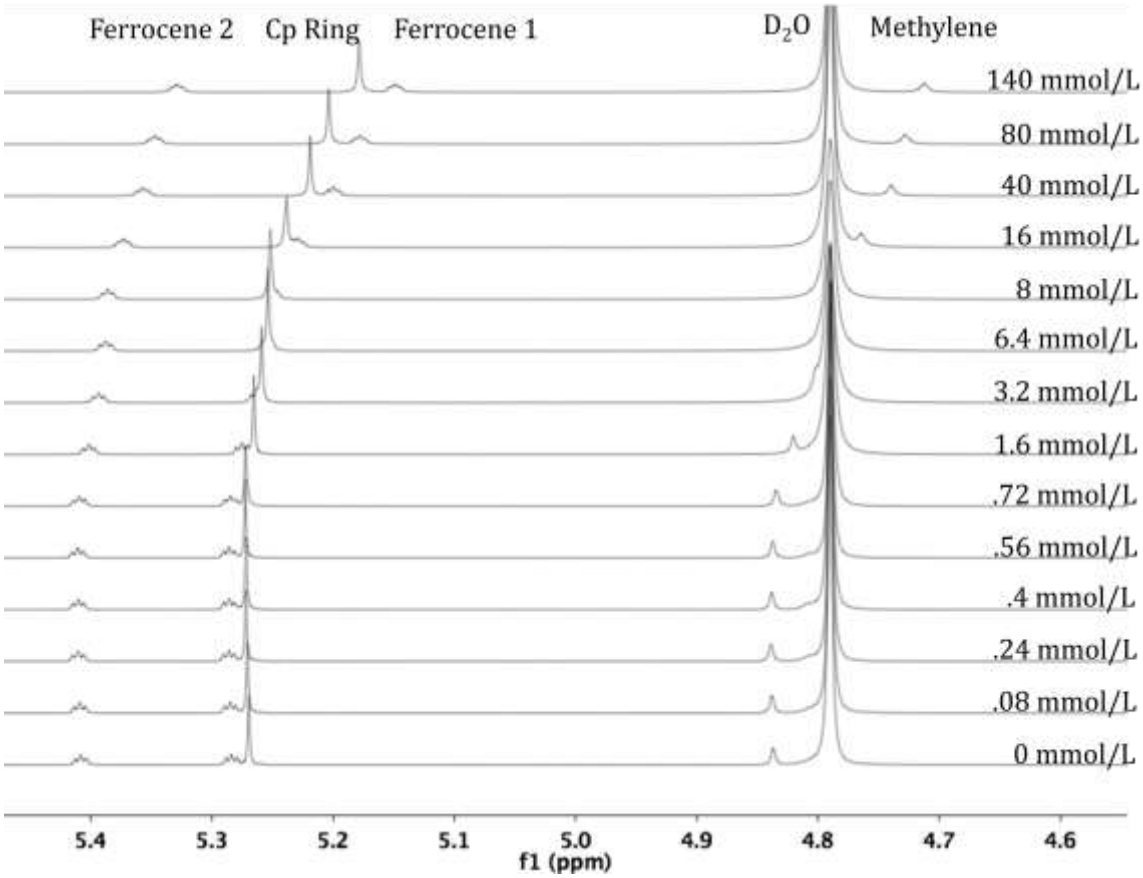
90% DMSO Cp Ring								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Cp Ring Trial 1	δ (ppm) Cp Ring Trial 2	δ (ppm) Cp Ring Trial 3
0.008	100	1	0	0	0	5.2695613	5.2713971	5.2718865
0.008	100	1	0.00008	20	0.01	5.2707871	5.2707730	5.2697427
0.008	100	1	0.00024	60	0.03	5.2719691	5.2704811	5.2762684
0.008	100	1	0.0004	100	0.05	5.2719446	5.2729633	5.2867472
0.008	100	1	0.00056	140	0.07	5.2724439	5.2725857	5.2724376
0.008	100	1	0.00072	180	0.09	5.2721623	5.2711497	5.2709993
0.008	100	1	0.0016	400	0.2	5.2655336	5.2665580	5.2663585
0.008	100	1	0.0032	800	0.4	5.2592465	5.2619540	5.2617361
0.008	100	1	0.0064	40	0.8	5.2537112	5.2546084	5.2544452
0.008	100	1	0.008	50	1	5.2518460	5.2500162	5.2521400
0.008	100	1	0.016	100	2	5.2385848	5.2398849	5.2398872
0.008	100	1	0.04	250	5	5.2190149	5.2190407	5.2191255
0.008	100	1	0.08	500	10	5.2035954	5.2037680	5.2034675
0.008	100	1	0.14	875	18.75	5.1785468	5.1785800	5.1794815

Cp Ring	Ka
Trial 1	19.81
Trial 2	21.97
Trial 3	21.95
Average	21.24
Standard Deviation	1.24
% Error	5.85

	Ka
Fc 1 Trial 1	29.93
Fc 1 Trial 2	31.08
Fc 1 Trial 3	32.31
Fc 2 Trial 1	41.29
Fc 2 Trial 2	45.21
Fc 2 Trial 3	44.12
Me Trial 1	86.75
Me Trial 2	79.29
Me Trial 3	81.66
Cp Trial 1	19.81
Cp Trial 2	21.97
Cp Trial 3	21.95
Average	44.62



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shifts for aminomethylferrocenium hydrochloride peaks for Trial 1.

Job plot determination of stoichiometry of binding for Aminomethylferrocenium Hydrochloride (3) and Potassium Benzoate (1) in 9:1 DMSO: D_2O

General Procedure: 8 mmol/L stock solutions were made of aminomethylferrocenium hydrochloride **3** (Host) and of potassium benzoate **1** (Guest). Contents were bound for two hours at 20˚C. The cyclopentadienyl ring and ferrocene 2 peaks of the host and five of the benzoate peaks of the guest were monitored. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400**.** Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

Sample	δ (ppm) Benzoate 1 Trial 1	δ (ppm) Benzoate 2 Trial 1	δ (ppm) Benzoate 3 Trial 1	δ (ppm) Benzoate 4 Trial 1	δ (ppm) Benzoate 5 Trial 1	$\chi_{(1\bullet3)}$	Amt. 3 (mL)	Amt. 1 (mL)
1						0	1	0
2	8.4986149	8.5166549	8.5354893	8.9795131	8.9986074	0.1	0.9	0.1
3	8.4486508	8.4673311	8.4858668	8.9563090	8.9750607	0.2	0.8	0.2
4	8.4212663	8.4391643	8.4579267	8.9448921	8.9620230	0.3	0.7	0.3
5	8.4016540	8.4189288	8.4374008	8.9348837	8.9515245	0.4	0.6	0.4
6	8.3861651	8.4030042	8.4218220	8.9280086	8.9446587	0.5	0.5	0.5
7	8.3746856	8.3912579	8.4100215	8.9226384	8.9389167	0.6	0.4	0.6
8	8.3652468	8.3817342	8.4003775	8.9182325	8.9343522	0.7	0.3	0.7
9	8.3553257	8.3714443	8.3900189	8.9134762	8.9295004	0.8	0.2	0.8
10	8.3455633	8.3615061	8.3795459	8.9090053	8.9246417	0.9	0.1	0.9
11	8.3317713	8.3463414	8.3652318	8.9031087	8.9184061	1	0	1

Sample	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_o-\delta_{obs.})$	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_{obs.}-\delta_o)$	$\chi_{(1\bullet3)}$	Amt. 3 (mL)	Amt. 1 mL)
1						0	1	0
2	0.1668436	0.1703135	0.1702575	0.0764044	0.0802013	0.1	0.9	0.1
3	0.1168795	0.1209897	0.1206350	0.0532003	0.0566546	0.2	0.8	0.2
4	0.0894950	0.0928229	0.0926949	0.0417834	0.0436169	0.3	0.7	0.3
5	0.0698827	0.0725874	0.0721690	0.0317750	0.0331184	0.4	0.6	0.4
6	0.0543938	0.0566628	0.0565902	0.0248999	0.0262526	0.5	0.5	0.5
7	0.0429143	0.0449165	0.0447897	0.0195297	0.0205106	0.6	0.4	0.6
8	0.0334755	0.0353928	0.0351457	0.0151238	0.0159461	0.7	0.3	0.7
9	0.0235544	0.0251029	0.0247871	0.0103675	0.0110943	0.8	0.2	0.8
10	0.0137920	0.0151647	0.0143141	0.0058966	0.0062356	0.9	0.1	0.9
11	0	0	0	0	0	1	0	1

Sample	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\chi_{(1•3)}$	χ_3	χ_1
1						0	1	0
2	0.0166843	0.0170313	0.0170257	0.0076404	0.0080201	0.1	0.9	0.1
3	0.0233759	0.0241979	0.0241270	0.0106400	0.0113309	0.2	0.8	0.2
4	0.0268485	0.0278468	0.0278084	0.0125350	0.0130850	0.3	0.7	0.3
5	0.0279530	0.0290349	0.0288676	0.0127100	0.0132473	0.4	0.6	0.4
6	0.0271969	0.0283314	0.0282951	0.0124499	0.0131263	0.5	0.5	0.5
7	0.0257485	0.0269499	0.0268738	0.0117178	0.0123063	0.6	0.4	0.6
8	0.0234328	0.0247749	0.0246019	0.0105866	0.0111622	0.7	0.3	0.7
9	0.0188435	0.0200823	0.0198296	0.0082940	0.0088754	0.8	0.2	0.8
10	0.0124128	0.0136482	0.0128826	0.0053069	0.0056120	0.9	0.1	0.9
11	0	0	0	0	0	1	0	1

Sample	δ (ppm) Cp Ring Trial 1	δ (ppm) Ferrocene 2 Trial 1	δ (ppm) Cp Ring Trial 2	δ (ppm) Ferrocene 2 Trial 2	$\chi_{(1•3)}$	Amt. 3 (mL)	Amt. 1 (mL)
1	5.2857550	5.4242767	5.2857900	5.4242761	0	1	0
2	5.2857696	5.4227833	5.2857765	5.4229379	0.1	0.9	0.1
3	5.2827071	5.4182016	5.2827107	5.4182591	0.2	0.8	0.2
4	5.2805775	5.4144530	5.2795791	5.4134018	0.3	0.7	0.3
5	5.2773120	5.4098135	5.2771589	5.4095353	0.4	0.6	0.4
6	5.2748949	5.4054343	5.2749443	5.4056433	0.5	0.5	0.5
7	5.2720590	5.4010662	5.2721887	5.4012208	0.6	0.4	0.6
8	5.2694422	5.3962584	5.2694944	5.3958071	0.7	0.3	0.7
9	5.2657318	5.3888918	5.2656372	5.3888168	0.8	0.2	0.8
10	5.2603933	5.3776598	5.2603933	5.3776598	0.9	0.1	0.9
11					1	0	1

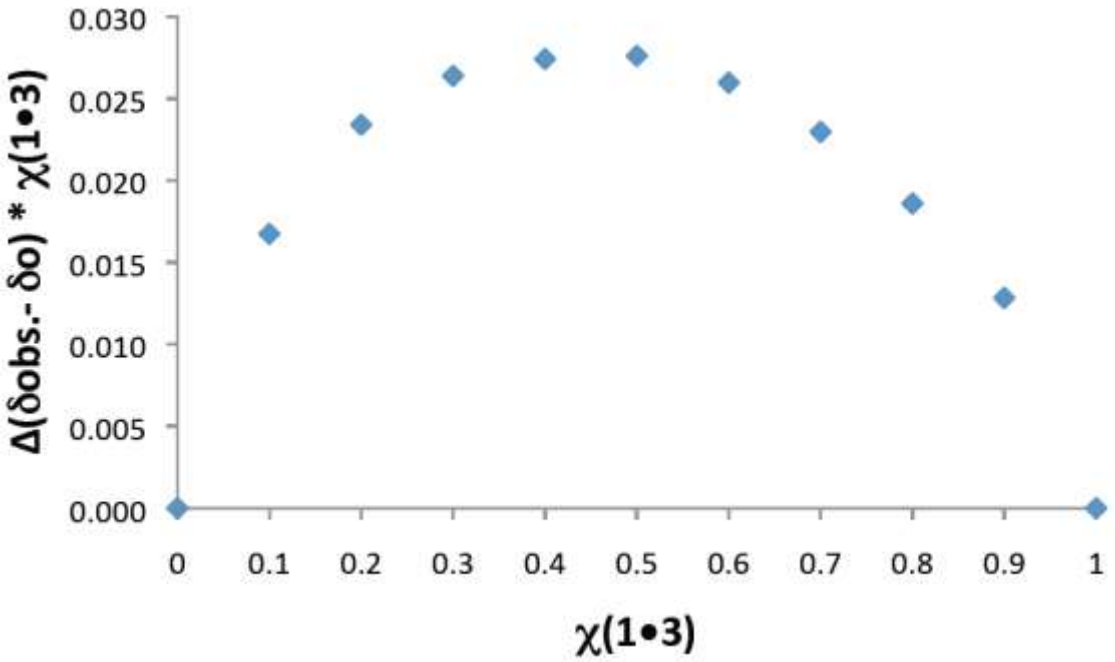
Sample	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\chi_{(1•3)}$	Amt. 3 (mL)	Amt. 1 (mL)
1	0	0	0	0	0	1	0
2	-0.0000146	0.0014934	0.0000135	0.0013382	0.1	0.9	0.1
3	0.0030479	0.0060751	0.0030793	0.0060170	0.2	0.8	0.2
4	0.0051775	0.0098237	0.0062109	0.0108743	0.3	0.7	0.3
5	0.0084430	0.0144632	0.0086311	0.0147408	0.4	0.6	0.4
6	0.0108601	0.0188424	0.0108457	0.0186328	0.5	0.5	0.5
7	0.0136960	0.0232105	0.0136013	0.0230553	0.6	0.4	0.6
8	0.0163128	0.0280183	0.0162956	0.0284690	0.7	0.3	0.7
9	0.0200232	0.0353849	0.0201528	0.0354593	0.8	0.2	0.8
10	0.0253617	0.0466169	0.0253967	0.0466163	0.9	0.1	0.9
11					1	0	1

Sample	$\Delta(\delta_o - \delta_{obs.}) * \chi_{(1•3)}$	$\Delta(\delta_o - \delta_{obs.}) * \chi_{(1•3)}$	$\Delta(\delta_o - \delta_{obs.}) * \chi_{(1•3)}$	$\Delta(\delta_o - \delta_{obs.}) * \chi_{(1•3)}$	$\chi_{(1•3)}$	χ_3	χ_1
1	0	0	0	0	0	1	0
2	-0.0000131	0.0013441	0.0000122	0.0012043	0.1	0.9	0.1
3	0.0024383	0.0048601	0.0024634	0.0048136	0.2	0.8	0.2
4	0.0036243	0.0068766	0.0043476	0.0076120	0.3	0.7	0.3
5	0.0050658	0.0086779	0.0051786	0.0088444	0.4	0.6	0.4
6	0.0054301	0.0094212	0.0054228	0.0093164	0.5	0.5	0.5
7	0.0054784	0.0092842	0.0054405	0.0092221	0.6	0.4	0.6
8	0.0048938	0.0084055	0.0048886	0.0085407	0.7	0.3	0.7
9	0.0040046	0.0070770	0.0040305	0.0070918	0.8	0.2	0.8
10	0.0025362	0.0046617	0.0025396	0.0046616	0.9	0.1	0.9
11					1	0	1

Sample	δ (ppm) Benzoate 1 Trial 1	δ (ppm) Benzoate 2 Trial 1	δ (ppm) Benzoate 3 Trial 1	δ (ppm) Benzoate 4 Trial 1	δ (ppm) Benzoate 5 Trial 1	$\chi_{(1•3)}$	Amt. 3 (mL)	Amt. 1 (mL)
1						0	1	0
2	8.4993797	8.5199788	8.5388516	8.9808590	8.9999963	0.1	0.9	0.1
3	8.4489214	8.4675359	8.4861685	8.9562874	8.9752546	0.2	0.8	0.2
4	8.4198680	8.4376986	8.4562192	8.9436635	8.9606540	0.3	0.7	0.3
5	8.4004536	8.4178124	8.4366374	8.9347674	8.9510351	0.4	0.6	0.4
6	8.3871265	8.4037681	8.4224548	8.9282314	8.9447642	0.5	0.5	0.5
7	8.3752007	8.3916452	8.4105316	8.9227320	8.9391921	0.6	0.4	0.6
8	8.3647274	8.3811699	8.3998833	8.9178120	8.9340376	0.7	0.3	0.7
9	8.3551677	8.3713934	8.3898384	8.9133990	8.9294912	0.8	0.2	0.8
10	8.3461843	8.3620514	8.3802386	8.9098582	8.9255747	0.9	0.1	0.9
11	8.3319223	8.3464520	8.3653178	8.9031885	8.9184301	1	0	1

Sample	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_{obs.} - \delta_o)$	$\Delta(\delta_{obs.} - \delta_o)$	$\chi_{(1•3)}$	Amt. 3 (mL)	Amt. 1 mL)
1						0	1	0
2	0.1674574	0.1735268	0.1735338	0.0776705	0.0815662	0.1	0.9	0.1
3	0.1169991	0.1210839	0.1208507	0.0530989	0.0568245	0.2	0.8	0.2
4	0.0879457	0.0912466	0.0909014	0.0404750	0.0422239	0.3	0.7	0.3
5	0.0685313	0.0713604	0.0713196	0.0315789	0.0326050	0.4	0.6	0.4
6	0.0552042	0.0573161	0.0571370	0.0250429	0.0263341	0.5	0.5	0.5
7	0.0432784	0.0451932	0.0452138	0.0195435	0.0207620	0.6	0.4	0.6
8	0.0328051	0.0347179	0.0345655	0.0146235	0.0156075	0.7	0.3	0.7
9	0.0232454	0.0249414	0.0245206	0.0102105	0.0110611	0.8	0.2	0.8
10	0.014262	0.0155994	0.0149208	0.0066697	0.0071446	0.9	0.1	0.9
11	0	0	0	0	0	1	0	1

Sample	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1•3)}$	$\chi_{(1•3)}$	χ_3	χ_1
1	0					0	1	0
2	0.0167457	0.0173526	0.0173533	0.0077670	0.0081566	0.1	0.9	0.1
3	0.0233998	0.0242167	0.0241701	0.0106197	0.0113649	0.2	0.8	0.2
4	0.0263837	0.0273739	0.0272704	0.0121425	0.0126671	0.3	0.7	0.3
5	0.0274125	0.0285441	0.0285278	0.0126315	0.0130420	0.4	0.6	0.4
6	0.0276021	0.0286580	0.0285685	0.0125214	0.0131670	0.5	0.5	0.5
7	0.0259670	0.0271159	0.0271282	0.0117261	0.0124572	0.6	0.4	0.6
8	0.0229635	0.0243025	0.0241958	0.0102364	0.0109252	0.7	0.3	0.7
9	0.0185963	0.0199531	0.0196164	0.0081684	0.0088488	0.8	0.2	0.8
10	0.0128358	0.0140394	0.0134287	0.0060027	0.0064301	0.9	0.1	0.9
11	0	0	0	0	0	1	0	1



Job Plot for Benzoate peak 1 from Trial 2 showing a maximum at mole fraction equal to 0.5, indicating a 1:1 stoichiometry between host and guest.

1,1'-di(aminomethyl)ferrocenium Hydrochloride (4) Bound to Potassium Benzoate (1) in 9:1 DMSO: D_2O

General Procedure for NMR Titrations:
8 mmol/L and 160 mmol/L stock solution of 1,1'-di(aminomethyl)ferrocenium hydrochloride **4** (Host) and potassium benzoate **1** (Guest) were made, respectively. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^1H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790). The two ferrocene triplets were monitored. Association constants were calculated for both signals, and the final association constant reported is the average of the local association constant values. The methylene singlet peak could not be monitored, due to its proximity to the D_2O solvent residual peak.

