Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.
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Supporting Information to

"Selective fluorescent turn-on sensing of sulfate in aqueous-organic mixtures by an uncharged bis(diamidocarbazole) receptor"

Krzysztof M. Bąk, Krystyna Masłowska and Michał J. Chmielewski*

2.4.7. Fluorescent titration of 10^{-5} M solution of receptor A in DMSO/10% H_2O with Na_2CO_3

2.4.8. Fluorescent titration of 10^{-5} M solution of receptor A in DMSO/10% H_2O with PhCOONa.

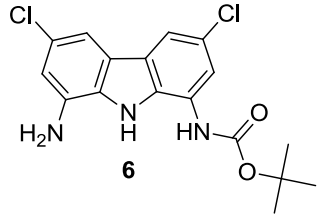
2.4.9. Fluorescent titration of 10^{-5} M solution of receptor A in DMSO/10% H_2O with NaCl.

1. Synthesis and characterisation of the model bis(diamidocarbazole) ligand A.

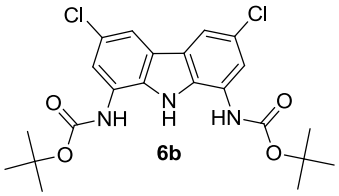
1.1 Instruments and methods. NMR spectra were recorded using Bruker AVANCE 500 MHz spectrometer at ambient temperature in DMSO-d_6 or DMSO-d_6/H_2O mixtures. Chemical shifts are reported in parts per million (ppm) and coupling constants J are given in hertz (Hz). Data are reported as follows: chemical shift, multiplicity (s-singlet, bs – broad singlet, d – doublet, dd – doublet of doublets), coupling constant and integration. The residual signal of DMSO-d_6 solvent was used as an internal reference standard (δH = 2.500 ppm and δC = 39.50 ppm). The ESI mass spectra were obtained using a Quattro (ESI TOF) mass spectrometer with methanol as a spray solvent. Elemental analysis was performed using a CHN analyser model Vario EL III Elementar Analyser. Chlorine content in all analysed samples was determined according to the Schöniger method.[1]

1.2. Synthesis. All precursors for the syntheses were obtained from Sigma-Aldrich and were used as received. TLC was carried out on Merck silica gel 60 F254 plates; Teledyne Isco CombiFlash system with RediSep Normal-phase Silica Flash Columns or Merck silica gel 60 (230 – 400 mesh) were used for preparative chromatography.

Mono-Boc-Protected 1,8-diamino-3,6-dichlorocarbazole 6. To a 100 ml two-neck round-bottom flask equipped with a magnetic stirrer, 1,8-diamino-3,6-dichlorocarbazole **5** (2.67 g, 10.0 mmol) was added. The flask was equipped with a reflux condenser connected to a check-valve bubbler and purged with argon. Afterwards, dry THF (from SPS, 60 ml) was added using syringe. After 20 min of bubbling argon through the solvent, di-*tert*-butyl dicarbonate (2.3 ml, 10.0 mmol) was slowly added dropwise via a syringe. Argon inlet was removed and the neck was closed with a glass stopper. The reaction was carried out at the boiling point of the solvent under reflux with stirring for 4 hours. After this time, the reaction mixture was cooled down to room temperature and the solvent was removed on rotary evaporator. The crude product was purified by column chromatography on 80 g of silica gel using gradient elution with CH_3OH/CH_2Cl_2 mixture, with methanol content varying from 0 to 1%. The progress of the chromatographic separation was monitored with TLC using 2% CH_3OH/CH_2Cl_2 as an eluent. Fractions containing pure product were combined and evaporated to yield 1.968 g (53.6%) of gray-violet solid (**6**) and 1.016 g (21.7 %) of orange solid (**6b**).