90% DMSO Ferrocene 1							
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 1	δ (ppm) Ferrocene 1 Trial 2
0.0008	100	1	0.0000	0	0	5.3296220	5.3320253
0.0008	100	1	0.0024	15	3	5.2619943	5.2644909
0.0008	100	1	0.0032	20	4	5.2545665	5.2581298
0.0008	100	1	0.0040	25	5	5.2511611	5.2545967
0.0008	100	1	0.0048	30	6	5.2441371	5.2493788
0.0008	100	1	0.0064	40	8	5.2398130	5.2443579
0.0008	100	1	0.0080	50	10	5.2394640	5.2394712
0.0008	100	1	0.0120	75	15	5.2237070	5.2330898
0.0008	100	1	0.0160	100	20	5.2209755	5.2248833
0.0008	100	1	0.0200	125	25	5.2177747	5.2132394
0.0008	100	1	0.0320	200	40	5.2015537	5.2054671
0.0008	100	1	0.0640	400	80	5.1831138	5.1889812
0.0008	100	1	0.0800	500	100	5.1786807	5.1799961
0.0008	100	1	0.1000	625	125	5.1665999	5.1702424
0.0008	100	1	0.1440	900	180	5.1572922	5.1595466

90% DMSO Ferrocene 1						
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 3
0.0008	100	1	0.0000	0	0	5.3758271
0.0008	100	1	0.0040	25	5	5.2982145
0.0008	100	1	0.0064	40	8	5.2856525
0.0008	100	1	0.0080	50	10	5.2774495
0.0008	100	1	0.0120	75	15	5.2694898
0.0008	100	1	0.0160	100	20	5.2616572
0.0008	100	1	0.0200	125	25	5.2569300
0.0008	100	1	0.0320	200	40	5.2399021
0.0008	100	1	0.0640	400	80	5.2199243
0.0008	100	1	0.1000	625	125	5.2004947
0.0008	100	1	0.1440	900	180	5.1992346

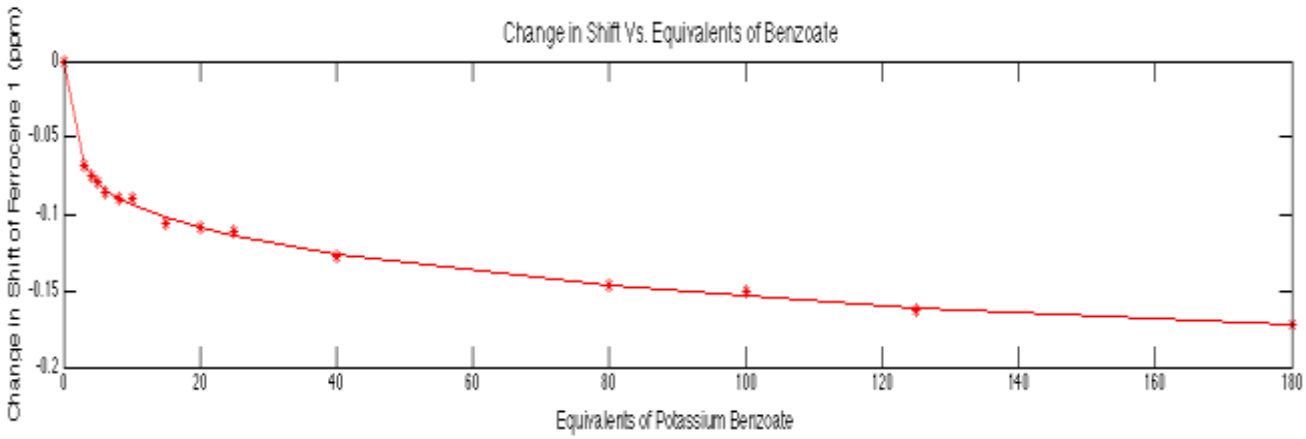
Ferrocene 1	K1	K2
Trial 1	849.09	11.18
Trial 2	829.13	11.55
Trial 3	953.20	20.79
Average	877.14	14.51
Standard Deviation	66.62	5.44
% Error	7.60	37.52

90% DMSO Ferrocene 2							
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 1	δ (ppm) Ferrocene 2 Trial 2
0.0008	100	1	0.0000	0	0	5.4159914	5.4177026
0.0008	100	1	0.0024	15	3	5.3426592	5.3437313
0.0008	100	1	0.0032	20	4	5.335690	5.3392491
0.0008	100	1	0.0040	25	5	5.3337675	5.3368968
0.0008	100	1	0.0048	30	6	5.3278255	5.3329145
0.0008	100	1	0.0064	40	8	5.3254475	5.3296472
0.0008	100	1	0.0080	50	10	5.3224865	5.3260672
0.0008	100	1	0.0120	75	15	5.3140831	5.3238299
0.0008	100	1	0.0160	100	20	5.3151927	5.3188827
0.0008	100	1	0.0200	125	25	5.3106821	5.3140151
0.0008	100	1	0.0320	200	40	5.3042590	5.3080664
0.0008	100	1	0.0640	400	80	5.2962987	5.3017180
0.0008	100	1	0.0800	500	100	5.2960259	5.2956486
0.0008	100	1	0.1000	625	125	5.2873924	5.2918155
0.0008	100	1	0.1440	900	180	5.2853804	5.2874674

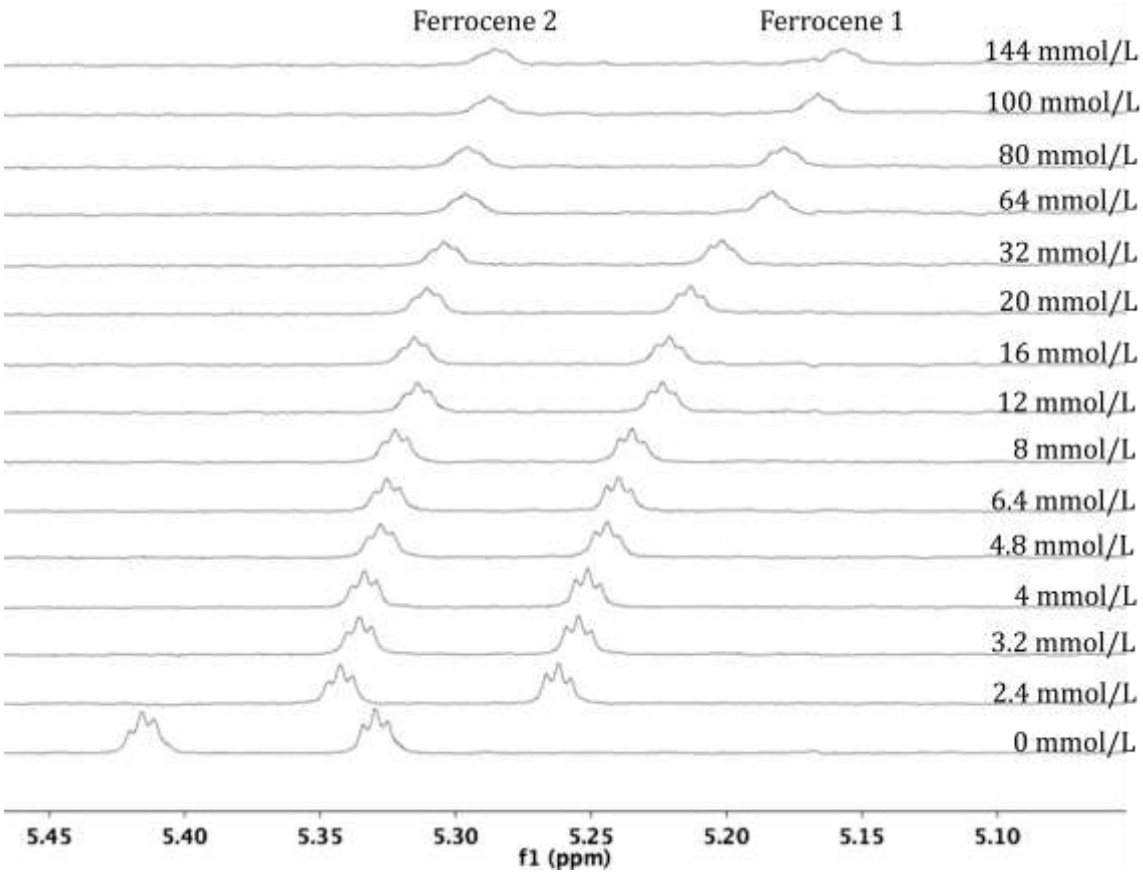
90% DMSO Ferrocene 2						
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 3
0.0008	100	1	0.0000	0	0	5.4666819
0.0008	100	1	0.0040	25	5	5.3805381
0.0008	100	1	0.0064	40	8	5.3705983
0.0008	100	1	0.0080	50	10	5.3653282
0.0008	100	1	0.0120	75	15	5.3614896
0.0008	100	1	0.0160	100	20	5.3593071
0.0008	100	1	0.0200	125	25	5.3540613
0.0008	100	1	0.0320	200	40	5.3484406
0.0008	100	1	0.0640	400	80	5.3365223
0.0008	100	1	0.1000	625	125	5.3267394
0.0008	100	1	0.1440	900	180	5.3259468

Ferrocene 2	K1	K2
Trial 1	1012.22	8.36
Trial 2	1443.45	14.17
Trial 3	1031.37	13.31
Average	1162.35	11.94
Standard Deviation	243.63	3.14
% Error	20.96	26.26

	K1	K2
Fc 1 Trial 1	849.09	11.18
Fc 1 Trial 2	829.13	11.55
Fc 1 Trial 3	953.20	20.79
Fc 2 Trial 1	1012.22	8.36
Fc 2 Trial 2	1443.45	14.17
Fc 2 Trial 3	1031.37	13.31
Average	1019.74	13.23



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shifts for 1,1'-di(aminomethylferrocenium) hydrochloride peaks for Trial 1.

Job plot determination of stoichiometry of binding for 1,1'-di(aminomethyl) ferrocenium Hydrochloride (4) and Potassium Benzoate (1) in 9:1 DMSO: D_2O

General Procedure for Trial 1:
8 mmol/L stock solutions were made of 1,1'-di(aminomethyl)ferrocenium hydrochloride **4** (host) and of potassium benzoate **1** (guest). Contents were bound for two hours at 21˚C. Five of the benzoate peaks of the guest and the three ferrocenyl peaks of the host were monitored. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

General Procedure for Trial 2:
8 mmol/L stock solutions were made of 1,1'-di(aminomethyl)ferrocenium hydrochloride **4** (host) and of potassium benzoate **1** (guest). Contents were bound for two hours at 22˚C. Five of the benzoate peaks of the guest and the three ferrocenyl peaks of the host were monitored. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

Sample	δ (ppm) Benzoate 1 Trial 1	δ (ppm) Benzoate 2 Trial 1	δ (ppm) Benzoate 3 Trial 1	δ (ppm) Benzoate 4 Trial 1	δ (ppm) Benzoate 5 Trial 1	$\chi_{(1\bullet4)}$	Amt. 4 (mL)	Amt. 1 (mL)
1						0	1	0
2	8.5068895	8.5276115	8.5472313	8.9894595	9.0085879	0.1	.9	0.1
3	8.4692318	8.4880285	8.5067471	8.9683032	8.9873123	0.2	.8	0.2
4	8.4434952	8.4621811	8.4809448	8.9545533	8.9733376	0.3	.7	0.3
5	8.4231516	8.4415033	8.4603314	8.9458877	8.9626661	0.4	.6	0.4
6	8.4076809	8.4254387	8.4442178	8.9388250	8.9552847	0.5	.5	0.5
7	8.3928687	8.4096755	8.4287581	8.9311943	8.9480564	0.6	.4	0.6
8	8.3765052	8.3955204	8.4123563	8.9209352	8.9411084	0.7	.3	0.7
9	8.3629353	8.3792754	8.3978940	8.9178810	8.9340240	0.8	.2	0.8
10	8.3477641	8.3636269	8.3822465	8.9114913	8.9272515	0.9	.1	0.9
11	8.3281484	8.3422185	8.3617475	8.9023276	8.9177961	1	0	1

Sample	$\Delta(\delta_{obs.}- \delta_o)$	$\Delta(\delta_{obs.}- \delta_o)$	$\Delta(\delta_{obs.}- \delta_o)$	$\Delta(\delta_{obs.}- \delta_o)$	$\Delta(\delta_{obs.}- \delta_o)$	$\chi_{(1\bullet4)}$	Amt. 4 (mL)	Amt. 1 mL)
1						0	1.0	0
2	0.1787411	0.1853930	0.1854838	0.0871319	0.0907918	0.1	0.9	0.1
3	0.1410834	0.1458100	0.1449996	0.0659756	0.0695162	0.2	0.8	0.2
4	0.1153468	0.1199626	0.1191973	0.0522257	0.0555415	0.3	0.7	0.3
5	0.0950032	0.0992848	0.0985839	0.0435601	0.0448700	0.4	0.6	0.4
6	0.0795325	0.0832202	0.0824703	0.0364974	0.0374886	0.5	0.5	0.5
7	0.0647203	0.0674570	0.0670106	0.0288667	0.0302603	0.6	0.4	0.6
8	0.0483568	0.0533019	0.0506088	0.0186076	0.0233123	0.7	0.3	0.7
9	0.0347869	0.0370569	0.0361465	0.0155534	0.0162279	0.8	0.2	0.8
10	0.0196157	0.0214084	0.0204990	0.0091637	0.0094554	0.9	0.1	0.9
11	0	0	0	0	0	1	0.0	1

Sample	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1\bullet4)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1\bullet4)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1\bullet4)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1\bullet4)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(1\bullet4)}$	$\chi_{(1\bullet4)}$	χ_4	χ_1
1						0	1.0	0
2	0.0178741	0.0185393	0.0185484	0.0087132	0.0090792	0.1	0.9	0.1
3	0.0282167	0.0291620	0.0289999	0.0131951	0.0139032	0.2	0.8	0.2
4	0.0346040	0.0359888	0.0357592	0.0156677	0.0166625	0.3	0.7	0.3
5	0.0380013	0.0397139	0.0394336	0.0174240	0.0179480	0.4	0.6	0.4
6	0.0397663	0.0416101	0.0412352	0.0182487	0.0187443	0.5	0.5	0.5
7	0.0388322	0.0404742	0.0402064	0.0173200	0.0181562	0.6	0.4	0.6
8	0.0338498	0.0373113	0.0354262	0.0130253	0.0163186	0.7	0.3	0.7
9	0.0278295	0.0296455	0.0289172	0.0124427	0.0129823	0.8	0.2	0.8
10	0.0176541	0.0192676	0.0184491	0.0082473	0.0085099	0.9	0.1	0.9
11	0	0	0	0	0	1	0.0	1

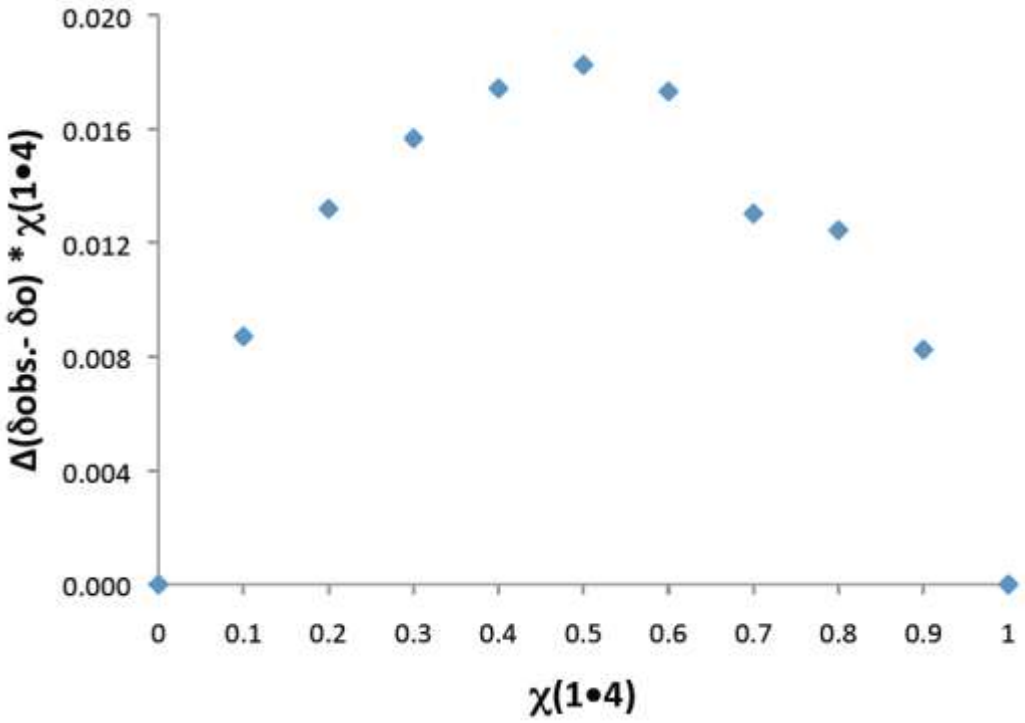
Sample	δ (ppm) Methylene Trial 1	δ (ppm) Ferrocene 1 Trial 1	δ (ppm) Ferrocene 2 Trial 2	$\chi_{(1•4)}$	Amt. 4 (mL)	Amt. 1 (mL)
1	4.8561235	5.3481445	5.4481895	0	1.0	0
2	4.8438664	5.3420354	5.4399153	0.1	0.9	0.1
3	4.8296752	5.3339646	5.4303305	0.2	0.8	0.2
4	4.8169053	5.3254419	5.4208141	0.3	0.7	0.3
5	4.8035640	5.3168932	5.4113609	0.4	0.6	0.4
6	4.7900000	5.3094352	5.4031682	0.5	0.5	0.5
7	4.7761514	5.3004624	5.3934428	0.6	0.4	0.6
8	4.7569697	5.2911419	5.3784886	0.7	0.3	0.7
9	4.7331981	5.2779431	5.3680080	0.8	0.2	0.8
10	4.6936322	5.2590780	5.3460804	0.9	0.1	0.9
11				1	0	1
Sample	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\chi_{(1•4)}$	χ_4	χ_1
1	0	0	0	0	1.0	0
2	0.0122571	0.0061091	0.0082742	0.1	0.9	0.1
3	0.0264483	0.0141799	0.0178590	0.2	0.8	0.2
4	0.0392182	0.0227026	0.0273754	0.3	0.7	0.3
5	0.0525595	0.0312513	0.0368286	0.4	0.6	0.4
6	0.0661235	0.0387093	0.0450213	0.5	0.5	0.5
7	0.0799721	0.0476821	0.0547467	0.6	0.4	0.6
8	0.0991538	0.0570026	0.0697009	0.7	0.3	0.7
9	0.1229254	0.0702014	0.0801815	0.8	0.2	0.8
10	0.1624913	0.0890665	0.1021091	0.9	0.1	0.9
11				1	0.0	1
Sample	$\Delta(\delta_o - \delta_{obs.}) * \chi_4$	$\Delta(\delta_o - \delta_{obs.}) * \chi_4$	$\Delta(\delta_o - \delta_{obs.}) * \chi_4$	$\chi_{(1•4)}$	χ_4	χ_1
1	0	0	0	0	1.0	0
2	0.0110314	0.0054982	0.0074468	0.1	0.9	0.1
3	0.0211586	0.0113439	0.0142872	0.2	0.8	0.2
4	0.0274527	0.0158918	0.0191628	0.3	0.7	0.3
5	0.0315357	0.0187508	0.0220972	0.4	0.6	0.4
6	0.0330617	0.0193546	0.0225107	0.5	0.5	0.5
7	0.0319888	0.0190728	0.0218987	0.6	0.4	0.6
8	0.0297461	0.0171008	0.0209103	0.7	0.3	0.7
9	0.0245851	0.0140403	0.0160363	0.8	0.2	0.8
10	0.0162491	0.0089067	0.0102109	0.9	0.1	0.9
11				1	0.0	1

Sample	δ (ppm) Benzoate 1 Trial 2	δ (ppm) Benzoate 2 Trial 2	δ (ppm) Benzoate 3 Trial 2	δ (ppm) Benzoate 4 Trial 2	δ (ppm) Benzoate 5 Trial 2	$\chi_{(1\bullet4)}$	Amt. 4 (mL)	Amt. 1 (mL)
1						0	1	0
2	8.3974328	8.4149407	8.4339440	8.9235707	8.9413275	0.46	0.54	0.46
3	8.3948399	8.4121261	8.4312104	8.9236919	8.9405333	0.49	0.51	0.49
4	8.3895494	8.4072058	8.4258503	8.9210898	8.9373988	0.52	0.48	0.52
5	8.3846196	8.4014278	8.4205818	8.9182519	8.9349379	0.55	0.45	0.55
6	8.3788922	8.3959570	8.4150783	8.9153913	8.9325397	0.58	0.42	0.58
7	8.3700121	8.3871423	8.4060616	8.9113275	8.9276705	0.64	0.36	0.64
8	8.3678244	8.3845867	8.4031402	8.9111031	8.9276749	0.67	0.33	0.67
9	8.3636618	8.3802068	8.3990839	8.9090123	8.9255481	0.7	0.3	0.7
10	8.3281484	8.3422185	8.3617475	8.9023276	8.9177961	1	0	1

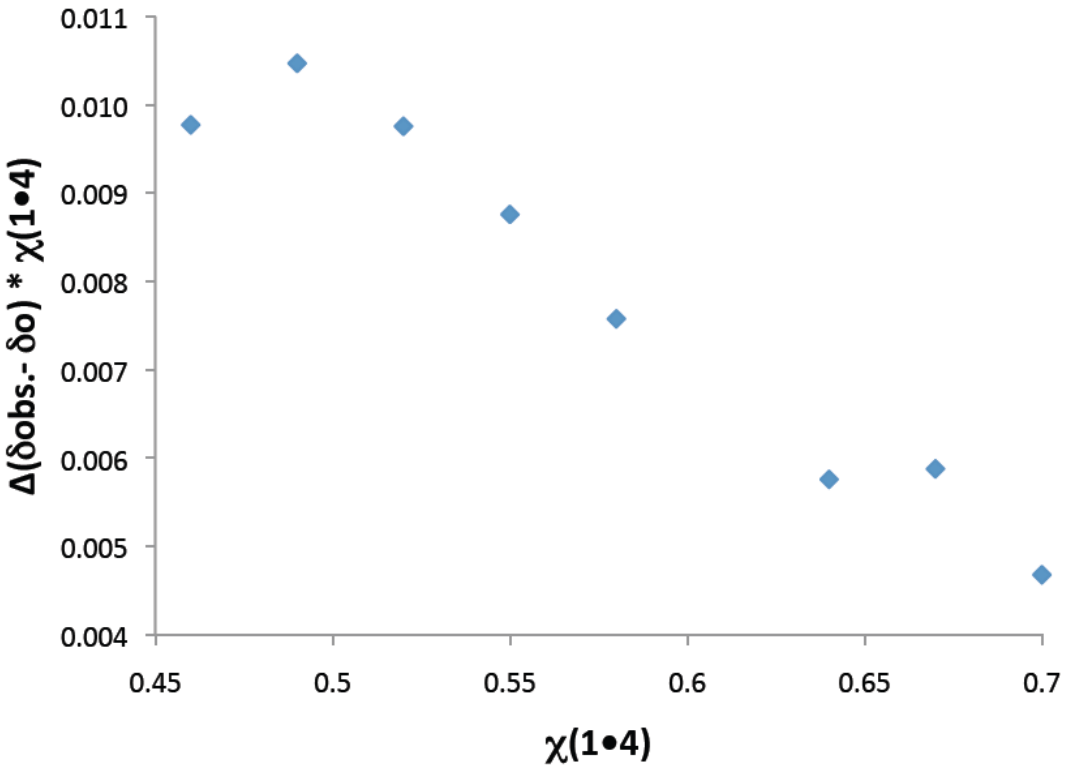
Sample	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_o-\delta_{obs.})$	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_{obs.}-\delta_o)$	$\chi_{(1\bullet4)}$	Amt. 4 (mL)	Amt. 1 mL)
1						0	1	0
2	0.0692844	0.0727222	0.0721965	0.0212431	0.0235314	0.46	0.54	0.46
3	0.0666915	0.0699076	0.0694629	0.0213643	0.0227372	0.49	0.51	0.49
4	0.0614010	0.0649873	0.0641028	0.0187622	0.0196027	0.52	0.48	0.52
5	0.0564712	0.0592093	0.0588343	0.0159243	0.0171418	0.55	0.45	0.55
6	0.0507438	0.0537385	0.0533308	0.0130637	0.0147436	0.58	0.42	0.58
7	0.0418637	0.0449238	0.0443141	0.0089999	0.0098744	0.64	0.36	0.64
8	0.0396760	0.0423682	0.0413927	0.0087755	0.0098788	0.67	0.33	0.67
9	0.0355134	0.0379883	0.0373364	0.0066847	0.0077520	0.7	0.3	0.7
10	0	0	0	0	0	1	0	1