6

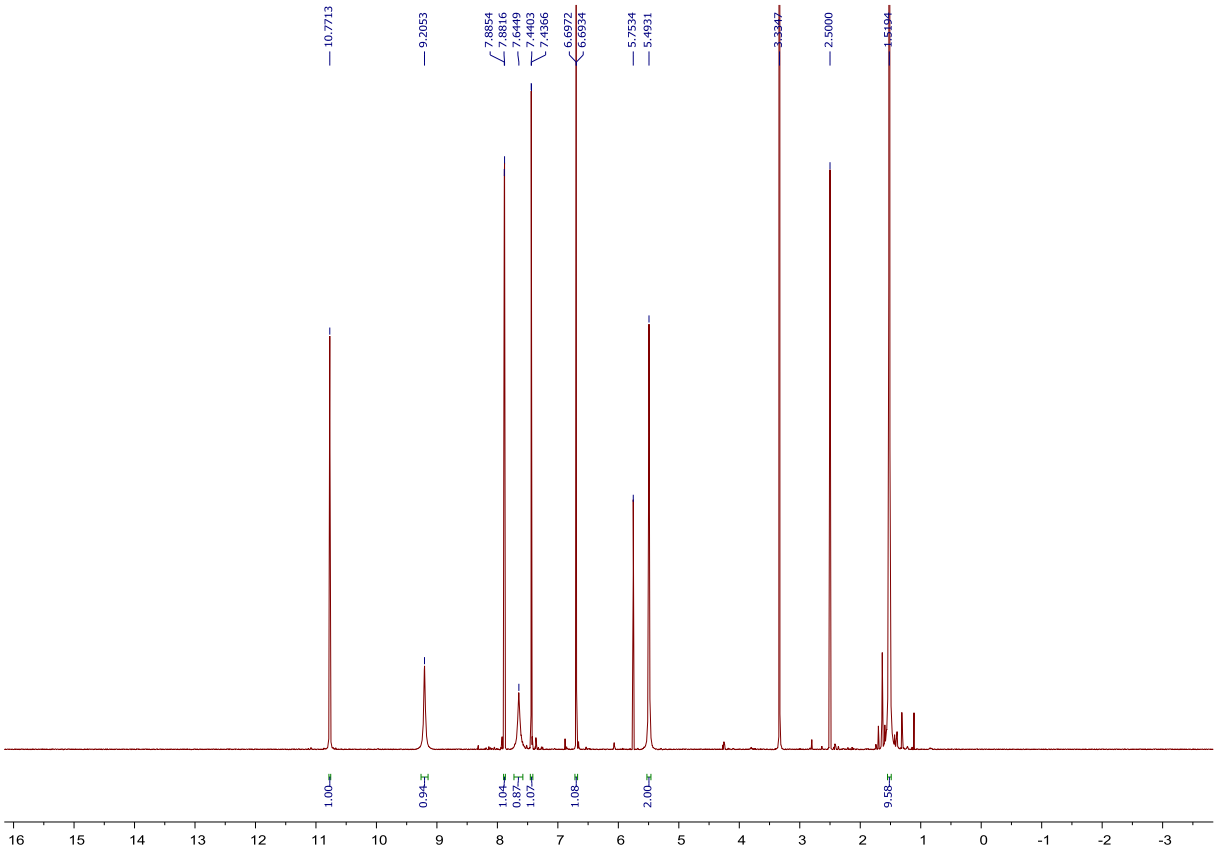


6b

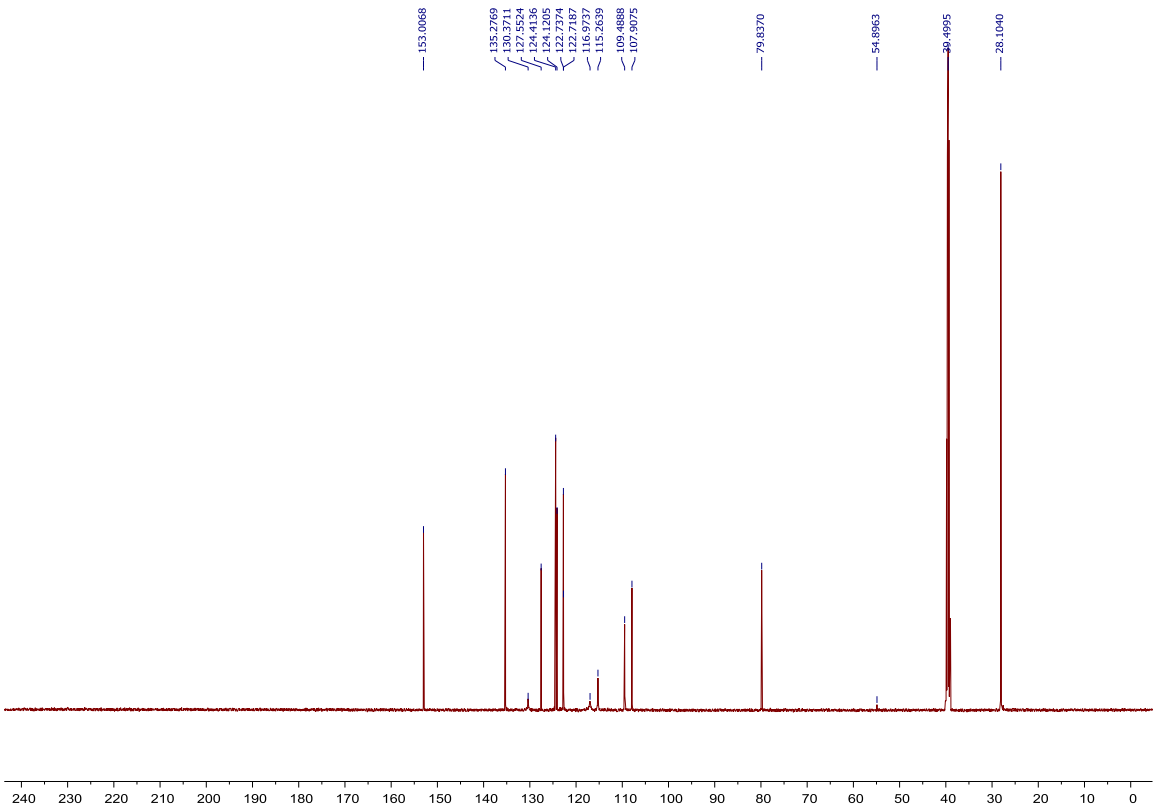
(6) ^{1}H NMR (DMSO-d_6) δ_{DMSO}: 10.77 (s; 1H); 9.20 (s; 1H); 7.88 (d; *J* = 1.9 Hz; 1H); 7.65 (bs; 1H); 7.44 (d; *J* = 1.9 Hz; 1H); 6.70 (d; *J* = 1.9 Hz; 1H); 5.49 (s; 2H); 1.52 (s; 9H).
^{13}C NMR (DMSO-d_6) δ_{DMSO}: 153.01; 135.28; 130.37; 127.55; 124.41; 124.12; 122.74; 122.72; 116.97; 115.26; 109.49; 107.91; 79.84; 28.10.
HR MS (ESI): m/z calcd. for $C_{17}H_{18}Cl_2N_3O_2$ $[M+H]^+$: 366.0776; found: 366.0771.
Elemental Analysis calcd. for $C_{17}H_{17}Cl_2N_3O_2$: C 55.75; H 4.68; N 11.47; Cl 19.36; found: C 55.48; H 4.38; N 11.33; Cl 19.35.
(6b) ^{1}H NMR (DMSO-d_6) δ_{DMSO}: 10.98 (s; 1H); 9.43 (bs; 2H); 8.00 (d; *J* = 2.0 Hz; 2H); 7.72 (bs; 2H); 1.52 (s; 18H).
^{13}C NMR (DMSO-d_6) δ_{DMSO}: 153.00; 130.20; 124.58; 123.56; 123.36; 117.44; 115.25; 79.95; 28.08.
HR MS (ESI): m/z calcd. for $C_{22}H_{25}Cl_2N_3O_4K$ $[M+K]^+$: 504.0859; found: 504.0854.
Elemental Analysis calcd. for $C_{22}H_{25}Cl_2N_3O_4$: C 56.66; H 5.4. N 9.01; Cl 15.2; found: C 56.41; H 5.24; N 8.99; Cl 15.5.

[1] Schöniger, W. *Mikrochim. Acta* **1956**, 869.

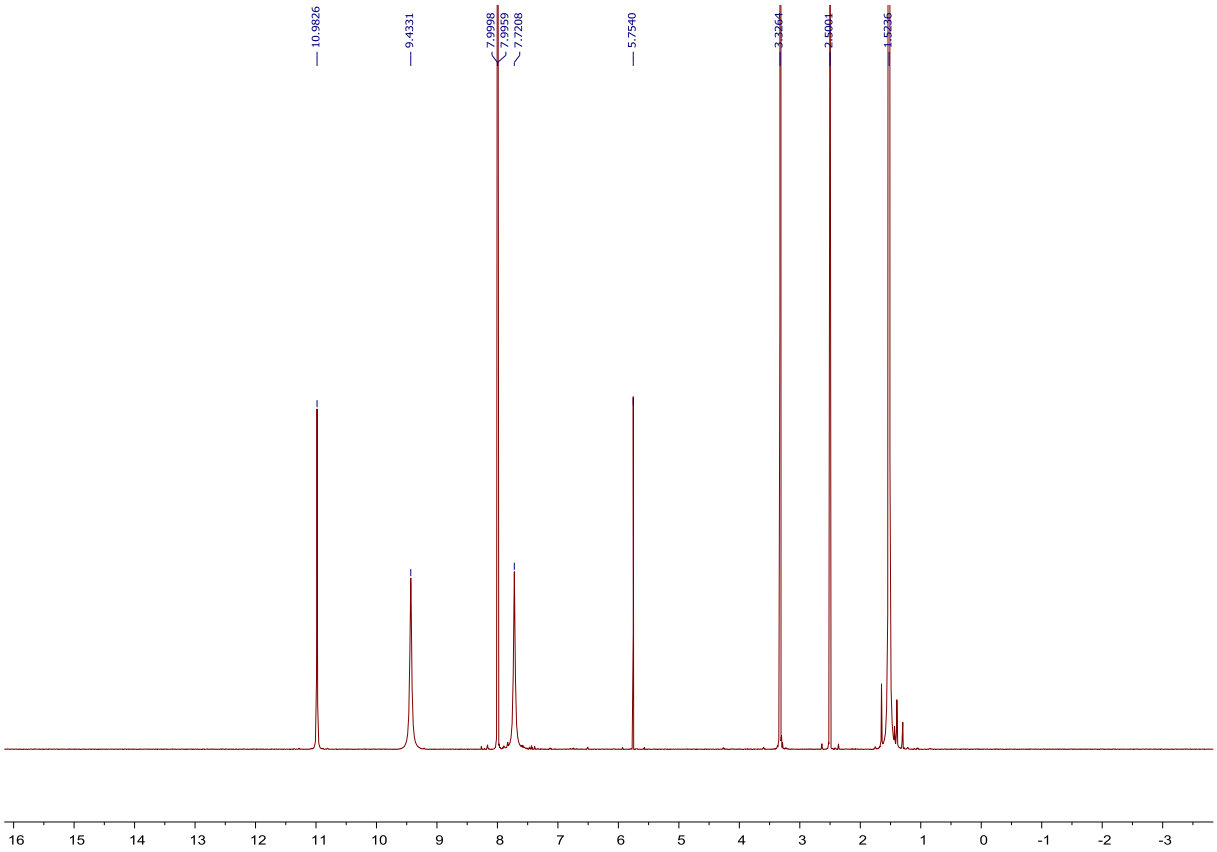
^{1}H NMR of 6 in DMSO-d_6:



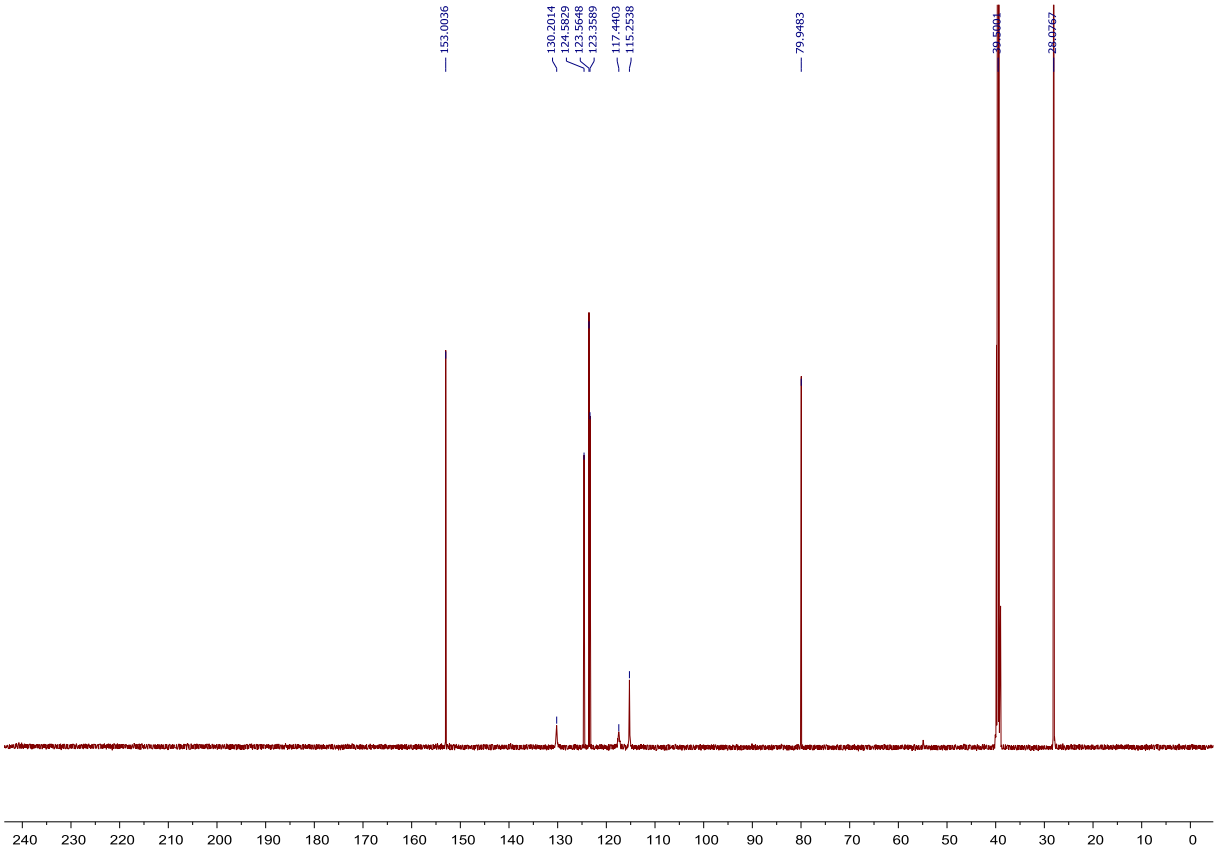
^{13}C NMR of 6 in DMSO-d_6



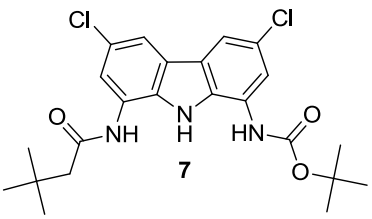
^{1}H NMR of 6b in DMSO-d_6:



^{13}C NMR of 6b in DMSO-d_6



Boc-Protected 1-(3,3-dimethylbutyrylamino)-8-amino-3,6-dichlorocarbazole 7. To a 50 ml round bottom flask equipped with a magnetic stirrer, **6** (0.737 g, 2.00 mmol) was added. The flask was closed with a septum and purged with argon. Afterwards, dry THF (from SPS, 15 ml), triethylamine (0.335 ml, 2.40 mmol) were added and to the resulting mixture *t*-butylacetyl chloride (0.334 ml, 2.40 mmol) was slowly added dropwise via a syringe. The reaction mixture was stirred for 1 hour at room temperature. The precipitated triethylamine hydrochloride was filtered off, and the filtrate was evaporated to dryness on rotary evaporator. The solid residue was separated by flash column chromatography (CombiFlash) on 24 g of silica gel using gradient elution with CH_3OH/CH_2Cl_2 mixtures (0 to 5% MeOH). Fractions containing pure product were combined and evaporated to yield 0.766 g (82.5%) of white solid.