Sample	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1\bullet4)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1\bullet4)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1\bullet4)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1\bullet4)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1\bullet4)}$	$\chi_{(1\bullet4)}$	χ_4	χ_1
1						0	1	0
2	0.0318708	0.0334522	0.0332104	0.0097718	0.0108244	0.46	0.54	0.46
3	0.0326788	0.0342547	0.0340368	0.0104685	0.0111412	0.49	0.51	0.49
4	0.0319285	0.0337934	0.0333335	0.0097563	0.0101934	0.52	0.48	0.52
5	0.0310592	0.0325651	0.0323589	0.0087584	0.0094280	0.55	0.45	0.55
6	0.0294314	0.0311683	0.0309319	0.0075769	0.0085513	0.58	0.42	0.58
7	0.0267928	0.0287512	0.0283610	0.0057599	0.0063196	0.64	0.36	0.64
8	0.0265829	0.0283867	0.0277331	0.0058796	0.0066188	0.67	0.33	0.67
9	0.0248594	0.0265918	0.0261355	0.0046793	0.0054264	0.7	0.3	0.7
10	0	0	0	0	0	1	0	1

Sample	δ (ppm) Methylene Trial 2	δ (ppm) Ferrocene 1 Trial 2	δ (ppm) Ferrocene 2 Trial 2	$\chi_{(1•4)}$	Amt. 4 (mL)	Amt. 1 (mL)
1	4.8561235	5.3481445	5.4481895	0	1	0
2	4.2160571	5.2973779	5.3910362	0.46	0.54	0.46
3	4.2171409	5.2963542	5.3898404	0.49	0.51	0.49
4	4.2171680	5.2935762	5.3869838	0.52	0.48	0.52
5	4.2172538	5.2906401	5.3839111	0.55	0.45	0.55
6	4.2183161	5.2879690	5.3806692	0.58	0.42	0.58
7	4.2173060	5.2818290	5.3740452	0.64	0.36	0.64
8	4.2195299	5.2806200	5.3726506	0.67	0.33	0.67
9	4.2195098	5.2774969	5.3692558	0.7	0.3	0.7
10				1	0	1
Sample	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\chi_{(1•4)}$	χ_4	χ_1
1	0.0000000	0.0000000	0.0000000	0	1	0
2	0.6400664	0.0507666	0.0571533	0.46	0.54	0.46
3	0.6389826	0.0517903	0.0583491	0.49	0.51	0.49
4	0.6389555	0.0545683	0.0612057	0.52	0.48	0.52
5	0.6388697	0.0575044	0.0642784	0.55	0.45	0.55
6	0.6378074	0.0601755	0.0675203	0.58	0.42	0.58
7	0.6388175	0.0663155	0.0741443	0.64	0.36	0.64
8	0.6365936	0.0675245	0.0755389	0.67	0.33	0.67
9	0.6366137	0.0706476	0.0789337	0.7	0.3	0.7
10				1	0	1
Sample	$\Delta(\delta_o - \delta_{obs.}) * \chi_4$	$\Delta(\delta_o - \delta_{obs.}) * \chi_4$	$\Delta(\delta_o - \delta_{obs.}) * \chi_4$	$\chi_{(1•4)}$	χ_4	χ_1
1	0.0000000	0.0000000	0.0000000	0	1	0
2	0.3456359	0.0274140	0.0308628	0.46	0.54	0.46
3	0.3258811	0.0264131	0.0297580	0.49	0.51	0.49
4	0.3066986	0.0261928	0.0293787	0.52	0.48	0.52
5	0.2874914	0.0258770	0.0289253	0.55	0.45	0.55
6	0.2678791	0.0252737	0.0283585	0.58	0.42	0.58
7	0.2299743	0.0238736	0.0266919	0.64	0.36	0.64
8	0.2100759	0.0222831	0.0249278	0.67	0.33	0.67
9	0.1909841	0.0211943	0.0236801	0.7	0.3	0.7
10				1	0	1



Job Plot in 9:1 DMSO: D_2O for Benzoate 4 Trial 1 indicating both a 1:1 and 1:2 stoichiometry between host and guest.



Job Plot for 9:1 DMSO: D_2O Trial 2 Benzoate 4 indicating both a 1:1 and 1:2 stoichiometry between host and guest.

1,1'-di(aminomethyl)ferrocenium Hydrochloride (4) Bound to Potassium Benzoate (1) in 1:1 DMSO: D_2O

General Procedure for NMR Titrations Trial 1:
8 mmol/L and 160 mmol/L stock solution of 1,1'-di(aminomethyl)ferrocene **4** (Host) and potassium benzoate **1** (Guest) were made, respectively. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

General Procedure for NMR Titrations Trials 2 and 3:
8 mmol/L and 160 mmol/L stock solution of 1,1'-di(aminomethyl)ferrocene **4** (Host) and potassium benzoate **1** (Guest) were made, respectively. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

General Procedure for NMR Titrations Trial 4:
An 8 mmol/L stock solution of 1,1'-di(aminomethyl)ferrocene **4** (Host) was made. 10 mmol/L and 400 mmol/L stock solutions of potassium benzoate **1** (Guest) were made. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. For samples 2-6, the 10 mmol/L stock solution of potassium benzoate was used. For samples 7-13, the 400 mmol/L stock solution of potassium benzoate was used. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

50% DMSO Ferrocene 1

Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 1
0.0008	100	1	0.0000	0	0	4.5429248
0.0008	100	1	0.0032	20	4	4.5388779
0.0008	100	1	0.0040	25	5	4.5367380
0.0008	100	1	0.0056	35	7	4.5349794
0.0008	100	1	0.0064	40	8	4.5322759
0.0008	100	1	0.0072	45	9	4.5326117
0.0008	100	1	0.0080	50	10	4.5328303
0.0008	100	1	0.0120	75	15	4.5292981
0.0008	100	1	0.0160	100	20	4.5249582
0.0008	100	1	0.0320	200	40	4.5140153
0.0008	100	1	0.0480	300	60	4.5054807
0.0008	100	1	0.0640	400	80	4.4975010
0.0008	100	1	0.0800	500	100	4.4899656
0.0008	100	1	0.1200	750	150	4.4746197
0.0008	100	1	0.1440	900	180	4.4648932

Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 2	δ (ppm) Ferrocene 1 Trial 3
0.0008	100	1	0.0000	0	0	4.5449581	4.5449581
0.0008	100	1	0.0040	25	5	4.5386050	4.5396279
0.0008	100	1	0.0080	50	10	4.5349396	4.5343568
0.0008	100	1	0.0160	100	20	4.5255992	4.5268936
0.0008	100	1	0.0320	200	40	4.5153924	4.5162854
0.0008	100	1	0.0480	300	60	4.5069096	4.5079722
0.0008	100	1	0.0640	400	80	4.4991306	4.4990476
0.0008	100	1	0.1000	625	125	4.4830173	4.4847433
0.0008	100	1	0.1440	900	180	4.4678326	4.4676486

Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 4
0.0008	100	1	0.0000	0	0	4.5401007
0.0008	100	1	0.0004	40	.5	4.5393850
0.0008	100	1	0.0008	80	1	4.5384826
0.0008	100	1	0.0016	160	2	4.5373431
0.0008	100	1	0.0032	320	4	4.5333823
0.0008	100	1	0.0048	480	6	4.5319857
0.0008	100	1	0.0100	25	12.5	4.5271940
0.0008	100	1	0.0192	48	24	4.5189307
0.0008	100	1	0.0400	100	50	4.5066067
0.0008	100	1	0.0800	200	100	4.4869223
0.0008	100	1	0.1600	400	200	4.4633034
0.0008	100	1	0.2400	600	300	4.4379934
0.0008	100	1	0.3600	900	450	4.4045979

Ferrocene 1	K1	K2
Trial 1	64.34	1.37
Trial 2	59.25	1.65
Trial 3	55.03	0.99
Trial 4	39.71	0.10
Average	54.58	1.03
Standard Deviation	10.62	0.67
% Error	19.46	65.57

50% DMSO Ferrocene 2						
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 1
0.0008	100	1	0.0000	0	0	4.6129643
0.0008	100	1	0.0032	20	4	4.6082522
0.0008	100	1	0.0040	25	5	4.6084272
0.0008	100	1	0.0056	35	7	4.6065355
0.0008	100	1	0.0064	40	8	4.6050775
0.0008	100	1	0.0072	45	9	4.6074361
0.0008	100	1	0.0080	50	10	4.6047651
0.0008	100	1	0.0120	75	15	4.6045439
0.0008	100	1	0.0160	100	20	4.6005195
0.0008	100	1	0.0320	200	40	4.5945987
0.0008	100	1	0.0480	300	60	4.5890553
0.0008	100	1	0.0640	400	80	4.5834927
0.0008	100	1	0.0800	500	100	4.5805425
0.0008	100	1	0.1200	750	150	4.5736649
0.0008	100	1	0.1440	900	180	4.5632561

Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 2	δ (ppm) Ferrocene 2 Trial 3
0.0008	100	1	0.0000	0	0	4.6162577	4.6112128
0.0008	100	1	0.0040	25	5	4.6116827	4.6094804
0.0008	100	1	0.0080	50	10	4.6077774	4.6062586
0.0008	100	1	0.0160	100	20	4.6030301	4.6040763
0.0008	100	1	0.0320	200	40	4.5964851	4.5962223
0.0008	100	1	0.0480	300	60	4.5915084	4.5924663
0.0008	100	1	0.0640	400	80	4.5860282	4.5869178
0.0008	100	1	0.1000	625	125	4.5764025	4.5764066
0.0008	100	1	0.1440	900	180	4.5668240	4.5656075

Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 4
0.0008	100	1	0.0000	0	0	4.6103373
0.0008	100	1	0.0004	40	.5	4.6094536
0.0008	100	1	0.0008	80	1	4.6093266
0.0008	100	1	0.0016	160	2	4.6082487
0.0008	100	1	0.0032	320	4	4.6043340
0.0008	100	1	0.0048	480	6	4.6035455
0.0008	100	1	0.0100	25	12.5	4.6007680
0.0008	100	1	0.0192	48	24	4.5951170
0.0008	100	1	0.0400	100	50	4.5877567
0.0008	100	1	0.0800	200	100	4.5751266
0.0008	100	1	0.1600	400	200	4.5591193
0.0008	100	1	0.2400	600	300	4.5437075
0.0008	100	1	0.3600	900	450	4.5238163

Ferrocene 2	K1	K2
Trial 1	70.48	0.00
Trial 2	103.75	2.03
Trial 3	70.81	1.38
Trial 4	92.76	0.89
Average	84.45	1.08
Standard Deviation	16.56	0.86
% Error	19.61	79.46

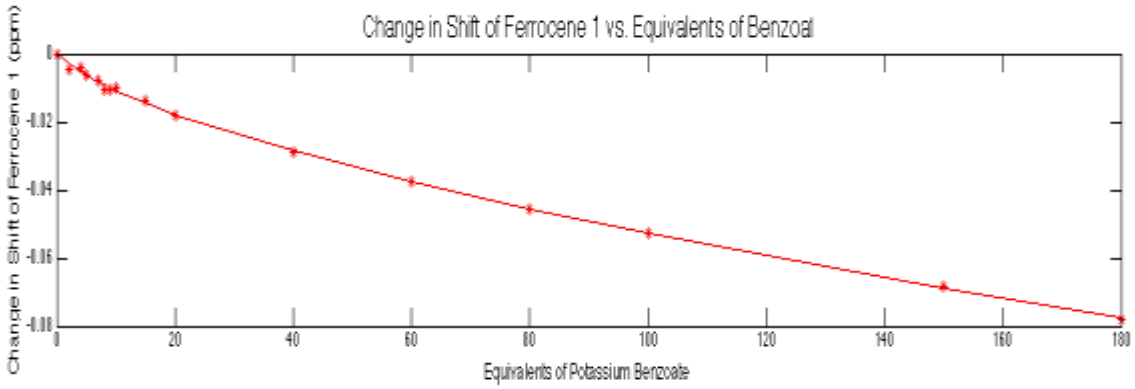
50% DMSO Methylene							
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Methylene Trial 1	
0.0008	100	1	0.0000	0	0	4.0837818	
0.0008	100	1	0.0032	20	4	4.0827489	
0.0008	100	1	0.0040	25	5	4.0815054	
0.0008	100	1	0.0056	35	7	4.0780151	
0.0008	100	1	0.0064	40	8	4.0794173	
0.0008	100	1	0.0072	45	9	4.0764971	
0.0008	100	1	0.0080	50	10	4.0763067	
0.0008	100	1	0.0120	75	15	4.0736496	
0.0008	100	1	0.0160	100	20	4.0745563	
0.0008	100	1	0.0320	200	40	4.0670769	
0.0008	100	1	0.0480	300	60	4.0641589	
0.0008	100	1	0.0640	400	80	4.0590984	
0.0008	100	1	0.0800	500	100	4.0553761	
0.0008	100	1	0.1200	750	150	4.0480917	
0.0008	100	1	0.1440	900	180	4.0446796	

Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Methylene Trial 2	δ (ppm) Methylene Trial 3
0.0008	100	1	0.0000	0	0	4.0909380	4.0909380
0.0008	100	1	0.0040	25	5	4.0861616	4.0847223
0.0008	100	1	0.0080	50	10	4.0819423	4.0847223
0.0008	100	1	0.0160	100	20	4.0773011	4.0738827
0.0008	100	1	0.0320	200	40	4.0719700	4.0701269
0.0008	100	1	0.0480	300	60	4.0686621	4.0673934
0.0008	100	1	0.0640	400	80	4.0633644	4.0641344
0.0008	100	1	0.1000	625	125	4.0573733	4.0555851
0.0008	100	1	0.1440	900	180	4.0487545	4.0467717

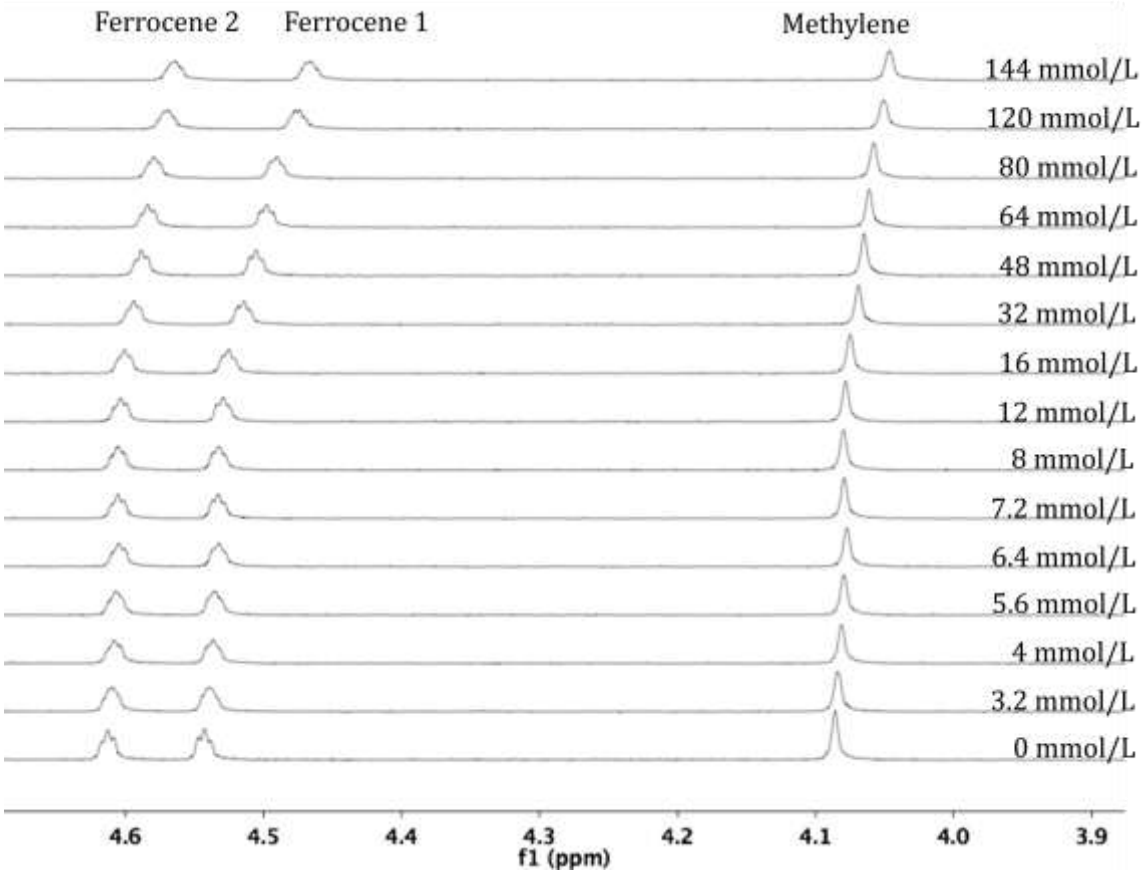
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Methylene Trial 4
0.0008	100	1	0.0000	0	0	4.0858939
0.0008	100	1	0.0004	40	.5	4.0843567
0.0008	100	1	0.0008	80	1	4.0836517
0.0008	100	1	0.0016	160	2	4.0821548
0.0008	100	1	0.0032	320	4	4.0756301
0.0008	100	1	0.0048	480	6	4.0746924
0.0008	100	1	0.0100	25	12.5	4.0749304
0.0008	100	1	0.0192	48	24	4.0689814
0.0008	100	1	0.0400	100	50	4.0645483
0.0008	100	1	0.0800	200	100	4.0539302
0.0008	100	1	0.1600	400	200	4.0457970
0.0008	100	1	0.2400	600	300	4.0325756
0.0008	100	1	0.3600	900	450	4.0164757

Methylene	K1	K2
Trial 1	331.27	4.15
Trial 2	332.03	1.47
Trial 3	341.11	0.00
Trial 4	249.94	0.47
Average	313.59	1.52
Standard Deviation	42.67	1.86
% Error	13.61	121.82

	K1	K2
Fc 1 Trial 1	64.34	1.37
Fc 1 Trial 2	59.25	1.65
Fc 1 Trial 3	55.03	0.99
Fc 1 Trial 4	39.71	0.10
Fc 2 Trial 1	70.48	0.00
Fc 2 Trial 2	103.75	2.03
Fc 2 Trial 3	70.81	1.38
Fc 2 Trial 4	92.76	0.89
Me Trial 1	331.27	4.15
Me Trial 2	332.03	1.47
Me Trial 3	341.11	0.00
Me Trial 4	249.94	0.47
Average	150.87	1.21



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shifts for 1,1'-di(aminomethylferrocenium) hydrochloride peaks for Trial 1.