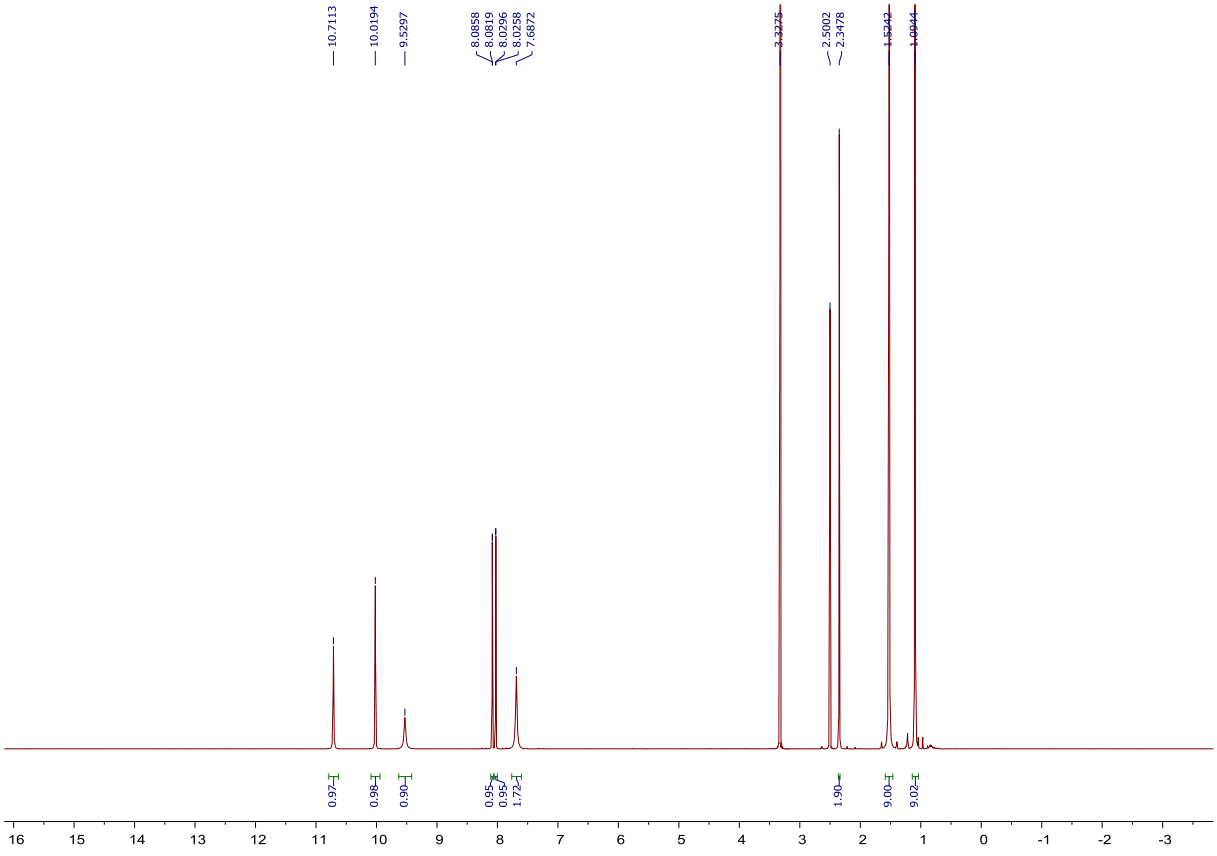
^{1}H NMR (DMSO-d_6) δ_{DMSO}: 10.71 (s; 1H); 10.02 (s; 1H); 9.53 (bs; 1H); 8.08 (d; *J* = 2.0 Hz; 1H); 8.03 (d; *J* = 1.9 Hz; 1H); 7.69 (bs; 2H); 2.35 (s; 2H); 1.52 (s; 9H); 1.09 (s; 9H).

^{13}C NMR (DMSO-d_6) δ_{DMSO}: 170.36; 153.03; 130.87; 130.24; 124.64; 124.16; 124.00; 123.78; 123.42; 123.15; 118.91; 117.66; 116.30; 115.33; 80.13; 49.13; 30.93; 29.64; 28.09.

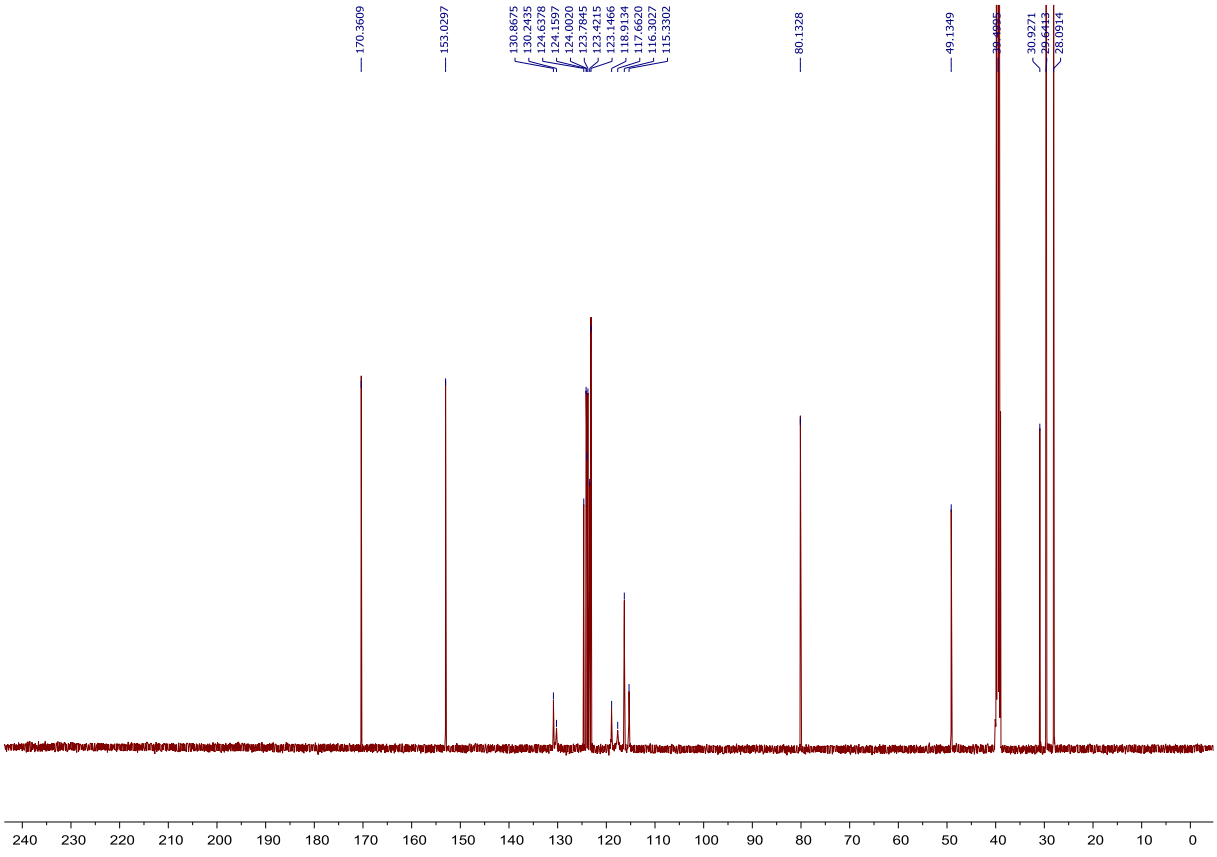
HR MS (ESI): m/z calcd. for $C_{23}H_{27}Cl_2N_3O_3Na$ $[M+Na]^+$: 486.1327; found: 486.1329.