1,1'-di(aminomethyl)ferrocenium Hydrochloride (4) Bound to Potassium Benzoate (1) in D_2O

General Procedure for NMR Titrations:
8 mmol/L and 400 mmol/L stock solution of 1,1'-di(aminomethyl)ferrocene **4** (Host) and potassium benzoate **1** (Guest) were made, respectively. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

D_2O Ferrocene 1								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 trial 1	δ (ppm) Ferrocene 1 trial 2	δ (ppm) Ferrocene 1 trial 3
0.0008	100	1	0.0000	0	0.0	4.3600684	4.3600684	4.3600684
0.0008	100	1	0.0100	25	12.5	4.3481284	4.3491007	4.3487178
0.0008	100	1	0.0192	48	24.0	4.3389218	4.3392523	4.3386278
0.0008	100	1	0.0400	100	50.0	4.3230507	4.3231180	4.3236711
0.0008	100	1	0.0800	200	100.0	4.2988775	4.2988353	4.2991707
0.0008	100	1	0.1600	400	200.0	4.2599788	4.2595126	4.2605251
0.0008	100	1	0.2800	700	350.0	4.2125417	4.2123165	4.2126492
0.0008	100	1	0.3600	900	450.0	4.1832583	4.1832315	4.1832875

Ferrocene 1	K1	K2
Trial 1	21.80	0.42
Trial 2	16.48	0.30
Trial 3	21.69	0.40
Average	19.99	0.37
Standard Deviation	3.04	0.06
% Error	15.19	16.43

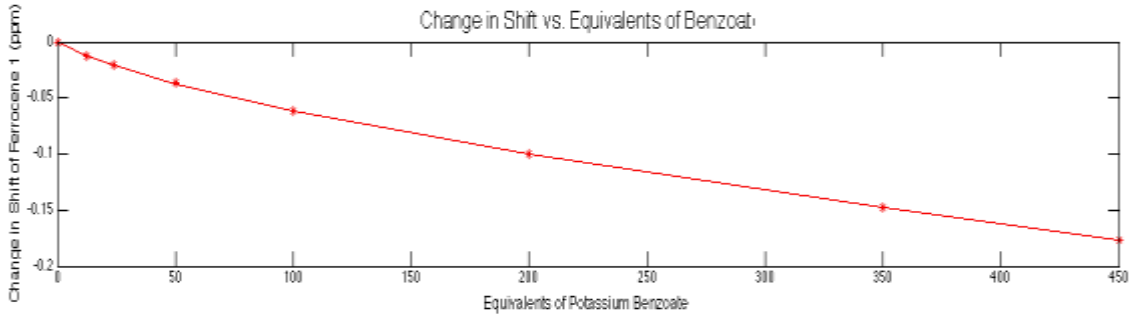
D_2O Ferrocene 2								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 1	δ (ppm) Ferrocene 2 Trial 2	δ (ppm) Ferrocene 2 Trial 3
0.0008	100	1	0.0000	0	0.0	4.4278341	4.4278341	4.4278341
0.0008	100	1	0.0100	25	12.5	4.4176249	4.4172731	4.4162861
0.0008	100	1	0.0192	48	24.0	4.4082179	4.4074095	4.4078750
0.0008	100	1	0.0400	100	50.0	4.3933961	4.3942189	4.3933130
0.0008	100	1	0.0800	200	100.0	4.3716848	4.3717069	4.3716455
0.0008	100	1	0.1600	400	200.0	4.3360612	4.3372853	4.3367400
0.0008	100	1	0.2800	700	350.0	4.2949773	4.2953198	4.2952163
0.0008	100	1	0.3600	900	450.0	4.2699167	4.2699455	4.2699893

Ferrocene 2	K1	K2
Trial 1	18.45	0.48
Trial 2	23.35	0.51
Trial 3	26.75	0.62
Average	22.85	0.54
Standard Deviation	4.17	0.07
% Error	18.26	13.29

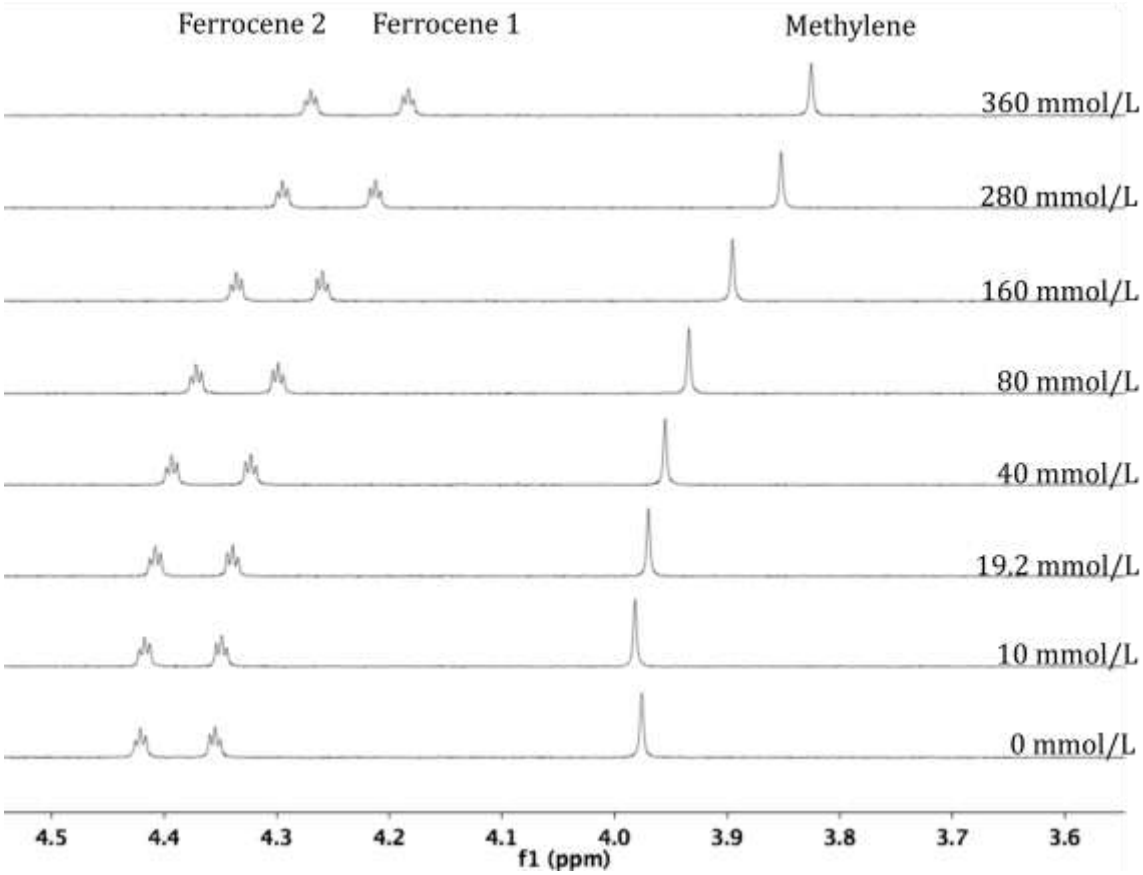
D_2O Methylene								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Methylene Trial 1	δ (ppm) Methylene Trial 2	δ (ppm) Methylene Trial 3
0.0008	100	1	0.0000	0	0.0	3.9931499	3.9758528	3.9725581
0.0008	100	1	0.0100	25	12.5	3.9786434	3.9817734	3.9816919
0.0008	100	1	0.0192	48	24.0	3.9701841	3.9699656	3.9684994
0.0008	100	1	0.0400	100	50.0	3.9549596	3.9551504	3.9577940
0.0008	100	1	0.0800	200	100.0	3.9340807	3.9341046	3.9334191
0.0008	100	1	0.1600	400	200.0	3.8965126	3.8952994	3.8971343
0.0008	100	1	0.2800	700	350.0	3.8526987	3.8519571	3.8528589
0.0008	100	1	0.3600	900	450.0	3.8255062	3.8254498	3.8254567

Methylene	K1	K2
Trial 1	56.39	0.79
Trial 2	54.15	0.89
Trial 3	64.05	0.79
Average	58.20	0.82
Standard Deviation	5.19	0.05
% Error	8.92	6.54

	K1	K2
Trial 1	21.80	0.42
Trial 2	16.48	0.30
Trial 3	21.69	0.40
Trial 1	18.45	0.48
Trial 2	23.35	0.51
Trial 3	26.75	0.62
Trial 1	56.39	0.79
Trial 2	54.15	0.89
Trial 3	64.05	0.79
Average	33.68	0.58



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shifts for 1,1'-di(aminomethylferrocenium) hydrochloride peaks for Trial 1.

(Guanidinylmethyl)ferrocenium Triflate (5) Bound to Potassium Benzoate (1) in 9:1 DMSO: D_2O

General Procedure for NMR titrations for trials 1-3:
A 8 mmol/L stock solution of (guanidinylmethyl)ferrocenium triflate **5** (Host) was made. 4 mmol/L and 50 mmol/L stock solutions of potassium benzoate **1** (Guest) were made. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. The 4 mmol/L stock solution of potassium benzoate was used for the first 9 samples for each three trials, and the 50 mmol/L stock solution of potassium benzoate was used for the last 4 samples for all three trials. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C.

General Procedure for NMR titrations for trials 4 and 5:
A 20 mmol/L stock solution of (guanidinylmethyl)ferrocenium triflate **5** (Host) was made. 16 mmol/L and 45 mmol/L stock solutions of potassium benzoate **1** (Guest) were made. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. The 20 mmol/L stock solution of potassium benzoate was used for the first 7 samples for each three trials, and the 45 mmol/L stock solution of potassium benzoate was used for the last sample for all three trials. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C.

All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790). The methylene peak, cyclopentadienyl ring peak, and the two ferrocene triplets were monitored. Association constants were calculated for all four signals, and the final association constant reported is the average of the local association constant values for each set of peak type.

90% DMSO Methylene								
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Methylene Trial 1	δ (ppm) Methylene Trial 2	δ (ppm) Methylene Trial 3
0.0008	100	1	0	0	0	5.1333255	5.1336957	5.1333399
0.0008	100	1	0.00008	20	0.1	5.1327520	5.1312916	5.1312065
0.0008	100	1	0.00016	40	0.2	5.1329717	5.1318149	5.1318220
0.0008	100	1	0.00032	80	0.4	5.1316892	5.1330305	5.1330269
0.0008	100	1	0.00064	160	0.8	5.1325833	5.1331744	5.1321747
0.0008	100	1	0.00096	240	1.2	5.1333228	5.1332170	5.1322833
0.0008	100	1	0.00128	320	1.6	5.1345411	5.1338045	5.1346979
0.0008	100	1	0.0016	400	2	5.1352583	5.1359627	5.1353207
0.0008	100	1	0.0032	800	4	5.1374759	5.1372615	5.1372199
0.0008	100	1	0.0064	128	8	5.1365271	5.1371424	5.1350888
0.0008	100	1	0.008	160	10	5.1364866	5.1382458	5.1365407
0.0008	100	1	0.016	320	20	5.1386094	5.1367429	5.1380720
0.0008	100	1	0.04	800	50	5.1368965	5.1349082	5.1348901

90% DMSO Methylene							
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Methylene Trial 4	δ (ppm) Methylene Trial 5
0.002	100	1	0	0	0	5.1308357	5.1310043
0.002	100	1	0.0008	50	0.4	5.1319901	5.1319472
0.002	100	1	0.001	62.5	0.5	5.1321050	5.1333008
0.002	100	1	0.002	125	1	5.1335031	5.1335451
0.002	100	1	0.004	250	2	5.1347185	5.1347709
0.002	100	1	0.008	500	4	5.1367020	5.1353974
0.002	100	1	0.01	625	5	5.1366193	5.1356258
0.002	100	1	0.02	444.4	10	5.1372918	5.1372105

Methylene	Ka
Trial 1	341.02
Trial 2	391.83
Trial 3	373.27
Trial 4	334.91
Trial 5	311.47
Average	350.50
Standard Deviation	31.95
% Error	9.12

90% DMSO Ferrocene 1								
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 1	δ (ppm) Ferrocene 1 Trial 2	δ (ppm) Ferrocene 1 Trial 3
0.0008	100	1	0	0	0	5.2411607	5.2417951	5.2420077
0.0008	100	1	0.00008	20	0.1	5.2400719	5.2386069	5.2394426
0.0008	100	1	0.00016	40	0.2	5.2399129	5.2388314	5.2383820
0.0008	100	1	0.00032	80	0.4	5.2377898	5.2377824	5.2389815
0.0008	100	1	0.00064	160	0.8	5.2355755	5.2374970	5.2360590
0.0008	100	1	0.00096	240	1.2	5.2360004	5.2344020	5.2338224
0.0008	100	1	0.00128	320	1.6	5.2362048	5.2344527	5.2350892
0.0008	100	1	0.0016	400	2	5.2336561	5.2345066	5.2334758
0.0008	100	1	0.0032	800	4	5.2289189	5.2280930	5.2287102
0.0008	100	1	0.0064	128	8	5.2190603	5.2188835	5.2178966
0.0008	100	1	0.008	160	10	5.2151208	5.2169346	5.2149558
0.0008	100	1	0.016	320	20	5.2055615	5.2042796	5.2054545
0.0008	100	1	0.04	800	50	5.1868563	5.1857015	5.1860812

90% DMSO Ferrocene 1							
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 4	δ (ppm) Ferrocene 1 Trial 5
0.002	100	1	0	0	0	5.2388055	5.2387860
0.002	100	1	0.0008	50	0.4	5.2359431	5.2359357
0.002	100	1	0.001	62.5	0.5	5.2352539	5.2364005
0.002	100	1	0.002	125	1	5.2319585	5.2315621
0.002	100	1	0.004	250	2	5.2250063	5.2250063
0.002	100	1	0.008	500	4	5.2171168	5.2160976
0.002	100	1	0.01	625	5	5.2136940	5.2123457
0.002	100	1	0.02	444.4	10	5.2019546	5.2013452

Ferrocene 1	Ka
Trial 1	64.84
Trial 2	66.37
Trial 3	75.42
Trial 4	70.14
Trial 5	72.20
Average	69.79
Standard Deviation	4.30
% Error	6.16

90% DMSO Cp Ring								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Cp Ring Trial 1	δ (ppm) Cp Ring Trial 2	δ (ppm) Cp Ring Trial 3
0.0008	100	1	0	0	0	5.2660147	5.2662250	5.2660925
0.0008	100	1	0.00008	20	0.1	5.2650732	5.2640345	5.2639628
0.0008	100	1	0.00016	40	0.2	5.2651000	5.2639628	5.2640035
0.0008	100	1	0.00032	80	0.4	5.2638435	5.2648242	5.2649375
0.0008	100	1	0.00064	160	0.8	5.2637034	5.2646957	5.2635786
0.0008	100	1	0.00096	240	1.2	5.2634653	5.2634733	5.2624293
0.0008	100	1	0.00128	320	1.6	5.2641310	5.2632069	5.2642024
0.0008	100	1	0.0016	400	2	5.2640398	5.2651155	5.2639839
0.0008	100	1	0.0032	800	4	5.2633535	5.2634097	5.2630050
0.0008	100	1	0.0064	128	8	5.2589130	5.2588503	5.2577823
0.0008	100	1	0.008	160	10	5.2572145	5.2583674	5.2573878
0.0008	100	1	0.016	320	20	5.2536171	5.2525790	5.2535790
0.0008	100	1	0.04	800	50	5.2435477	5.2424606	5.2423905

90% DMSO Cp Ring							
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Cp Ring Trial 4	δ (ppm) Cp Ring Trial 5
0.002	100	1	0	0	0	5.2637692	5.2638696
0.002	100	1	0.0008	50	0.4	5.2634168	5.2633776
0.002	100	1	0.001	62.5	0.5	5.2632034	5.2643238
0.002	100	1	0.002	125	1	5.2627806	5.2627148
0.002	100	1	0.004	250	2	5.2607461	5.2607487
0.002	100	1	0.008	500	4	5.2584182	5.2573947
0.002	100	1	0.01	625	5	5.2570157	5.2558251
0.002	100	1	0.02	444.4	10	5.2520956	5.2519272

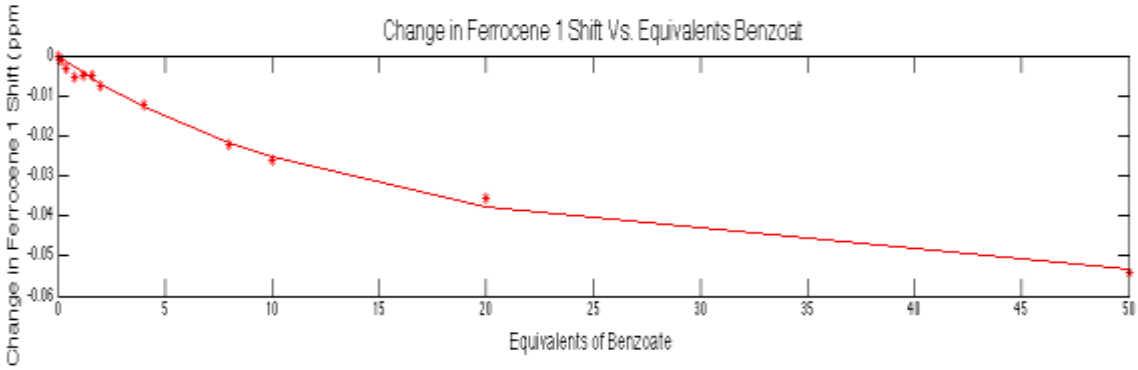
Cp Ring	Ka
Trial 1	33.04
Trial 2	28.61
Trial 3	33.74
Trial 4	31.63
Trial 5	32.26
Average	31.86
Standard Deviation	1.98
% Error	6.21

90% DMSO Ferrocene 2								
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 1	δ (ppm) Ferrocene 2 Trial 2	δ (ppm) Ferrocene 2 Trial 3
0.0008	100	1	0	0	0	5.3188659	5.3202557	5.3191627
0.0008	100	1	0.00008	20	0.1	5.3190460	5.3174183	5.3178008
0.0008	100	1	0.00016	40	0.2	5.3193569	5.3179111	5.3174302
0.0008	100	1	0.00032	80	0.4	5.3176644	5.3198191	5.3197092
0.0008	100	1	0.00064	160	0.8	5.3183884	5.3203892	5.3188254
0.0008	100	1	0.00096	240	1.2	5.3192894	5.3193765	5.3186457
0.0008	100	1	0.00128	320	1.6	5.3217084	5.3204729	5.3207836
0.0008	100	1	0.0016	400	2	5.3222485	5.3237731	5.3222505
0.0008	100	1	0.0032	800	4	5.3249980	5.3248233	5.3251829
0.0008	100	1	0.0064	128	8	5.3248719	5.3243181	5.3238541
0.0008	100	1	0.008	160	10	5.3263200	5.3261209	5.3258153
0.0008	100	1	0.016	320	20	5.3297088	5.3274535	5.3281044
0.0008	100	1	0.04	800	50	5.3268207	5.3264053	5.3258421

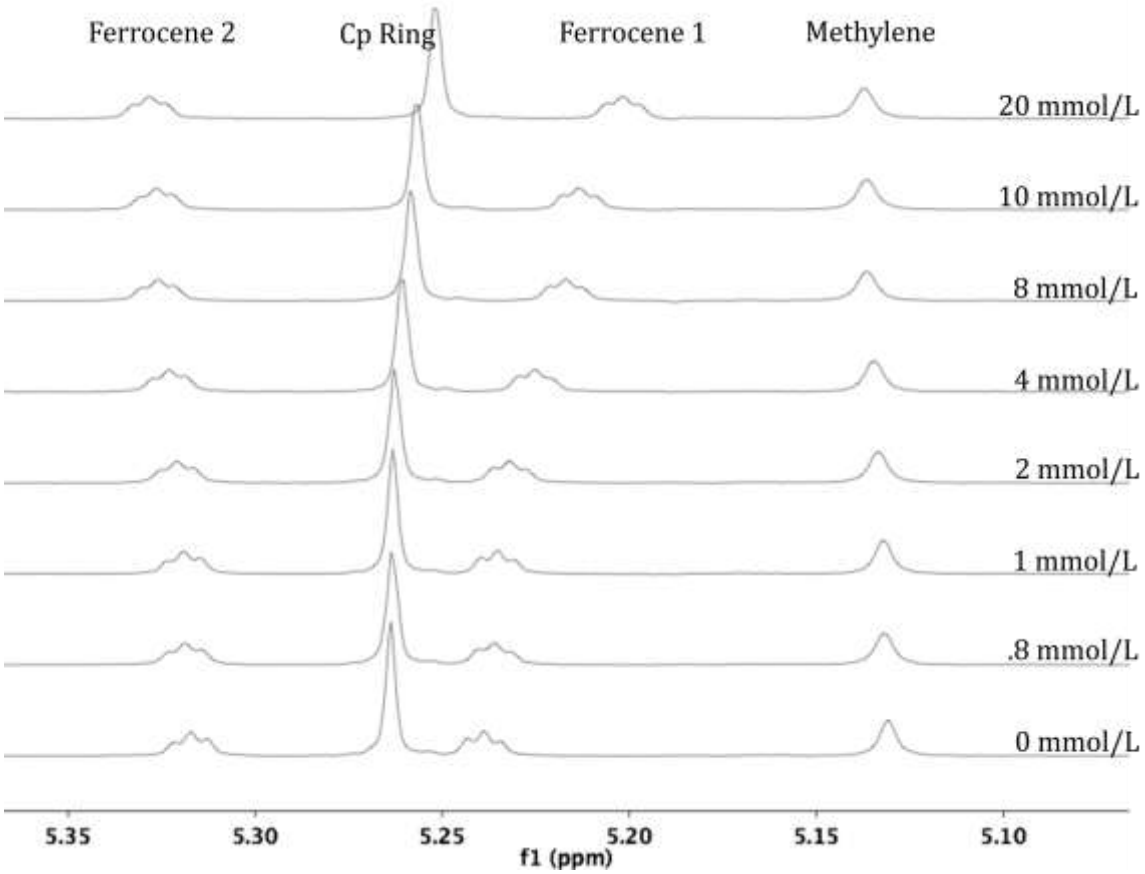
90% DMSO Ferrocene 2							
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 4	δ (ppm) Ferrocene 2 Trial 5
0.002	100	1	0	0	0	5.3172252	5.3174637
0.002	100	1	0.0008	50	0.4	5.3189397	5.3186784
0.002	100	1	0.001	62.5	0.5	5.3190915	5.3203651
0.002	100	1	0.002	125	1	5.3209568	5.3210628
0.002	100	1	0.004	250	2	5.3229615	5.3229277
0.002	100	1	0.008	500	4	5.3262143	5.3249881
0.002	100	1	0.01	625	5	5.3267666	5.3256699
0.002	100	1	0.02	444.4	10	5.3282222	5.3285189

Ferrocene 2	Ka
Trial 1	294.79
Trial 2	232.27
Trial 3	289.71
Trial 4	258.51
Trial 5	221.58
Average	259.37
Standard Deviation	32.93
% Error	12.70

	Ka
Me Trial 1	341.02
Me Trial 2	391.83
Me Trial 3	373.27
Me Trial 4	334.91
Me Trial 5	311.47
Fc 1 Trial 1	64.84
Fc 1 Trial 2	66.37
Fc 1 Trial 3	75.42
Fc 1 Trial 4	70.14
Fc 1 Trial 5	72.20
Cp Trial 1	33.04
Cp Trial 2	28.61
Cp Trial 3	33.74
Cp Trial 4	31.63
Cp Trial 5	32.26
Fc 2 Trial 1	294.79
Fc 2 Trial 2	232.27
Fc 2 Trial 3	289.71
Fc 2 Trial 4	258.51
Fc 2 Trial 5	221.58
Average	177.88



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shift for (Guanidinylmethyl)ferrocenium peaks for Trial 4.