Elemental Analysis calcd. for $C_{23}H_{27}Cl_2N_3O_3$: C 59.49; H 5.86; N 9.05; Cl 15.27; found: C 59.3; H 5.72; N 9.01; Cl 15.26.

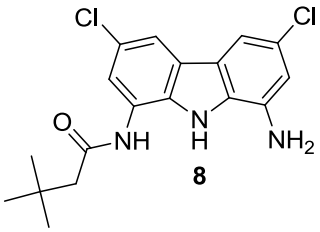
^{1}H NMR of 7 in DMSO-d_6:



^{13}C NMR of 7 in DMSO-d_6:



1-(3,3-dimethylbutyrylamino)-8-amino-3,6-dichlorocarbazole 8. To a 50 ml round bottom flask equipped with a magnetic stirrer, **7** (0.200 g, 0.43 mmol) was added. The flask was closed with a septum and purged with argon. Afterwards, dry CH_2Cl_2 (from SPS) and trifluoroacetic acid (1.00 ml, 13.1 mmol) were added using syringes. The reaction mixture was stirred for 2 hours at room temperature. After this time, solvent was removed by rotary evaporation. Dry residue was redissolved in DCM/MeOH and neutralized with TEA. Water was added to precipitate the product, and the precipitate was filtered off, washed with 2 portions of water (in total *ca.* 3 ml) and 2 portions of CH_3OH (in total *ca.* 1 ml) and dried thoroughly to yield 0.117 g (75%) of pure product as a white powder.



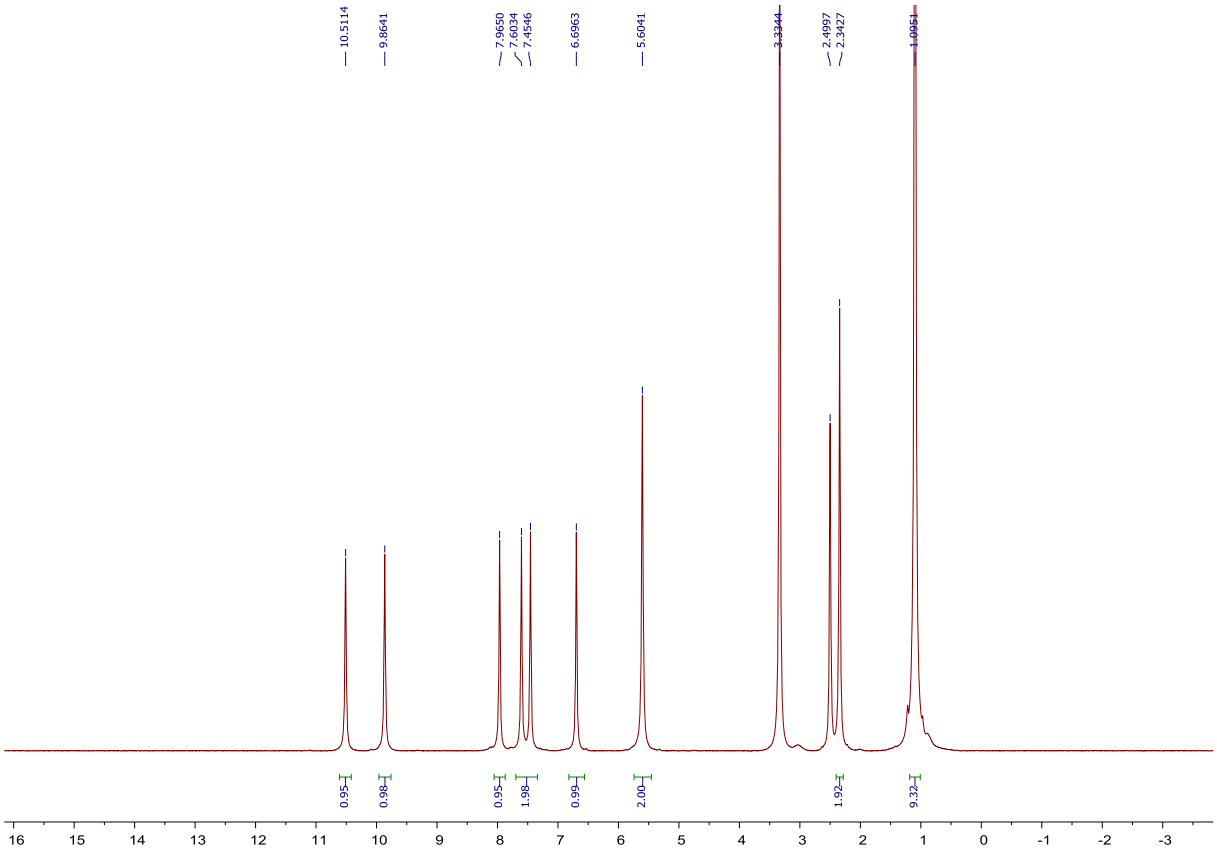
8

^{1}H NMR (DMSO-d_6) $\delta_{DMSO:}$ 10.51 (bs; 1H); 9.86 (bs; 1H); 7.96 (bs; 1H); 7.60 (bs; 1H); 7.45 (bs; 1H); 6.70 (bs; 1H); 5.60 (bs; 2H); 2.34 (bs; 2H); 1.10 (bs; 9H).

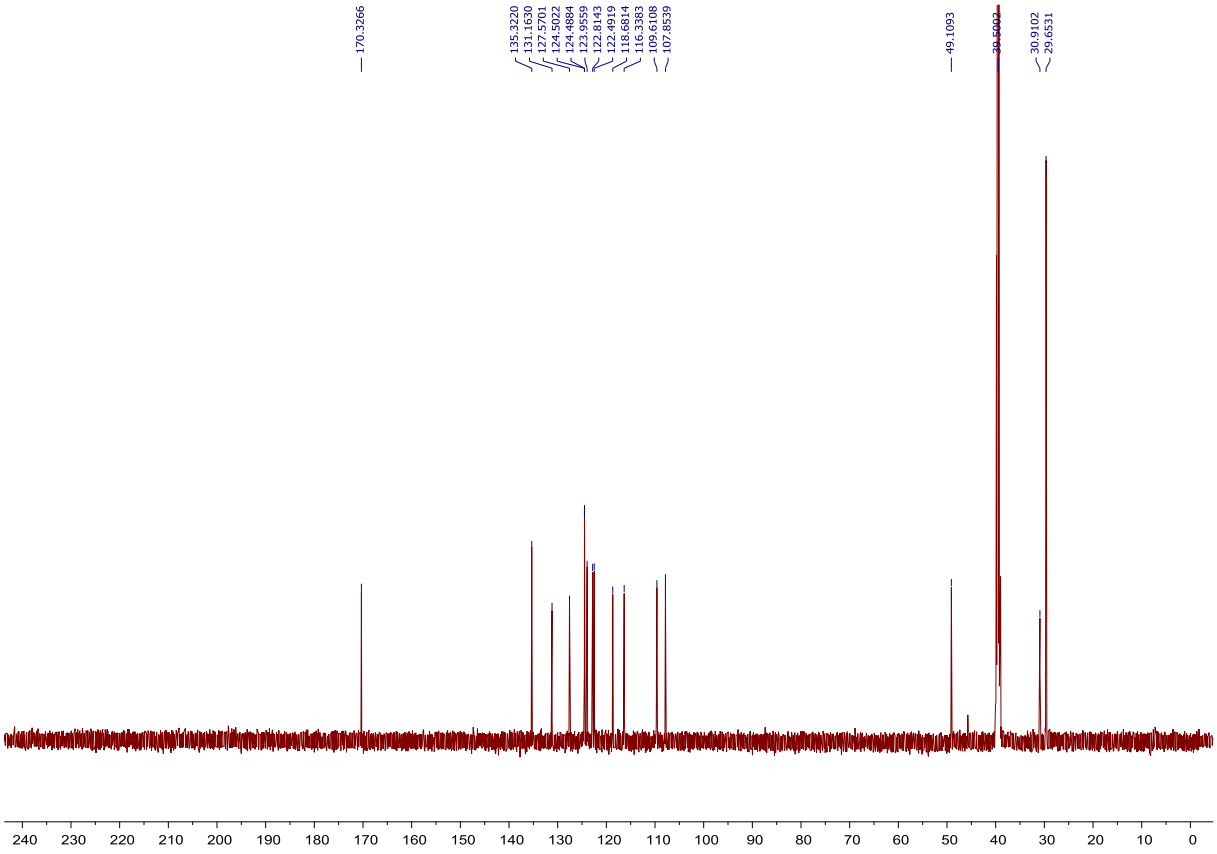
^{13}C NMR (DMSO-d_6) $\delta_{DMSO:}$ 170.33; 135.32; 131.16; 127.57; 124.50; 124.49; 123.96; 122.81; 122.49; 118.68; 116.34; 109.61; 107.85; 49.11; 30.91; 29.65.

HR MS (ESI): m/z calcd. for $C_{18}H_{20}Cl_2N_3O$: 364.0983; found: 364.0979.

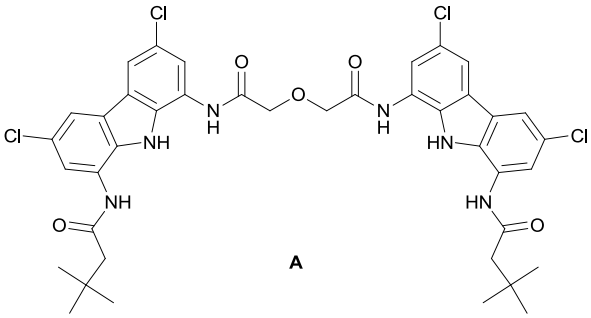
^{1}H NMR of 8 in DMSO-d_6:



^{13}C NMR of 8 in DMSO-d_6:



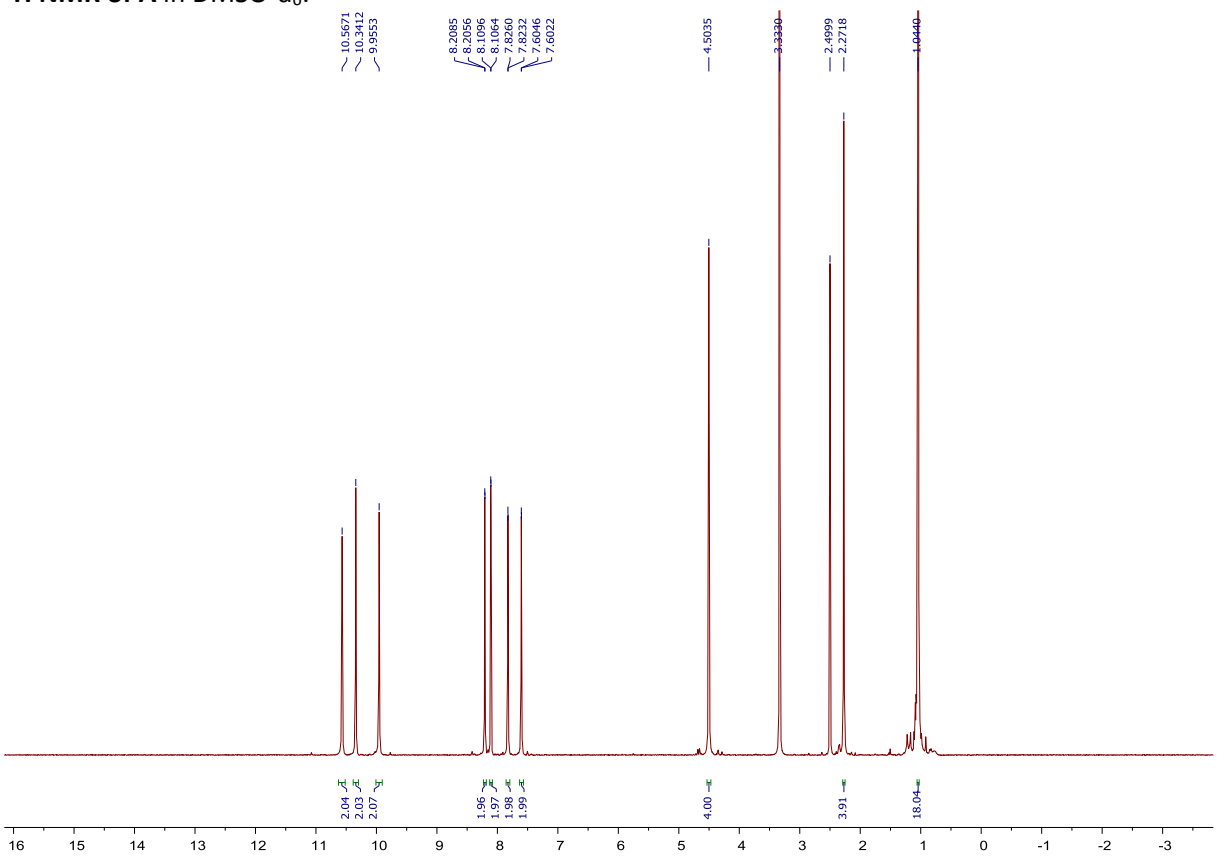
2,2'-oxydiacetylbis(1-amino-8-(3,3-dimethylbutyrylamino)-3,6-dichlorocarbazole) A. To a 25 ml round bottom flask equipped with a magnetic stirrer, **8** (0.100 g, 0.275 mmol) was added. The flask was closed with a septum and purged with argon. Afterwards, dry THF (from SPS, 10 ml) and triethylamine (40 µl, 0.30 mmol) were added and to the resulting solution diglycolyl chloride (16 µl, 0.14 mmol) was slowly added dropwise via a microsyringe. The reaction mixture was stirred for 22 hours at room temperature. The next day the reaction was quenched by the addition of water (20 ml). The flask was put into a refrigerator for 1 hour. After this time the precipitate was filtered off, washed with water (2 ml) and 2 portions of CH_3CN (in total *ca.* 2 ml) and dried thoroughly to yield 0.97 g (85.5%) of white solid.