Job's Method for Stoichiometry Determination of (Guanidinymethyl)ferrocenium Triflate (5) and Potassium Benzoate (1) in 9:1 DMSO: D_2O

General Procedure for Trials 1 and 2: 4.2 mmol/ L stock solutions were made of (guanidinylmethyl)ferrocenium triflate **5** (host) and of potassium benzoate **1** (guest). Contents were bound for two hours at 20˚C. The four ferrocenyl peaks of the host were monitored. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

Sample	δ (ppm) Methylene Trial 1	δ (ppm) Ferrocene 1 Trial 1	δ (ppm) Cp Ring Trial 1	δ (ppm) Ferrocene 2 Trial 1	$\chi_{(1•5)}$	Amt. 5 (mL)	Amt. 1 (mL)
1	5.1333255	5.2411607	5.2660147	5.3202557	0	1	0
2	5.1308503	5.2308503	5.2606021	5.3181990	0.43	0.57	0.43
3	5.1303736	5.2280643	5.2592817	5.3178566	0.49	0.51	0.49
4	5.1303397	5.2272070	5.2590497	5.3181155	0.55	0.45	0.55
5	5.1309290	5.2267313	5.2590569	5.3184047	0.61	0.39	0.61
6	5.1311773	5.2262526	5.2590050	5.3187839	0.64	0.36	0.64
7	5.1313701	5.2258880	5.2588151	5.3190795	0.67	0.33	0.67
8	5.1321910	5.2238645	5.2585650	5.3201757	0.8	0.2	0.8
9	5.1328175	5.2225617	5.2581709	5.3208002	0.9	0.1	0.9
10					1	0	1

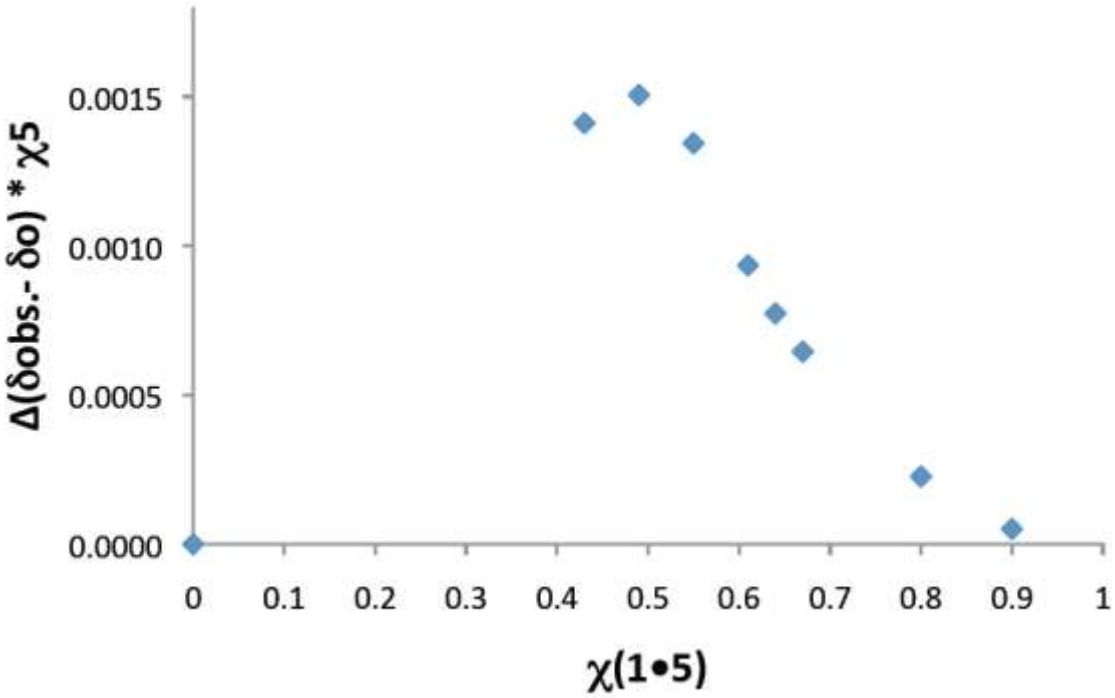
Sample	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\chi_{(1•5)}$	χ_5	χ_1
1	0	0	0	0	0	1	0
2	0.0024752	0.0103104	0.0054126	0.0020567	0.43	0.57	0.43
3	0.0029519	0.0130964	0.0067330	0.0023991	0.49	0.51	0.49
4	0.0029858	0.0139537	0.0069650	0.0021402	0.55	0.45	0.55
5	0.0023965	0.0144294	0.0069578	0.0018510	0.61	0.39	0.61
6	0.0021482	0.0149081	0.0070097	0.0014718	0.64	0.36	0.64
7	0.0019554	0.0152727	0.0071996	0.0011762	0.67	0.33	0.67
8	0.0011345	0.0172962	0.0074497	0.0000800	0.8	0.2	0.8
9	0.0005080	0.0185990	0.0078438	-0.0005445	0.9	0.1	0.9
10					1	0	1

Sample	$\Delta(\delta_o - \delta_{obs.}) * \chi_5$	$\Delta(\delta_o - \delta_{obs.}) * \chi_5$	$\Delta(\delta_o - \delta_{obs.}) * \chi_5$	$\Delta(\delta_o - \delta_{obs.}) * \chi_5$	$\chi_{(1•5)}$	χ_5	χ_1
1	0	0	0	0	0	1	0
2	0.0014108	0.0058769	0.0030851	0.0011723	0.43	0.57	0.43
3	0.0015054	0.0066791	0.0034338	0.0012235	0.49	0.51	0.49
4	0.0013436	0.0062791	0.0031342	0.0009630	0.55	0.45	0.55
5	0.0009346	0.0056274	0.0027135	0.0007218	0.61	0.39	0.61
6	0.0007733	0.0053669	0.0025234	0.0005298	0.64	0.36	0.64
7	0.0006452	0.0050399	0.0023758	0.0003881	0.67	0.33	0.67
8	0.0002269	0.0034592	0.0014899	0.0000160	0.8	0.2	0.8
9	0.0000508	0.0018599	0.0007843	-0.0000544	0.9	0.1	0.9
10					1	0	1

Sample	δ (ppm) Methylene Trial 2	δ (ppm) Ferrocene 1 Trial 2	δ (ppm) Cp Ring Trial 2	δ (ppm) Ferrocene 2 Trial 2	$\chi_{(1•5)}$	Amt. 5 (mL)	Amt. 1 (mL)
1	5.1336957	5.2417951	5.2662250	5.3202557	0	1	0
2	5.1309320	5.2305040	5.2605401	5.3182354	0.43	0.57	0.43
3	5.1301543	5.2283671	5.2594661	5.3176872	0.49	0.51	0.49
4	5.1304569	5.2274359	5.2591089	5.3179838	0.55	0.45	0.55
5	5.1310239	5.2266921	5.2590585	5.3185838	0.61	0.39	0.61
6	5.1312621	5.2261501	5.2590110	5.3187923	0.64	0.36	0.64
7	5.1313959	5.2257402	5.2585956	5.3189750	0.67	0.33	0.67
8	5.1322409	5.2241556	5.2585840	5.3201282	0.8	0.2	0.8
9	5.1328176	5.2225714	5.2581447	5.3208267	0.9	0.1	0.9
10					1	0	1

Sample	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\Delta(\delta_o - \delta_{obs.})$	$\chi_{(1•5)}$	χ_5	χ_1
1	0	0	0	0	0	1	0
2	0.0027637	0.0112911	0.0056849	0.0020203	0.43	0.57	0.43
3	0.0035414	0.0134280	0.0067589	0.0025685	0.49	0.51	0.49
4	0.0032388	0.0143592	0.0071161	0.0022719	0.55	0.45	0.55
5	0.0026718	0.0151030	0.0071665	0.0016719	0.61	0.39	0.61
6	0.0024336	0.0156450	0.0072140	0.0014634	0.64	0.36	0.64
7	0.0022998	0.0160549	0.0076294	0.0012807	0.67	0.33	0.67
8	0.0014548	0.0176395	0.0076410	0.0001275	0.8	0.2	0.8
9	0.0008781	0.0192237	0.0080803	-0.0005710	0.9	0.1	0.9
10					1	0	1

Sample	$\Delta(\delta_o - \delta_{obs.}) * \chi_5$	$\Delta(\delta_o - \delta_{obs.}) * \chi_5$	$\Delta(\delta_o - \delta_{obs.}) * \chi_5$	$\Delta(\delta_o - \delta_{obs.}) * \chi_5$	$\chi_{(1•5)}$	χ_5	χ_1
1	0	0	0	0	0	1	0
2	0.0015753	0.0064359	0.0032403	0.0011515	0.43	0.57	0.43
3	0.0018061	0.0068482	0.0034470	0.0013099	0.49	0.51	0.49
4	0.0014574	0.0064616	0.0032022	0.0010223	0.55	0.45	0.55
5	0.0010420	0.0058901	0.0027949	0.0006520	0.61	0.39	0.61
6	0.0008760	0.0056322	0.0025970	0.0005268	0.64	0.36	0.64
7	0.0007589	0.0052981	0.0025177	0.0004226	0.67	0.33	0.67
8	0.0002909	0.0035279	0.0015282	0.0000255	0.8	0.2	0.8
9	0.0000878	0.0019223	0.0008080	-0.0000571	0.9	0.1	0.9
10					1	0	1



Job Plot for the Methylene peak from Trial 1 depicting a maximum at mole fraction equal to 0.5, indicating a 1:1 stoichiometry between host and guest.

1,1'-bis(guanidinylmethyl)ferrocenium Hydrochloride (6) Bound to Potassium Benzoate (1) in 9:1 DMSO: D_2O

General Procedure for NMR Titrations:
An 8 mmol/ stock solution of 1,1'-bis(guanidinylmethyl)ferrocenium hydrochloride **6** (Host) was made. 4 mmol/L and 20 mmol/L stock solutions of potassium benzoate **1** (Guest) were made. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. The 4 mmol/L stock solution of benzoate was used for samples 2-10, and the 20 mmol/L stock solution of benzoate was used for samples 11-13. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

90% DMSO Ferrocene 1								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 1	δ (ppm) Ferrocene 1 Trial 2	δ (ppm) Ferrocene 1 Trial 3
0.0008	100	1	0.00000	0	0	5.2794828	5.2794828	5.2794828
0.0008	100	1	0.00004	10	0.05	5.2794319	5.2794902	5.2794603
0.0008	100	1	0.00008	20	0.1	5.2794087	5.2794945	5.2793928
0.0008	100	1	0.00024	60	0.3	5.2793613	5.2794016	5.2794534
0.0008	100	1	0.00040	100	0.5	5.2793531	5.2793028	5.2793613
0.0008	100	1	0.00056	140	0.7	5.2780132	5.2796052	5.2787376
0.0008	100	1	0.00072	180	0.9	5.2779706	5.2778628	5.2786858
0.0008	100	1	0.00080	200	1	5.2759995	5.2774682	5.2770285
0.0008	100	1	0.00160	400	2	5.2727130	5.2723199	5.2726290
0.0008	100	1	0.00320	800	4	5.2667051	5.2668839	5.2668571
0.0008	100	1	0.00640	320	8	5.2594595	5.2584833	5.2584719
0.0008	100	1	0.00800	400	10	5.2577428	5.2576377	5.2577646
0.0008	100	1	0.01600	800	20	5.2483762	5.2484438	5.2475246

Ferrocene 1	K1	K2
Trial 1	11320.00	128.17
Trial 2	10279.10	156.24
Trial 3	10384.80	133.56
Average	10661.30	139.32
Standard Deviation	572.89	14.90
% Error	5.37	10.69

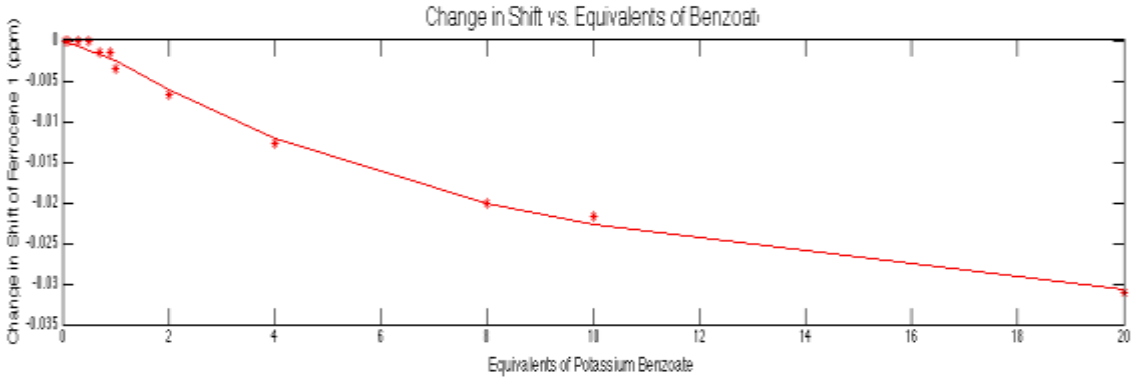
90% DMSO Ferrocene 2								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 1	δ (ppm) Ferrocene 2 Trial 2	δ (ppm) Ferrocene 2 Trial 3
0.0008	100	1	0.00000	0	0	5.3405515	5.3405515	5.3392839
0.0008	100	1	0.00004	10	0.05	5.3392920	5.3393212	5.3393110
0.0008	100	1	0.00008	20	0.1	5.3392470	5.3393647	5.3394202
0.0008	100	1	0.00024	60	0.3	5.3394701	5.3393936	5.3395066
0.0008	100	1	0.00040	100	0.5	5.3392661	5.3393476	5.3393309
0.0008	100	1	0.00056	140	0.7	5.3386526	5.3406766	5.3394463
0.0008	100	1	0.00072	180	0.9	5.3400666	5.3401926	5.3411335
0.0008	100	1	0.00080	200	1	5.3392862	5.3401883	5.3405672
0.0008	100	1	0.00160	400	2	5.3415490	5.3416216	5.3414836
0.0008	100	1	0.00320	800	4	5.3431914	5.3434596	5.3434658
0.0008	100	1	0.00640	320	8	5.3445131	5.3434747	5.3434401
0.0008	100	1	0.00800	400	10	5.3458432	5.3456018	5.3456352
0.0008	100	1	0.01600	800	20	5.3466566	5.3468579	5.3456192

Ferrocene 2	K1	K2
Trial 1	11842.20	320.17
Trial 2	11464.00	354.49
Trial 3	11540.00	401.48
Average	11615.40	358.72
Standard Deviation	200.06	40.82
% Error	1.72	11.38

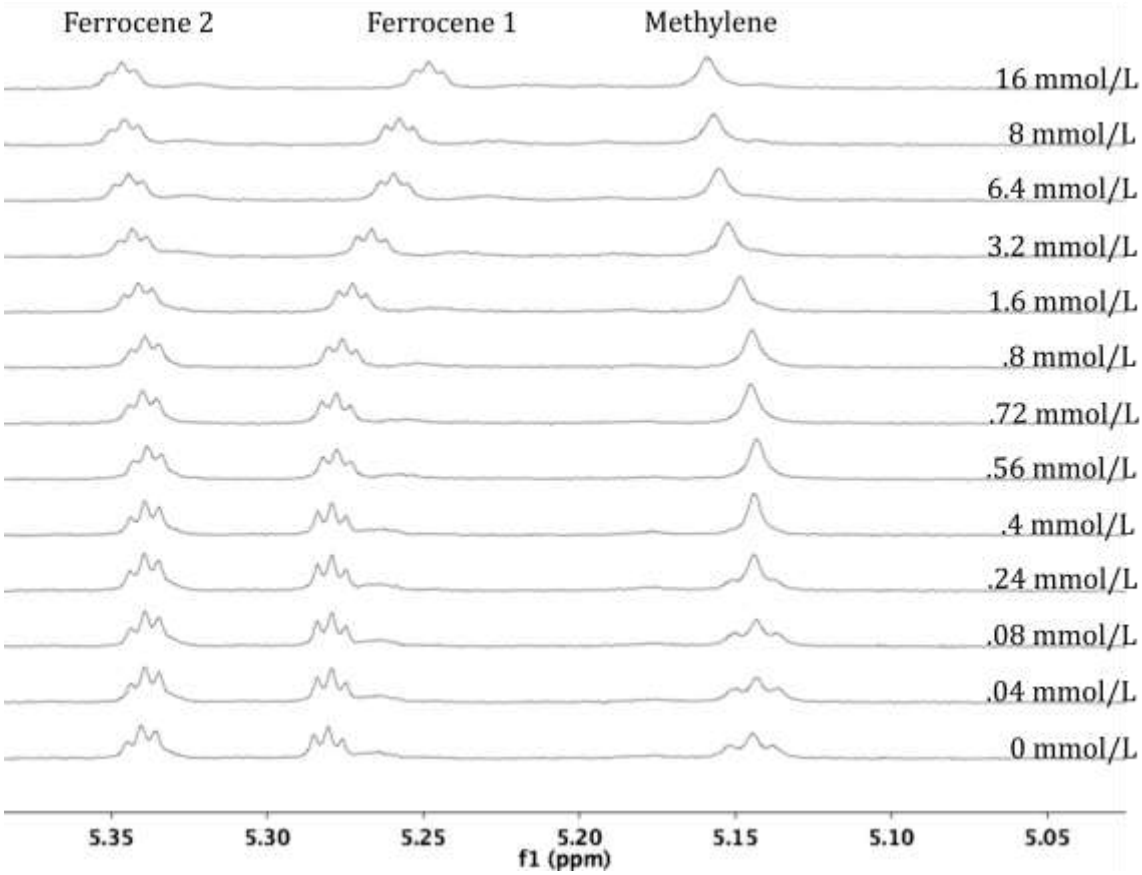
90% DMSO Methylene								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	Methylene Trial 1	Methylene Trial 2	Methylene Trial 3
0.0008	100	1	0.00000	0	0	5.1445823	5.1445823	5.1445823
0.0008	100	1	0.00004	10	0.05	5.1434397	5.1432502	5.1434961
0.0008	100	1	0.00008	20	0.1	5.1433850	5.1434397	5.1435443
0.0008	100	1	0.00024	60	0.3	5.1441403	5.1437399	5.1435664
0.0008	100	1	0.00040	100	0.5	5.1439873	5.1439291	5.1439644
0.0008	100	1	0.00056	140	0.7	5.1431423	5.1454423	5.1442175
0.0008	100	1	0.00072	180	0.9	5.1450041	5.1451716	5.1462299
0.0008	100	1	0.00080	200	1	5.1447444	5.1454984	5.1458599
0.0008	100	1	0.00160	400	2	5.1484529	5.1485750	5.1485174
0.0008	100	1	0.00320	800	4	5.1524825	5.1525703	5.1525189
0.0008	100	1	0.00640	320	8	5.1552312	5.1541692	5.1541060
0.0008	100	1	0.00800	400	10	5.1569493	5.1569641	5.1568649
0.0008	100	1	0.01600	800	20	5.1589833	5.1589578	5.1580164

Methylene	K1	K2
Trial 1	9845.14	470.59
Trial 2	13266.10	448.30
Trial 3	10193.40	403.07
Average	11101.55	440.66
Standard Deviation	1882.63	34.40
% Error	16.96	7.81

	K1	K2
Fc 1 Trial 1	11320.00	128.17
Fc 1 Trial 2	10279.10	156.24
Fc 1 Trial 3	10384.80	133.56
Fc 2 Trial 1	11842.20	320.17
Fc 2 Trial 2	11464.00	354.49
Fc 2 Trial 3	11540.00	401.48
Me Trial 1	9845.14	470.59
Me Trial 2	13266.10	448.30
Me Trial 3	10193.40	403.07
Average	11126.08	312.90



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shift for 1,1'-bis(guanidinylmethyl)ferrocenium peaks for Trial 1.

Job's Method for Stoichiometry Determination of 1,1-bis(guanidinylmethyl) ferrocenium Hydrochoride (6) and Potassium Benzoate (1) in 9:1 DMSO: D_2O

General Procedure for Trials 1 and 2: .8 mmol/ L stock solutions were made of 1,1'-bis(guanidinylmethyl)ferrocenium hydrochloride **6** (host) and of potassium benzoate **1** (guest). Contents were bound for two hours at 21˚C. Three of the ferrocenyl peaks of the host were monitored as well as two benzoate peaks. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400**.** Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

Sample	δ (ppm) Benzoate 1 Trial 1	δ (ppm) Benzoate 2 Trial 1	δ (ppm) Benzoate 3 Trial 1	δ (ppm) Benzoate 4 Trial 1	δ (ppm) Benzoate 5 Trial 1	$\chi_{(1•6)}$	Amt. 6 (mL)	Amt. 1 (mL)
1						0	1	0
2	8.5630848	8.5822162	8.6015548	9.0047966	9.0244229	.1	.9	.1
3	8.5632442	8.5823344	8.6012671	9.0053380	9.0245560	.2	.8	.2
4	8.5612398	8.5803877	8.5993430	9.0034229	9.0225183	.3	.7	.3
5	8.5624067	8.5814656	8.6003413	9.0043011	9.0235848	.4	.6	.4
6	8.5637183	8.5802308	8.5990017	9.0025192	9.0222025	.5	.5	.5
7	8.5637500	8.5822639	8.6013164	9.0053329	9.0243350	.6	.4	.6
8	8.5637595	8.5826336	8.6015968	9.0061022	9.0251371	.7	.3	.7
9	8.5020936	8.5213274	8.5406195	8.9781411	8.9972342	.8	.2	.8
10	8.4036062	8.4206569	8.4400297	8.9354500	8.9527782	.9	.1	.9
11	8.3402374	8.3543683	8.3742584	8.9163798	8.9315440	1	0	1

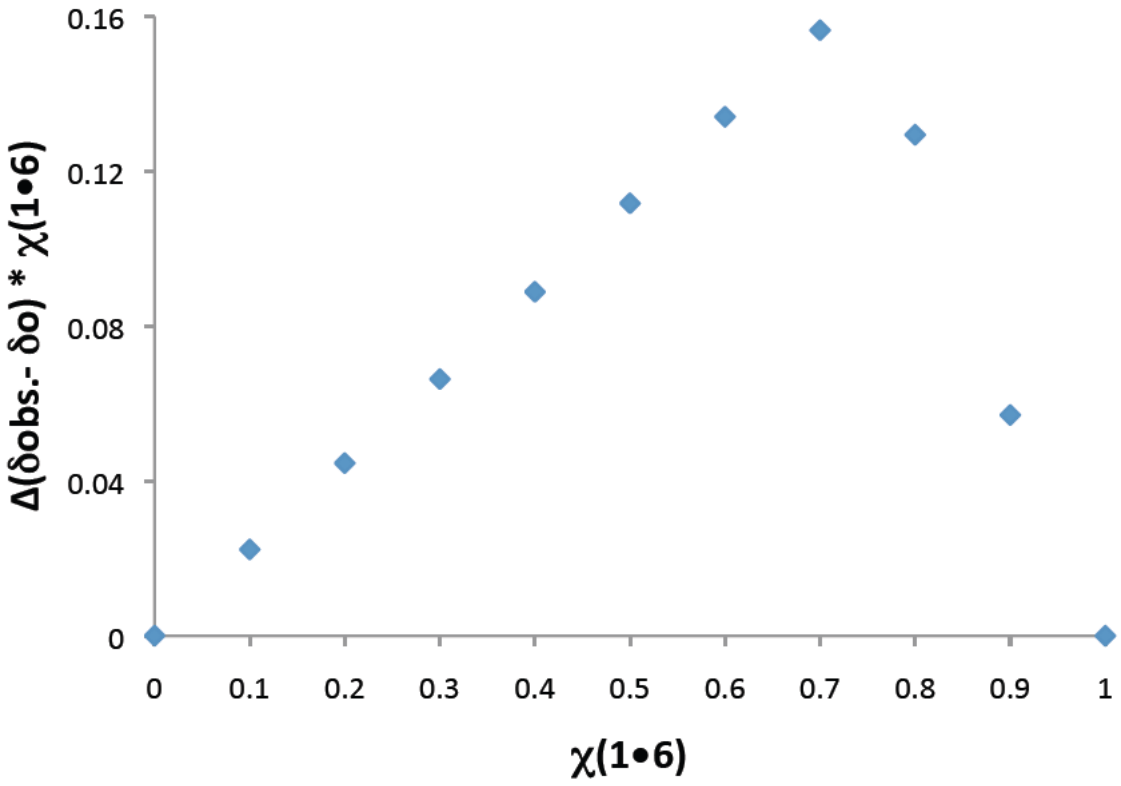
Sample	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_o-\delta_{obs.})$	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_{obs.}-\delta_o)$	$\chi_{(1•6)}$	Amt. 6 (mL)	Amt. 1 mL)
1						0	1	0
2	0.2228474	0.2278479	0.2272964	0.0884168	0.0928789	.1	.9	.1
3	0.2230068	0.2279661	0.2270087	0.0889582	0.0930120	.2	.8	.2
4	0.2210024	0.2260194	0.2250846	0.0870431	0.0909743	.3	.7	.3
5	0.2221693	0.2270973	0.2260829	0.0879213	0.0920408	.4	.6	.4
6	0.2234809	0.2258625	0.2247433	0.0861394	0.0906585	.5	.5	.5
7	0.2235126	0.2278956	0.2270580	0.0889531	0.0927910	.6	.4	.6
8	0.2235221	0.2282653	0.2273384	0.0897224	0.0935931	.7	.3	.7
9	0.1618562	0.1669591	0.1663611	0.0617613	0.0656902	.8	.2	.8
10	0.0633688	0.0662886	0.0657713	0.0190702	0.0212342	.9	.1	.9
11	0	0	0	0	0	1	0	1

Sample	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\chi_{(1•6)}$	χ_6	χ_1
1						0	1	0
2	0.0222847	0.0227847	0.0227296	0.0088416	0.0092878	.1	.9	.1
3	0.0446013	0.0455932	0.0454017	0.0177916	0.0186024	.2	.8	.2
4	0.0663007	0.0678058	0.0675253	0.0261129	0.0272922	.3	.7	.3
5	0.0888677	0.0908389	0.0904331	0.0351685	0.0368163	.4	.6	.4
6	0.1117404	0.1129312	0.1123716	0.0430697	0.0453292	.5	.5	.5
7	0.1341075	0.1367373	0.1362348	0.0533718	0.0556746	.6	.4	.6
8	0.1564654	0.1597857	0.1591368	0.0628056	0.0655151	.7	.3	.7
9	0.1294849	0.1335672	0.1330888	0.0494090	0.0525521	.8	.2	.8
10	0.0570319	0.0596597	0.0591941	0.0171631	0.0191107	.9	.1	.9
11	0	0	0	0	0	1	0	1

Sample	δ (ppm) Benzoate 1 Trial 2	δ (ppm) Benzoate 2 Trial 2	δ (ppm) Benzoate 3 Trial 2	δ (ppm) Benzoate 4 Trial 2	δ (ppm) Benzoate 5 Trial 2	$\chi_{(1•6)}$	Amt. 6 (mL)	Amt. 1 (mL)
1						0	1	0
2	8.5630198	8.5822706	8.6011489	9.0043448	9.0244229	.1	.9	.1
3	8.5635267	8.5823985	8.6013534	9.00533	9.0247517	.2	.8	.2
4	8.5621917	8.5810696	8.6001917	9.0039139	9.0236476	.3	.7	.3
5	8.5623851	8.5813632	8.6003089	9.0043452	9.0233866	.4	.6	.4
6	8.5617675	8.5805609	8.5996192	9.0045209	9.0218351	.5	.5	.5
7	8.5624188	8.5815304	8.6006572	9.0045457	9.0238496	.6	.4	.6
8	8.5670076	8.582987	8.5992681	9.0076307	9.026251	.7	.3	.7
9	8.4850561	8.5039793	8.5230367	8.9708756	8.9899772	.8	.2	.8
10	8.3962854	8.4140673	8.4326757	8.9314268	8.9489937	.9	.1	.9
11	8.3276583	8.3419521	8.3611416	8.9018381	8.9170365	1	0	1

Sample	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_o-\delta_{obs.})$	$\Delta(\delta_{obs.}-\delta_o)$	$\Delta(\delta_{obs.}-\delta_o)$	$\chi_{(1•6)}$	Amt. 6 (mL)	Amt. 1 mL)
1						0	1	0
2	0.2353615	0.2403185	0.2400073	0.1025067	0.1073864	0.1	0.9	0.1
3	0.2358684	0.2404464	0.2402118	0.1034919	0.1077152	0.2	0.8	0.2
4	0.2345334	0.2391175	0.2390501	0.1020758	0.1066111	0.3	0.7	0.3
5	0.2347268	0.2394111	0.2391673	0.1025071	0.1063501	0.4	0.6	0.4
6	0.2341092	0.2386088	0.2384776	0.1026828	0.1047986	0.5	0.5	0.5
7	0.2347605	0.2395783	0.2395156	0.1027076	0.1068131	0.6	0.4	0.6
8	0.2393493	0.2410349	0.2381265	0.1057926	0.1092145	0.7	0.3	0.7
9	0.1573978	0.1620272	0.1618951	0.0690375	0.0729407	0.8	0.2	0.8
10	0.0686271	0.0721152	0.0715341	0.0295887	0.0319572	0.9	0.1	0.9
11	0	0	0	0	0	1	0	1

Sample	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\Delta(\delta_{obs.}-\delta_o) * \chi_{(1•6)}$	$\chi_{(1•6)}$	χ_6	χ_1
1						0	1	0
2	0.0235361	0.0240318	0.0240007	0.0102506	0.0107386	0.1	0.9	0.1
3	0.0471736	0.0480892	0.0480423	0.0206983	0.0215430	0.2	0.8	0.2
4	0.0703600	0.0717352	0.0717150	0.0306227	0.0319833	0.3	0.7	0.3
5	0.0938907	0.0957644	0.0956669	0.0410028	0.0425400	0.4	0.6	0.4
6	0.1170546	0.1193044	0.1192388	0.0513414	0.0523993	0.5	0.5	0.5
7	0.1408563	0.1437469	0.1437093	0.0616245	0.0640878	0.6	0.4	0.6
8	0.1675445	0.1687244	0.1666885	0.0740548	0.0764501	0.7	0.3	0.7
9	0.1259182	0.1296217	0.1295160	0.0552300	0.0583525	0.8	0.2	0.8
10	0.0617643	0.0649036	0.0643806	0.0266298	0.0287614	0.9	0.1	0.9
11	0	0	0	0	0	1	0	1



Job Plot for Benzoate peak 1 from Trial 1 indicating a 1:2 stoichiometry between host and guest.

1,1'-bis(guanidinylmethyl)ferrocenium Hydrochloride (6) Bound to Potassium Benzoate (1) in 1:1 DMSO: D_2O

General Procedure for NMR Titrations:
An 8 mmol/ stock solution of 1,1'-bis(guanidinylmethyl)ferrocenium hydrochloride **6** (Host) was made. 4 mmol/L and 160 mmol/L stock solutions of potassium benzoate **1** (Guest) were made. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. The 4 mmol/L stock solution of benzoate was used for samples 2-9, and the 160 mmol/L stock solution of benzoate was used for samples 10-12. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

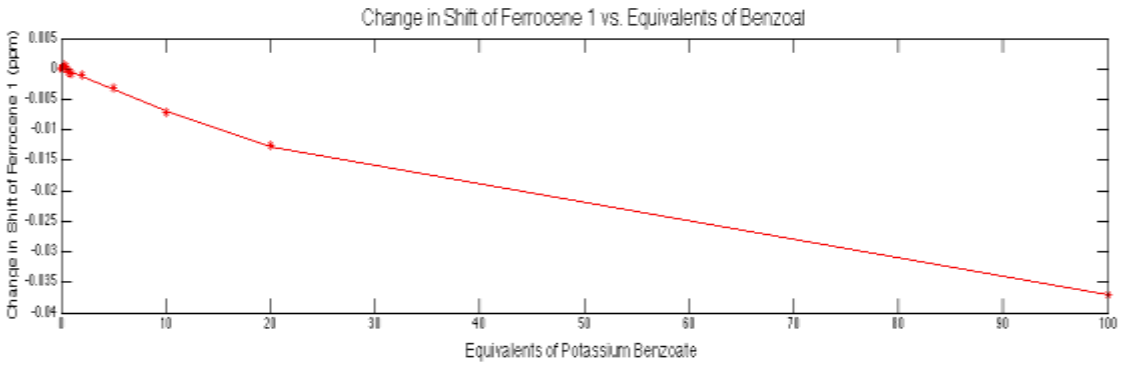
50% DMSO Ferrocene 1								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 1	δ (ppm) Ferrocene 1 Trial 2	δ (ppm) Ferrocene 1 Trial 3
0.0008	100	1	0.00000	0	0	4.4672405	4.4669255	4.4673527
0.0008	100	1	0.00004	10	0.05	4.4673941	4.4672926	4.4673941
0.0008	100	1	0.00008	20	0.1	4.4673686	4.4673967	4.4677859
0.0008	100	1	0.00024	60	0.3	4.4677859	4.4677859	4.4677859
0.0008	100	1	0.00040	100	0.5	4.4676017	4.4677859	4.4675704
0.0008	100	1	0.00056	140	0.7	4.4667213	4.4675149	4.4676257
0.0008	100	1	0.00072	180	0.9	4.4667065	4.4667606	4.4671473
0.0008	100	1	0.00080	200	1	4.4663683	4.4670495	4.4670326
0.0008	100	1	0.00160	400	2	4.4662196	4.4659864	4.4655005
0.0008	100	1	0.00400	25	5	4.4640094	4.4630360	4.4633327
0.0008	100	1	0.00800	50	10	4.4601104	4.4606758	4.4603521
0.0008	100	1	0.01600	100	20	4.4545857	4.4544923	4.4547478
0.0008	100	1	0.08000	500	100	4.4302182	4.4302100	4.4306782

Ferrocene 1	K1	K2
Trial 1	4376.95	15.18
Trial 2	4390.39	16.49
Trial 3	4350.79	12.32
Average	4372.71	14.66
Standard Deviation	20.14	2.13
% Error	0.46	14.54

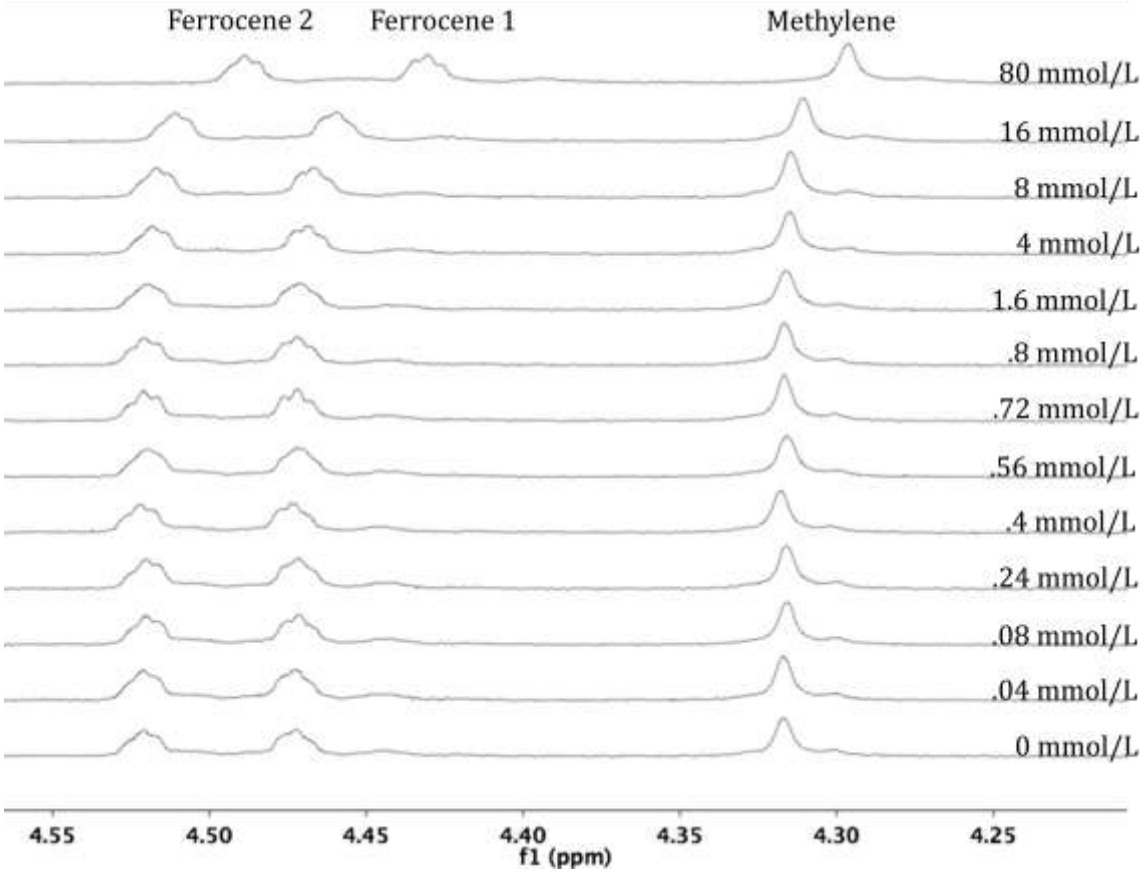
50% DMSO Ferrocene 2								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 1	δ (ppm) Ferrocene 2 Trial 2	δ (ppm) Ferrocene 2 Trial 3
0.0008	100	1	0.00000	0	0	4.5159782	4.5163315	4.5161860
0.0008	100	1	0.00004	10	0.05	4.5157471	4.5157730	4.5158283
0.0008	100	1	0.00008	20	0.1	4.5163032	4.5160459	4.5161939
0.0008	100	1	0.00024	60	0.3	4.5162326	4.5162326	4.5162326
0.0008	100	1	0.00040	100	0.5	4.5162326	4.5164682	4.5164368
0.0008	100	1	0.00056	140	0.7	4.5154081	4.5163212	4.5160126
0.0008	100	1	0.00072	180	0.9	4.5159698	4.5161744	4.5161606
0.0008	100	1	0.00080	200	1	4.5166070	4.5160554	4.5162351
0.0008	100	1	0.00160	400	2	4.5148695	4.5149125	4.5147840
0.0008	100	1	0.00400	25	5	4.5135754	4.5130653	4.5133299
0.0008	100	1	0.00800	50	10	4.5113041	4.5108673	4.5108841
0.0008	100	1	0.01600	100	20	4.5060807	4.5061204	4.5060046
0.0008	100	1	0.08000	500	100	4.4885921	4.4885112	4.4888090

Ferrocene 2	K1	K2
Trial 1	4039.05	16.75
Trial 2	4165.45	17.48
Trial 3	4971.22	18.28
Average	4391.91	17.50
Standard Deviation	505.67	0.76
% Error	11.51	4.36

	K1	K2
Fc 1 Trial 1	4376.95	15.18
Fc 1 Trial 2	4390.39	16.49
Fc 1 Trial 3	4350.79	12.32
Fc 2 Trial 1	4039.05	16.75
Fc 2 Trial 2	4165.45	17.48
Fc 2 Trial 3	4971.22	18.28
Average	4382.31	16.08



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked NMR spectra depicting NMR shift for 1,1'-bis(guanidinylmethyl)ferrocenium peaks for Trial 1.

1,1'-bis(guanidinylmethyl)ferrocenium Hydrochloride (6) Bound to Potassium Benzoate (1) in D_2O

General Procedure for NMR Titrations:
An 8 mmol/ stock solution of 1,1'-bis(guanidinylmethyl)ferrocenium hydrochloride **6** (Host) was made. 4 mmol/L and 160 mmol/L stock solutions of potassium benzoate **1** (Guest) were made. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. The 4 mmol/L stock solution of benzoate was used for samples 2-8, and the 160 mmol/L stock solution of benzoate was used for samples 9-13. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 21°C. All ^1H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

D_2O Ferrocene 1								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 1 Trial 1	δ (ppm) Ferrocene 1 Trial 2	δ (ppm) Ferrocene 1 Trial 3
0.0008	100	1	0.00000	0	0	4.29187300	4.29187300	4.29187300
0.0008	100	1	0.00008	20	0.1	4.29194920	4.29190390	4.29194733
0.0008	100	1	0.00024	60	0.3	4.29162960	4.29130260	4.29143490
0.0008	100	1	0.00040	100	0.5	4.29141760	4.29141440	4.29137553
0.0008	100	1	0.00056	140	0.7	4.29102600	4.29131020	4.29122797
0.0008	100	1	0.00072	180	0.9	4.29107600	4.29097960	4.29102733
0.0008	100	1	0.00080	200	1	4.29062480	4.29058120	4.29066203
0.0008	100	1	0.00160	400	2	4.28958140	4.28928870	4.28930263
0.0008	100	1	0.00400	25	5	4.28554120	4.28512520	4.28531670
0.0008	100	1	0.00800	50	10	4.27966790	4.27917850	4.27950477
0.0008	100	1	0.04000	250	50	4.24878880	4.24841800	4.24854470
0.0008	100	1	0.08000	500	100	4.22325460	4.22239810	4.22295763
0.0008	100	1	0.14400	900	180	4.19171160	4.19161340	4.19133127

Ferrocene 1	K1	K2
Trial 1	40.43	1.08
Trial 2	44.21	2.07
Trial 3	49.74	1.43
Average	44.79	1.52
Standard Deviation	4.68	0.50
% Error	10.45	33.01

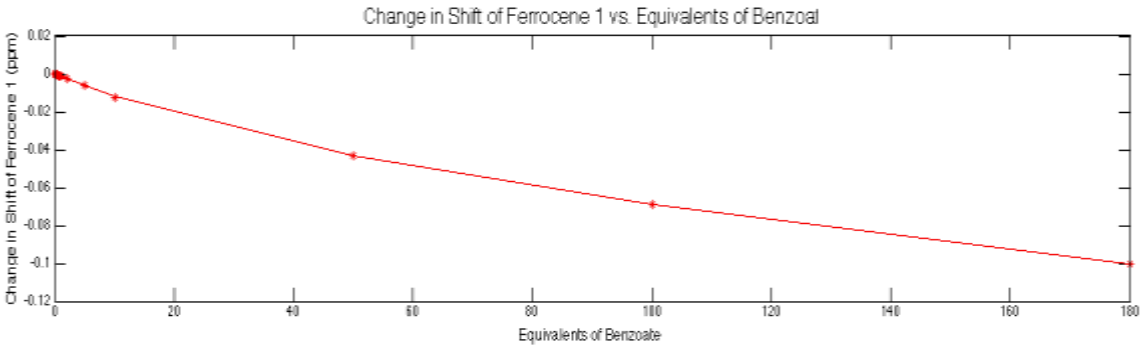
D_2O Ferrocene 2								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene 2 Trial 1	δ (ppm) Ferrocene 2 Trial 2	δ (ppm) Ferrocene 2 Trial 3
0.0008	100	1	0.00000	0	0	4.3417328	4.3417204	4.3417328
0.0008	100	1	0.00008	20	0.1	4.3419718	4.3419028	4.3420306
0.0008	100	1	0.00024	60	0.3	4.3415457	4.3412077	4.3413622
0.0008	100	1	0.00040	100	0.5	4.3413335	4.3412424	4.3412856
0.0008	100	1	0.00056	140	0.7	4.3409690	4.3410469	4.3410797
0.0008	100	1	0.00072	180	0.9	4.3409720	4.3408009	4.3408669
0.0008	100	1	0.00080	200	1	4.3403497	4.3403942	4.3403788
0.0008	100	1	0.00160	400	2	4.3390644	4.3388490	4.3387712
0.0008	100	1	0.00400	25	5	4.3338708	4.3336345	4.3338173
0.0008	100	1	0.00800	50	10	4.3271115	4.3267292	4.3269377
0.0008	100	1	0.04000	250	50	4.2900640	4.2893160	4.2894944
0.0008	100	1	0.08000	500	100	4.2579103	4.2580578	4.2582678
0.0008	100	1	0.14400	900	180	4.2202020	4.2209356	4.2199981

Ferrocene 2	K1	K2
Trial 1	69.66	3.00
Trial 2	68.52	2.57
Trial 3	49.48	1.61
Average	62.55	2.39
Standard Deviation	11.34	0.71
% Error	18.12	29.74