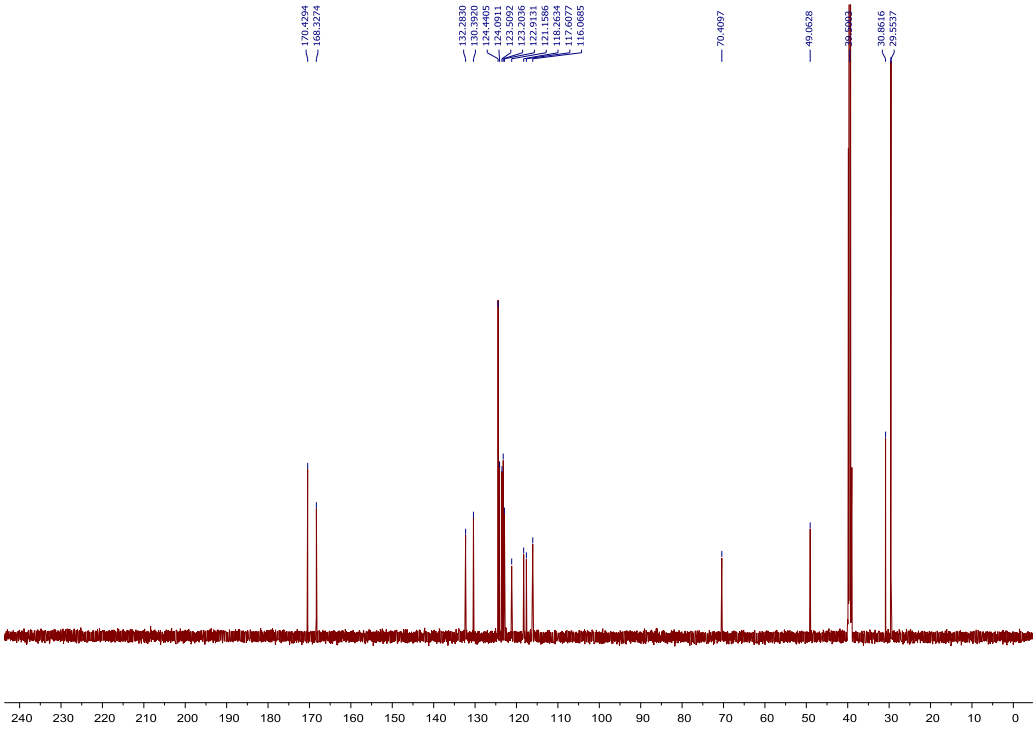
A

^{1}H NMR (DMSO-d_6) δ_{DMSO}: 10.57 (s; 2H); 10.34 (s; 2H); 9.96 (s; 2H); 8.21 (d; *J* = 2.1 Hz; 2H); 8.11 (d; *J* = 2.0 Hz; 2H); 7.82 (d; *J* = 2.1 Hz; 2H); 7.60 (d; *J* = 2.0 Hz; 2H); 4.50 (s; 4H); 2.27 (s; 4H); 1.04 (s; 18H);
^{13}C NMR (DMSO-d_6) δ_{DMSO}: 170.43; 168.33; 132.28; 130.39; 124.44; 124.09; 123.51; 123.20; 122.91; 121.16; 118.26; 117.61; 116.07; 70.41; 49.06; 30.86; 29.55.
HR MS (ESI): m/z calcd. for $C_{40}H_{40}Cl_4N_6O_5Na$ $[M+Na]^+$: 847.1712; found: 847.1704.
Elemental Analysis calcd. for $C_{40}H_{40}Cl_4N_6O_5$: C 58.12; H 4.88; N 10.17; found: C 57.87; H 4.9; N 9.97.

^{1}H NMR of A in DMSO-d_6:



^{13}C NMR of A in DMSO-d_6:



2. Binding studies.

2.1. Materials:

Tetrabutylammonium sulphate was purchased from Alfa Aesar as a 50% aqueous solution. Before drying, the pH of this solution was checked and found to be neutral (pH=7.3 upon dilution to 1M concentration), confirming that the sample is essentially free from hydrogensulphate. Anhydrous salt was obtained in the following way: *ca.* 1g of the 50% solution was transferred to a 25 ml round-bottom flask and most of the water was removed on rotary evaporator with gentle heating over a few hours. Viscous residue was then further dried under high vacuum over KOH to a constant mass (in total *ca.* 47% loss of weight was reached). The resulting white crystalline solid was stored in a vacuum desiccator over KOH and used for titrations.

Tetrabutylammonium chloride, tetrabutylammonium benzoate and tetrabutylammonium dihydrogen phosphate were obtained from Sigma-Aldrich and used as received.

DMSO (anhydrous, ≥99.9%) was purchased from Sigma-Aldrich. DMSO-d_6 (99.8% isotopic purity, containing less than 0.02% water) was obtained from Eurisotop in septum-sealed vials and used as received. DMSO/H_2O mixtures were obtained using Milli-Q H_2O and their concentrations were expressed as weight-weight percentage.

Mettler Toledo Excellence XA105DU analytical balance (d = 0.01 mg) was used for weighing all the samples.