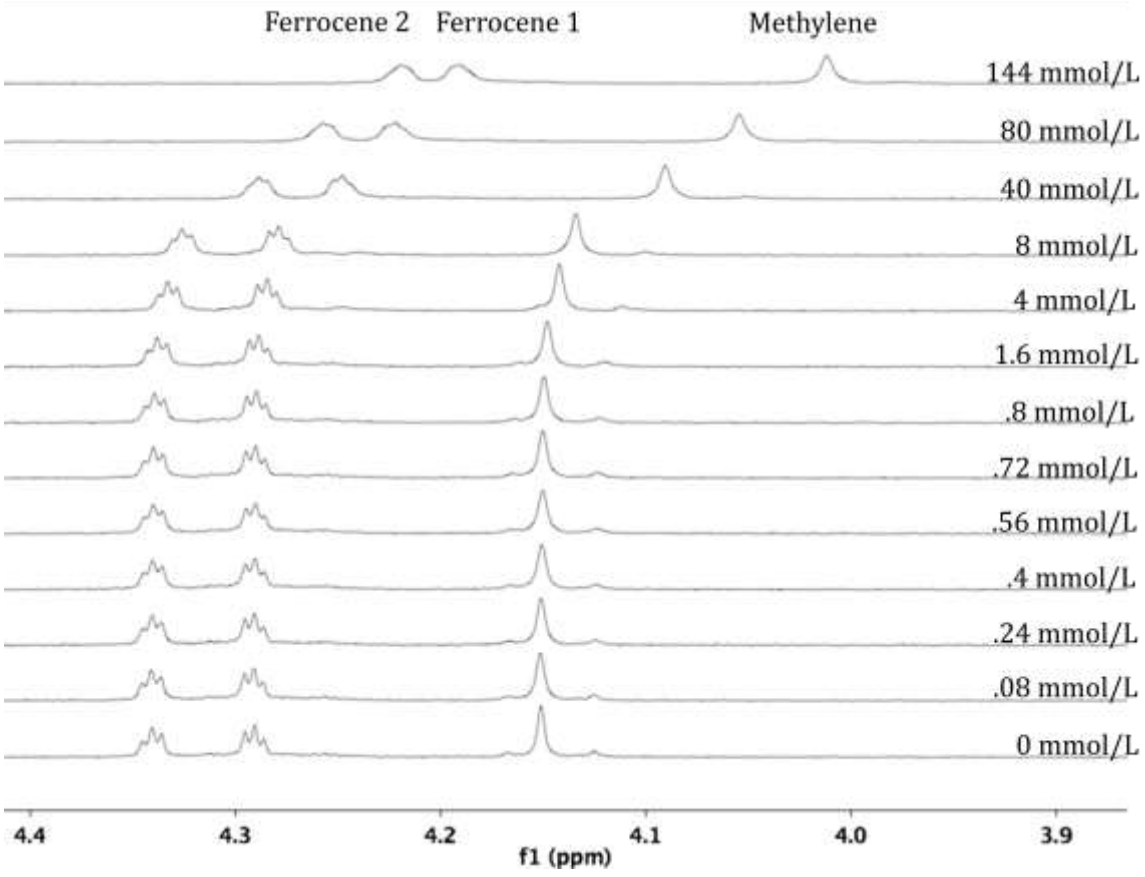
D_2O Methylene								
Host Conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest Conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Methylene Trial 1	δ (ppm) Methylene Trial 2	δ (ppm) Methylene Trial 3
0.0008	100	1	0.00000	0	0	4.1522261	4.1522261	4.1522261
0.0008	100	1	0.00008	20	0.1	4.1524145	4.1523440	4.1524024
0.0008	100	1	0.00024	60	0.3	4.1520029	4.1514356	4.1517044
0.0008	100	1	0.00040	100	0.5	4.1518280	4.1517951	4.1517734
0.0008	100	1	0.00056	140	0.7	4.1512939	4.1513831	4.1513709
0.0008	100	1	0.00072	180	0.9	4.1511685	4.1509462	4.1510446
0.0008	100	1	0.00080	200	1	4.1508148	4.1505550	4.1507436
0.0008	100	1	0.00160	400	2	4.1492155	4.1488447	4.1488531
0.0008	100	1	0.00400	25	5	4.1431732	4.1427979	4.1430288
0.0008	100	1	0.00800	50	10	4.1352842	4.1347948	4.1351211
0.0008	100	1	0.04000	250	50	4.0916172	4.0912919	4.0913813
0.0008	100	1	0.08000	500	100	4.0555360	4.0555299	4.0555643
0.0008	100	1	0.14400	900	180	4.0128810	4.0129747	4.0125656

Methylene	K1	K2
Trial 1	42.77	1.90
Trial 2	60.18	2.29
Trial 3	43.74	1.63
Average	48.89	1.94
Standard Deviation	9.78	0.33
% Error	20.01	17.00

Ferrocene 1	K1	K2
Fc 1 Trial 1	40.43	1.08
Fc 1 Trial 2	44.21	2.07
Fc 1 Trial 3	49.74	1.43
Fc 2 Trial 1	69.66	3.00
Fc 2 Trial 2	68.52	2.57
Fc 2 Trial 3	49.48	1.61
Me Trial 1	42.77	1.90
Me Trial 2	60.18	2.29
Me Trial 3	43.74	1.63
Average	52.08	1.95



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.

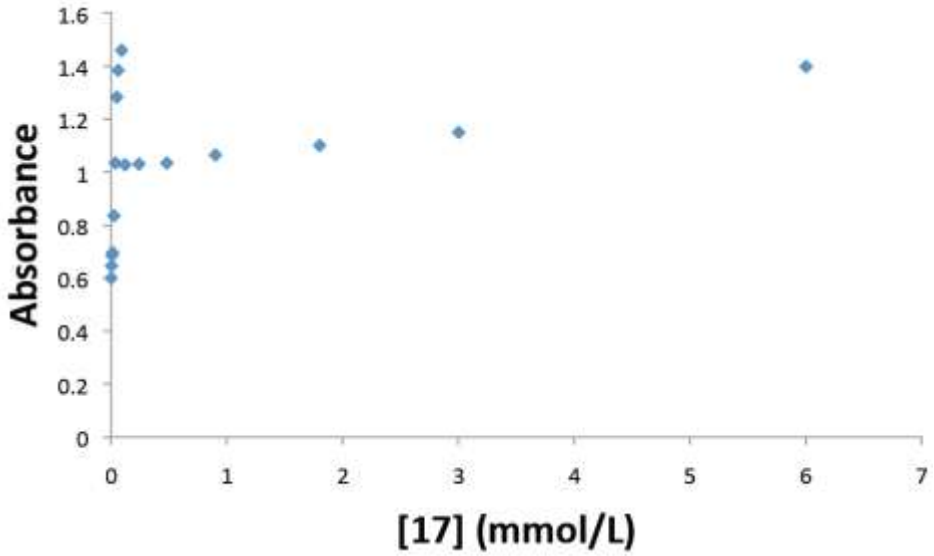


Stacked NMR spectra depicting NMR shifts for 1,1'-bis(guanidinylmethyl)ferrocenium peaks for Trial 1

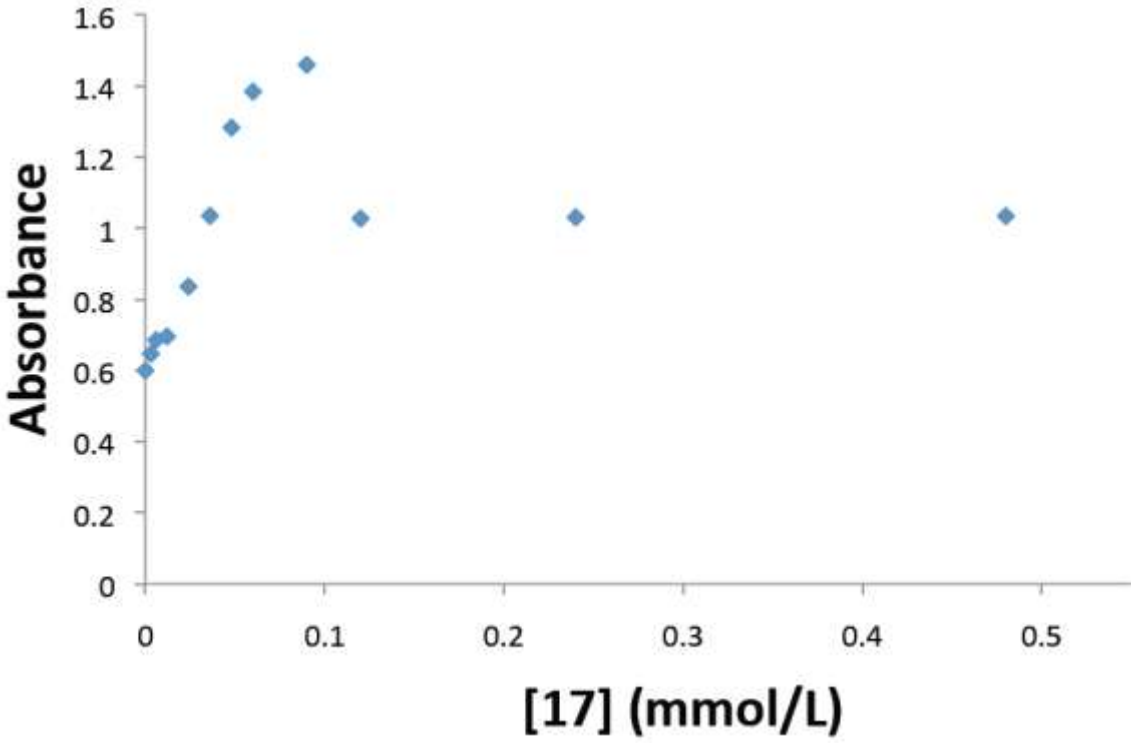
1,1'-bis(acetylguanidinyl)ferrocenium Hydrochloride (10) Bound to Potassium Acetate (17) in 9:1 DMSO: D_2O

General Procedure:
A 3 mmol/L stock solution of 1,1'-bis(acetylguanidinyl)ferrocenium hydrochloride **10** (Host) was made. 0.1 mmol/L and 8 mmol/L stock solutions of potassium acetate **17** (Guest) were made. 100 uL of Host were added to a vial, followed by and amount of Guest indicated in the table. The 0.1 mmol/L stock solution of potassium acetate was used for samples 2-9, and the 8 mmol/L stock solution of potassium acetate was used for samples 10-16. Contents were diluted to a final volume of 5 mL and allowed to bind for two hours at 20°C. All Absorbance spectra were recorded at 325 nm with a Varian Cary 50 spectrophotometer.

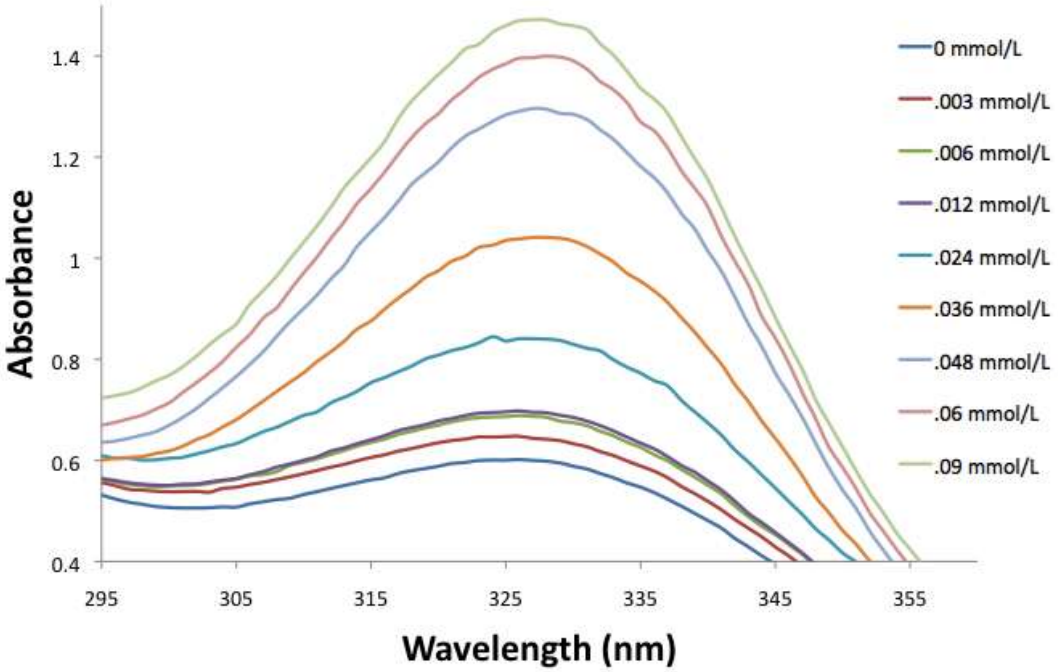
90% DMSO								
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	Abs. Trial 1	Abs. Trial 2	Abs. Trial 3
6.00E-05	100	5	0	0	0	0.6003765	0.5663859	0.6042576
6.00E-05	100	5	0.000003	150	0.05	0.6469800	0.5942549	0.6759570
6.00E-05	100	5	0.000006	300	0.1	0.6865492	0.6264567	0.6898023
6.00E-05	100	5	0.000012	600	0.2	0.6959016	0.6317630	0.7055580
6.00E-05	100	5	0.000024	1200	0.4	0.8360804	0.7410572	0.8909351
6.00E-05	100	5	0.000036	1800	0.6	1.0350655	0.9124368	1.0416101
6.00E-05	100	5	0.000048	2400	0.8	1.2834766	1.1786060	1.3265686
6.00E-05	100	5	0.00006	3000	1	1.3845763	1.2948190	1.4457713
6.00E-05	100	5	0.00009	4500	1.5	1.4598309	1.3686138	1.5215263
6.00E-05	100	5	0.00012	75	2	1.0279443	1.0852702	1.2783529
6.00E-05	100	5	0.00024	150	4	1.0310315	1.1143578	1.3794469
6.00E-05	100	5	0.00048	300	8	1.0347663	1.1052700	1.4284889
6.00E-05	100	5	0.0009	562.5	15	1.0648937	1.1086087	1.4653276
6.00E-05	100	5	0.0018	1125	30	1.1007910	1.1945864	1.5216446
6.00E-05	100	5	0.003	1875	50	1.1503022	1.2434702	1.5929444
6.00E-05	100	5	0.006	3750	100	1.3985047	1.4906242	1.6718638



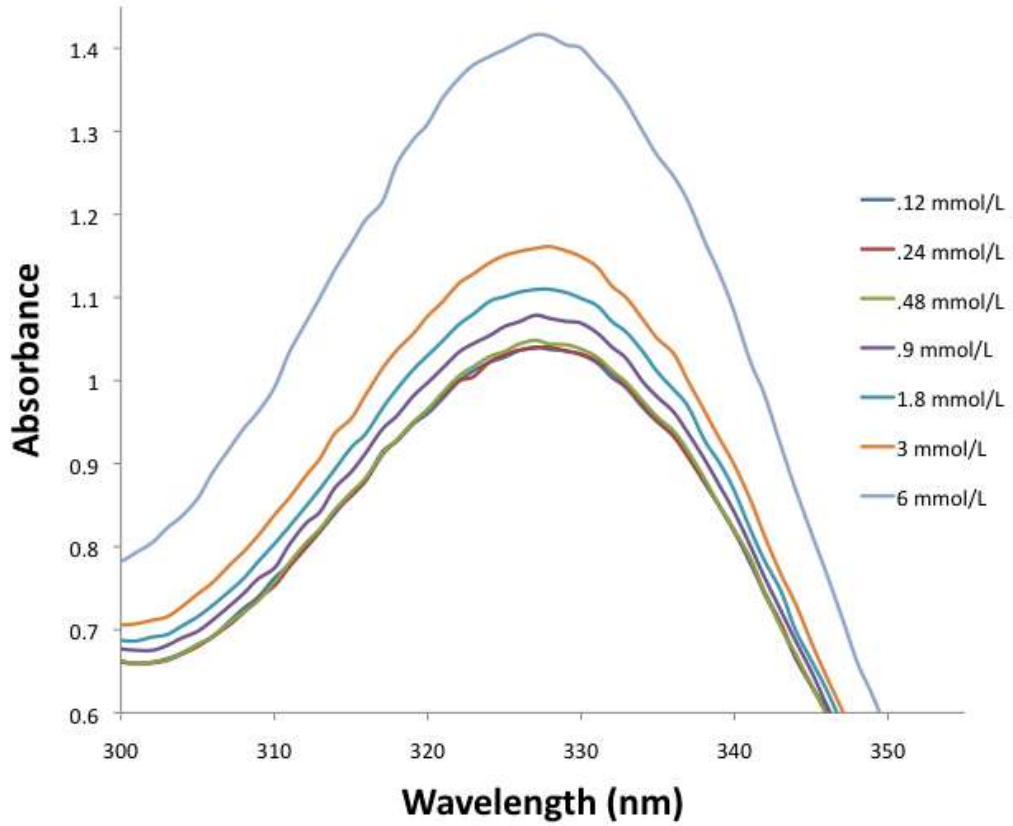
Full graph of the absorbance of **10** bound to **17** versus **[17]** in 9:1 DMSO: D_2O at 325 nm wavelength.



Zoomed in graph of the Absorbance of **10** bound to **17** versus **[17]** in 9:1 DMSO: D_2O at 325 nm wavelength depicting sharp increase in absorbance at equivalents of **17** less than 2, followed by sharp decrease in absorbance at equivalents of **17** equal to or greater than 2.



Absorbance of **10** bound to **17** in 9:1 DMSO: D_2O for samples 1-9.



Absorbance of **10** bound to **17** in 9:1 DMSO: D_2O for samples 10-16

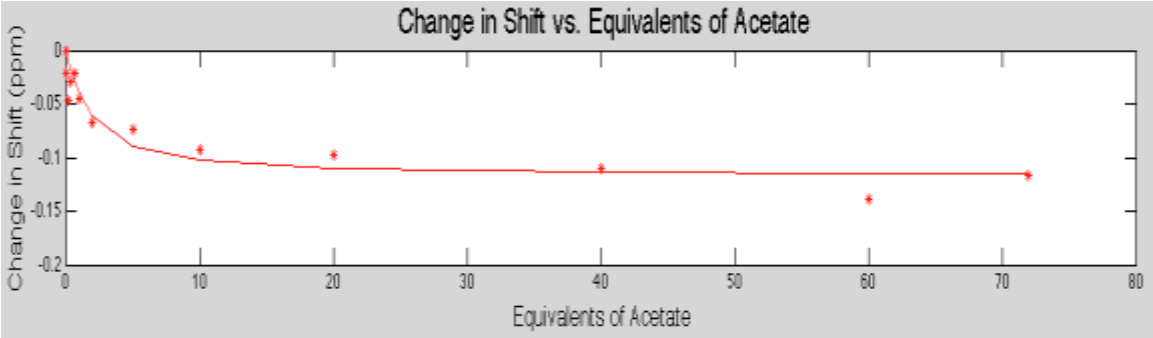
1,1'-bis(acetylguanidinyl)ferrocenium Hydrochloride (10) Bound to Potassium Acetate (17) in 1:1 DMSO: D_2O

General Procedure:
A 2 mmol/ stock solution of 1,1'-bis(acetylguanidinyl)ferrocenium hydrochloride **10** (Host) was made. 4 mmol/L and 160 mmol/L stock solutions of potassium acetate **17** (Guest) were made. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. The 4 mmol/L stock solution of potassium acetate was used for samples 2-6, and the 160 mmol/L stock solution of potassium acetate was used for samples 7-13. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 20°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400**.** Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

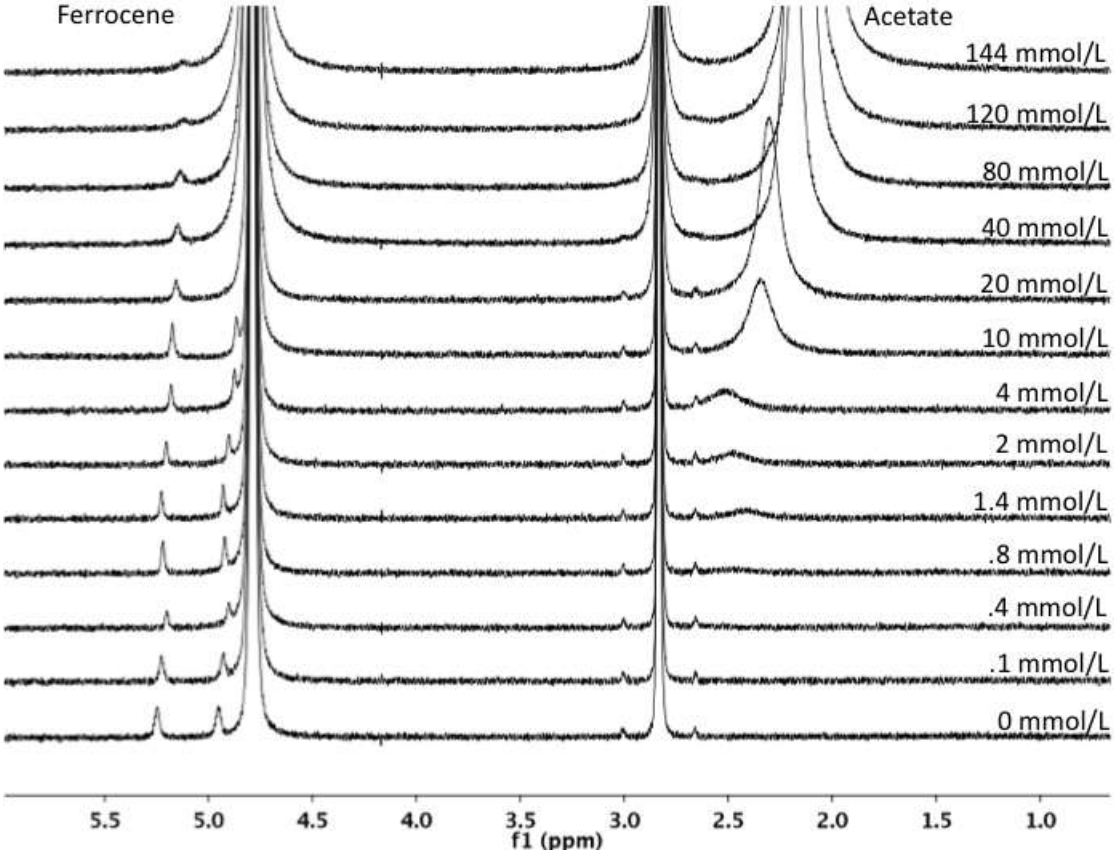
Only one ferrocene peak was analyzed, due to the proximity of the second ferrocene peak to the D_2O signal. The acetate peak was not analyzed, since it was not visible by NMR until 0.7 equivalents of acetate were present, and because of its close proximity to the DMSO satellite peaks.

50% DMSO Ferrocene								
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene Trial 1	δ (ppm) Ferrocene Trial 2	δ (ppm) Ferrocene Trial 3
0.002	100	1	0	0	0	5.2473266	5.2137216	5.2264572
0.002	100	1	0.0001	25	0.05	5.2254746	5.2145643	5.2128902
0.002	100	1	0.0004	100	0.2	5.2006663	5.1994911	5.1988953
0.002	100	1	0.0008	200	0.4	5.2186389	5.2058181	5.2090499
0.002	100	1	0.0014	350	0.7	5.2262971	5.2090935	5.2122095
0.002	100	1	0.002	500	1	5.2024777	5.1784944	5.1917888
0.002	100	1	0.004	25	2	5.1795118	5.2013235	5.1867753
0.002	100	1	0.01	62.5	5	5.1737767	5.1763040	5.1716435
0.002	100	1	0.02	125	10	5.1545871	5.1578324	5.1581964
0.002	100	1	0.04	250	20	5.1489486	5.1521203	5.1514031
0.002	100	1	0.08	500	40	5.1365258	5.1364511	5.1365407
0.002	100	1	0.12	750	60	5.1084307	5.1436921	5.1277446
0.002	100	1	0.144	900	72	5.1310884	5.1212956	5.1232812

Ferrocene	K1	K2
Trial 1	39304.40	77.71
Trial 2	39556.00	49.95
Trial 3	37612.90	57.41
Average	38824.43	61.69
Standard Deviation	1056.73	14.37
% Error	2.72	23.29



Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.



Stacked spectra for **10** bound to **17** in 1:1 DMSO: D_2O for Trial 1.

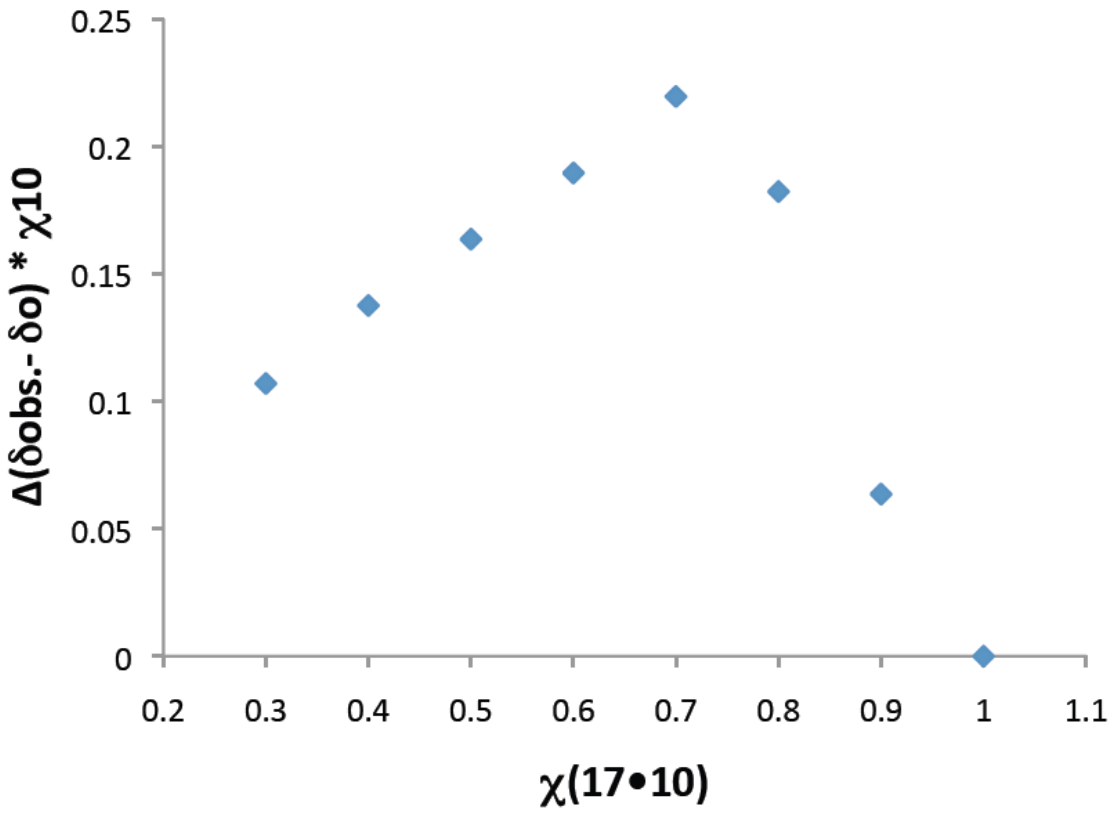
Job's Method for Stoichiometry Determination of 1,1'-bis(acetylguanidinyl) ferrocenium Hydrochloride (10) and Potassium Acetate (17) in 1:1 DMSO: D_2O

General Procedure for Trials 1 and 2: 4 mmol/ L stock solutions were made of 1,1'-bis(acetylguanidinyl)ferrocenium hydrochloride **10** (Host) and of potassium acetate **17** (Guest). Contents were bound for two hours at 20˚C. The potassium acetate peak was monitored. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400. Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

Sample	δ (ppm) Acetate Trial 1	δ (ppm) Acetate Trial 2	$\chi_{(17•10)}$	Amt. 10 (mL)	Amt. 17 (mL)
1	2.3733758	2.3302695	.3	.7	.3
2	2.3607917	2.3425884	.4	.6	.4
3	2.3440328	2.3107198	.5	.5	.5
4	2.3327484	2.3015742	.6	.4	.6
5	2.3305003	2.298281	.7	.3	.7
6	2.2447053	2.2196856	.8	.2	.8
7	2.0875294	2.1098724	.9	.1	.9
8	2.0168722	2.0158891	1	0	1

Sample	$\Delta(\delta_{obs.}- \delta_o)$	$\Delta(\delta_{obs.}- \delta_o)$	$\chi_{(17•10)}$	Amt. 10 (mL)	Amt. 1 mL)
1	0.3565036	0.3143804	.3	.7	.3
2	0.3439195	0.3266993	.4	.6	.4
3	0.3271606	0.2948307	.5	.5	.5
4	0.3158762	0.2856851	.6	.4	.6
5	0.3136281	0.2823919	.7	.3	.7
6	0.2278331	0.2037965	.8	.2	.8
7	0.0706572	0.0939833	.9	.1	.9
8	0	0	1	0	1

Sample	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(17•10)}$	$\Delta(\delta_{obs.}- \delta_o) * \chi_{(17•10)}$	$\chi_{(17•10)}$	χ_{10}	χ_{17}
1	0.1069511	0.0943141	.3	.7	.3
2	0.1375678	0.1306797	.4	.6	.4
3	0.1635803	0.1474154	.5	.5	.5
4	0.1895257	0.1714111	.6	.4	.6
5	0.2195397	0.1976743	.7	.3	.7
6	0.1822665	0.1630372	.8	.2	.8
7	0.0635915	0.0845850	.9	.1	.9
8	0	0	1	0	1



Job Plot for Potassium Acetate Trial 1 depicting a maximum at mole fraction equal to 0.7, indicating a 2:1 stoichiometry between guest and host.

1,1'-bis(acetylguanidinyl)ferrocenium Hydrochloride (10) Bound to Potassium Acetate (17) in D_2O

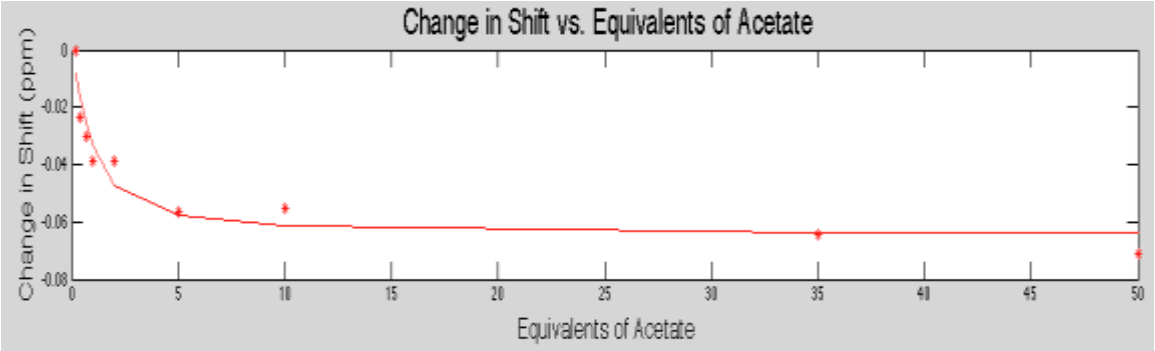
General Procedure:
A 2 mmol/ stock solution of 1,1'-bis(acetylguanidinyl)ferrocenium hydrochloride **10** (Host) was made. 4 mmol/L and 200 mmol/L stock solutions of potassium acetate **17** (Guest) were made. 100 uL of Host were added to a vial, followed by the amount of Guest indicated in the table. The 4 mmol/L stock solution of potassium acetate was used for samples 2-6, and the 200 mmol/L stock solution of potassium acetate was used for samples 7-11. Contents were diluted to a final volume of 1 mL and allowed to bind for 2 hours at 20°C. All ^{1}H NMR spectra were recorded at 400 MHz with a Varian MR-400**.** Chemical shifts are reported in ppm with reference to D_2O solvent signal (4.790).

Only the association constant of the potassium acetate peak was analyzed. The sharp rise and fall of the ferrocene peak made fitting the data difficult. The second ferrocene peak was not analyzed due to its proximity to the water signal. By samples 10 and 11, both of the ferrocene peaks were hidden behind the water signal.

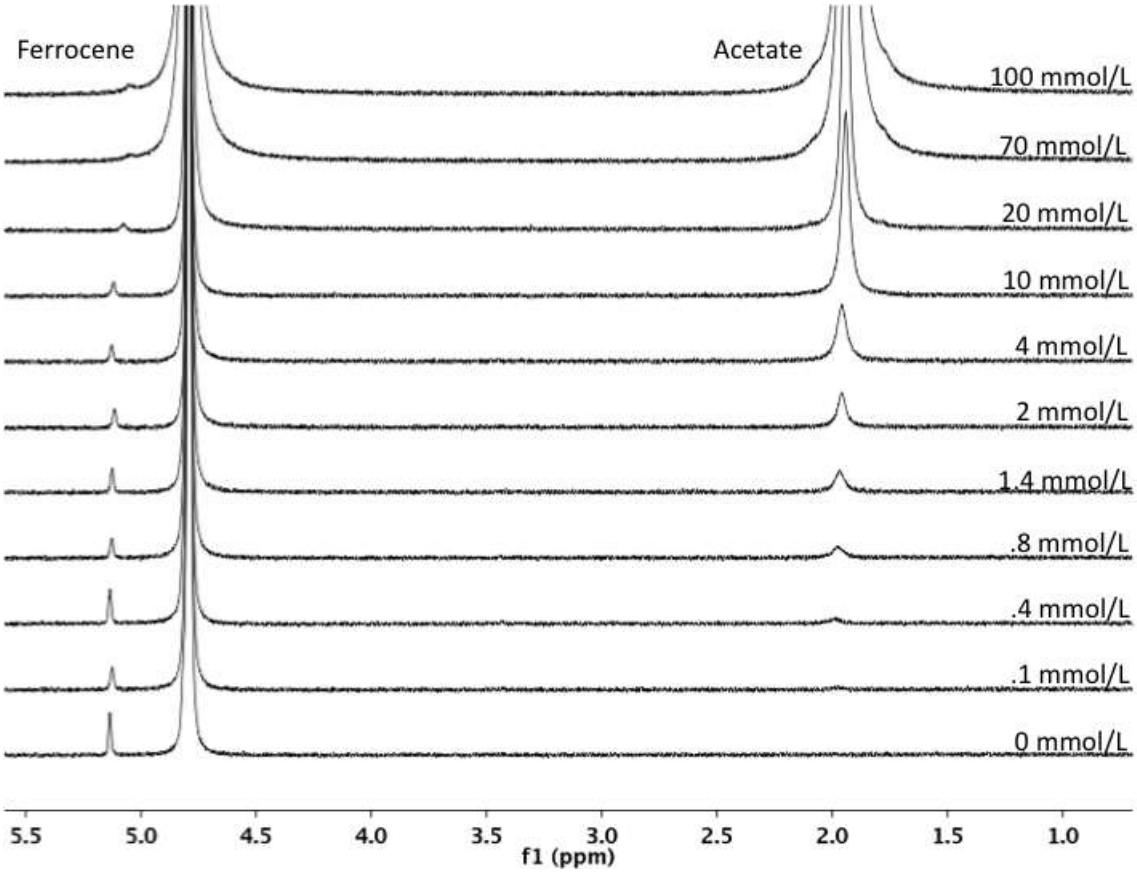
D_2O Ferrocene								
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Ferrocene Trial 1	δ (ppm) Ferrocene Trial 2	δ (ppm) Ferrocene Trial 3
0.002	100	1	0	0	0	5.0856694	5.1144114	5.1214986
0.002	100	1	0.0001	25	0.05	5.1299713	5.1295210	5.1334541
0.002	100	1	0.0004	100	0.2	5.1302073	5.1289372	5.1340389
0.002	100	1	0.0008	200	0.4	5.1254972	5.1245199	5.1266273
0.002	100	1	0.0014	350	0.7	5.1229486	5.1264738	5.1254653
0.002	100	1	0.002	500	1	5.1205127	5.1222585	5.1148967
0.002	100	1	0.004	20	2	5.1160614	5.1191609	5.1140936
0.002	100	1	0.01	50	5	5.1089978	5.1094684	5.0999858
0.002	100	1	0.02	100	10	5.1050778	5.0903666	5.0881255
0.002	100	1	0.07	350	35			
0.002	100	1	0.1	500	50			

D_2O Acetate								
Host conc. (M)	Amt. Host Added (uL)	Final Vol. (mL)	Guest conc. (M)	Amt. Guest Added (uL)	Equiv. of Guest	δ (ppm) Acetate Trial 1	δ (ppm) Acetate Trial 2	δ (ppm) Acetate Trial 3
0.002	100	1	0	0	0			
0.002	100	1	0.0001	25	0.05			
0.002	100	1	0.0004	100	0.2	1.9969624	1.9730960	1.9763878
0.002	100	1	0.0008	200	0.4	1.9735295	1.9568085	1.9680813
0.002	100	1	0.0014	350	0.7	1.9669594	1.9670026	1.9634344
0.002	100	1	0.002	500	1	1.9583295	1.9634929	1.9575618
0.002	100	1	0.004	20	2	1.9582746	1.9578059	1.9542921
0.002	100	1	0.01	50	5	1.9407444	1.9480958	1.9430060
0.002	100	1	0.02	100	10	1.9417046	1.9388015	1.9345413
0.002	100	1	0.07	350	35	1.9324409	1.9282704	1.9245177
0.002	100	1	0.1	500	50	1.9258105	1.9250304	1.9253732

Acetate	K1	K2
Trial 1	848.34	69.33
Trial 2	798.83	39.54
Trial 3	886.55	81.40
Average	844.57	63.42
Standard Deviation	43.98	21.55
% Error	5.21	33.97

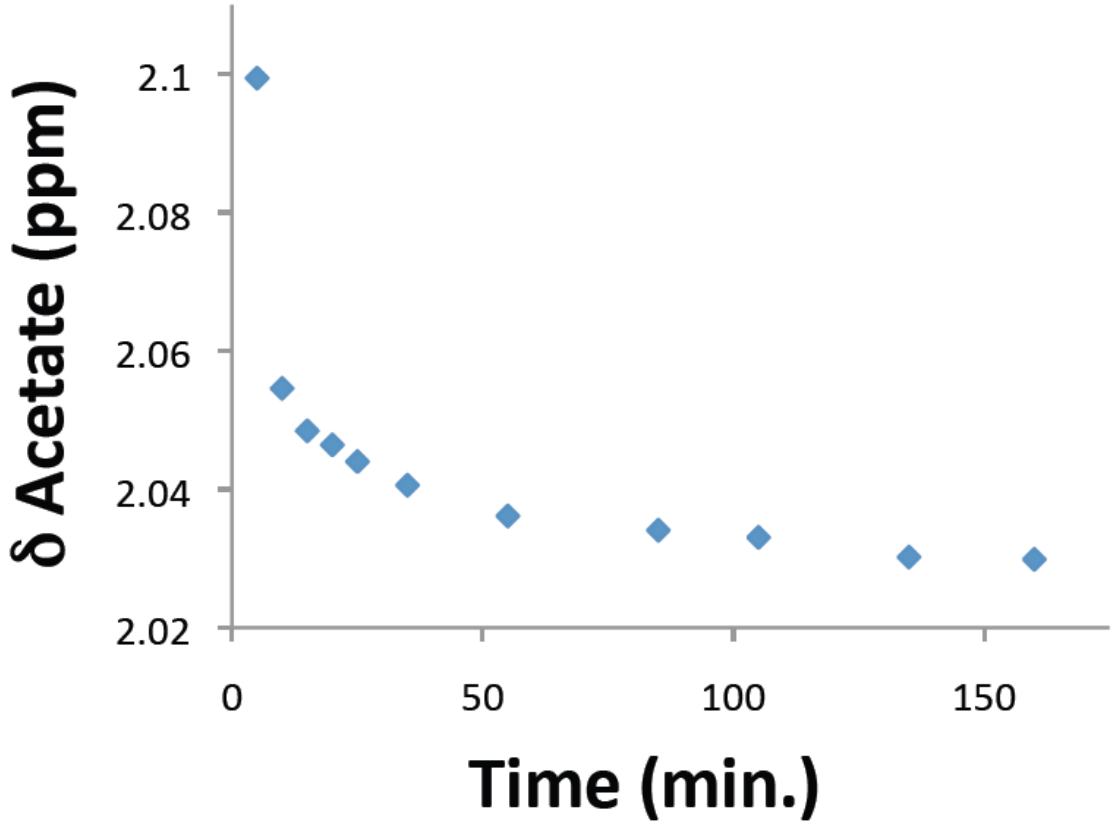


Example plot from Thordarson's Matlab NMR titration fitting software for Trial 1 data.

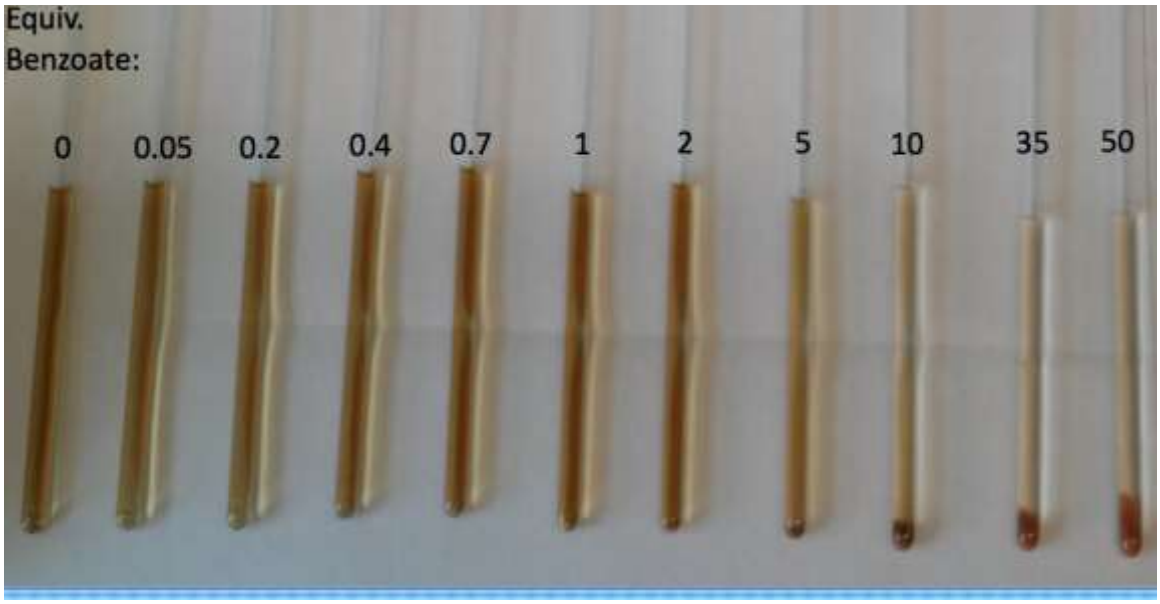


Stacked spectra of **10** bound to **17** in D_2O for Trial 1.

NMR Kinetics study of 10 bound to 17 in D_2O



NMR shift of **10** bound to **17** in D_2O versus time depicting the slow binding event, making it necessary to allow all samples to bind for two hours prior to analysis by NMR or UV-Vis.



NMR Tubes with 1,1'-bis(acetylguanidinyl)ferrocenium Hydrochloride **10** bound to Potassium Benzoate **1** in D_2O, showing visible precipitate when more than 2 equivalents of potassium benzoate are present, precluding any binding studies between **10** and **1**.