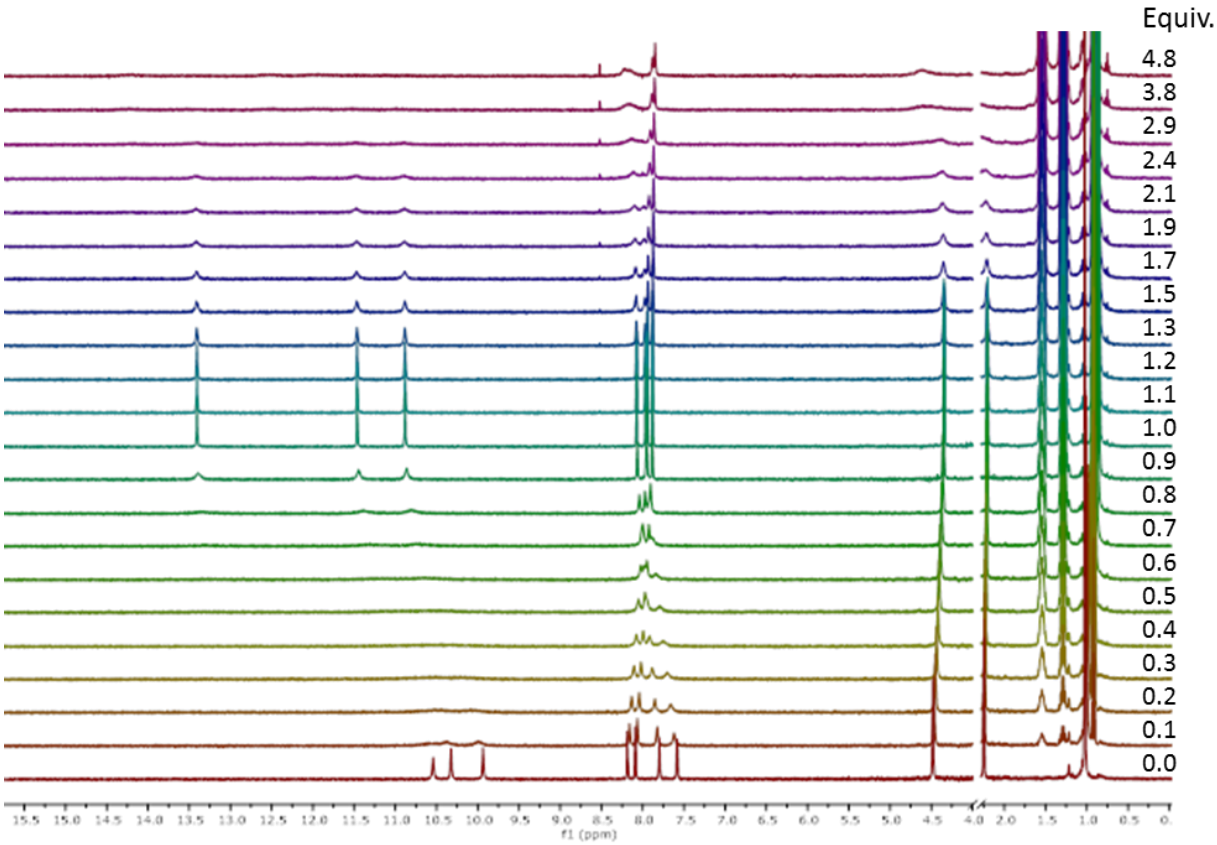
2.2. ^{1}H NMR titration procedure.

To a solution of host (600μl, 0.001M) in a septum-sealed screw-cap NMR tube, appropriate aliquots of titrant (0.015M, dissolved in the solution of host to avoid dilution) were added with a 25 μl gas-tight microsyringe. NMR spectra were measured on Agilent 400 MHz spectrometer. Nonlinear curve fit was carried out using the WinEQNMR2 software if possible.[2] Association constants $ß_{1:1}$ and $ß_{2:1}$ and chemical shifts of both 1:1 and 2:1 complexes were set as free parameters for fitting, whereas chemical shifts of free ligands were constrained to be equal to experimentally measured values.

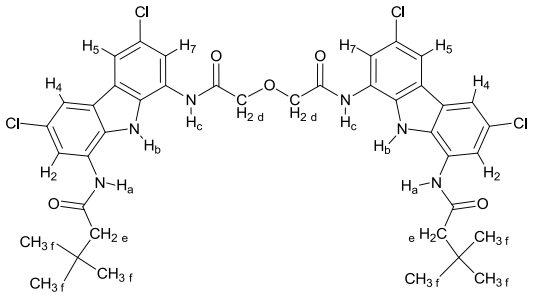
[2] M. J. Hynes, *J. Chem. Soc. Dalton. Trans.* **1993**, 311-312.

2.2.1. ^{1}H NMR titration of 0.001M solution of receptor **A** in DMSO-d_6 + 0.5% H_2O with 0.015M $(TBA)_2SO_4$.

a) ^{1}H NMR spectra



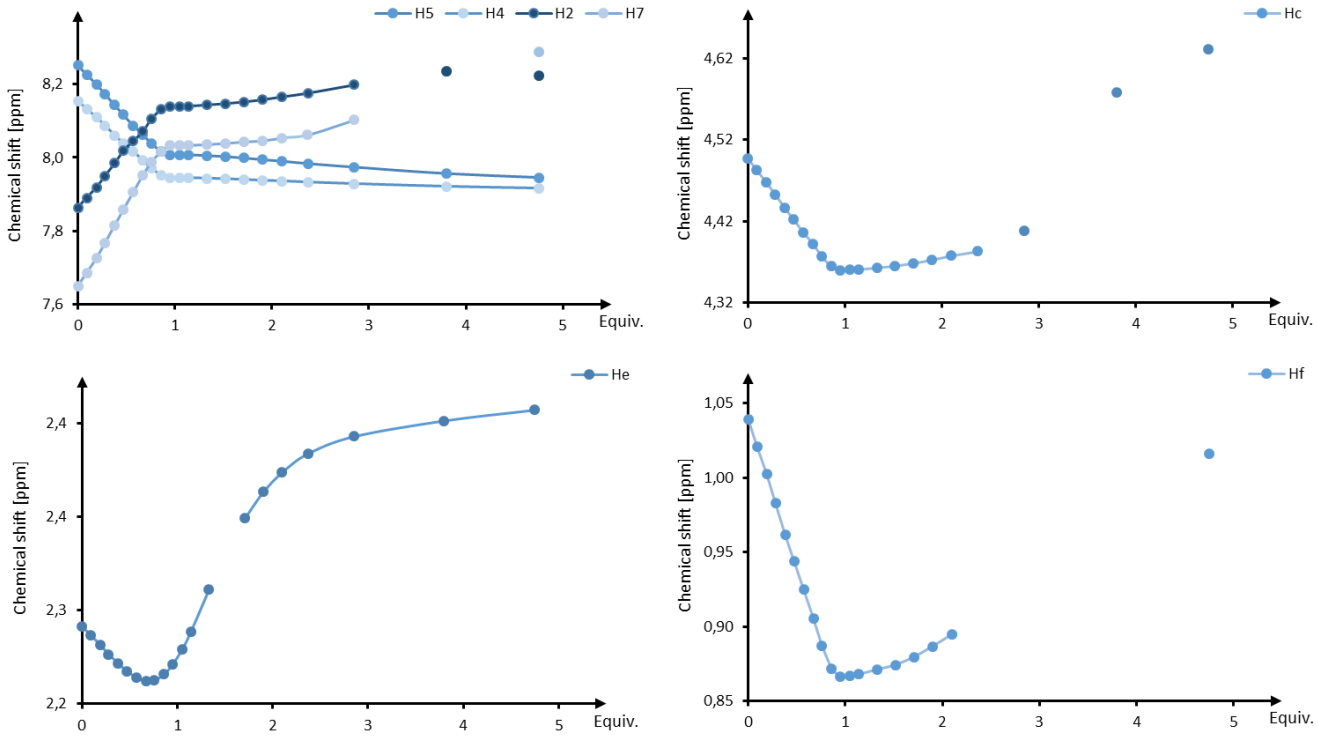
b) Raw data



Added volume of titrant solution [µl]	Equivalents of $(TBA)_2SO_4$	Hb	Hc	Ha	H5	H4	H2	H7	Hc	He	Hf
0.0	0.00	10.5580	10.3409	9.9527	8.20155	8.1037	7.8136	7.59975	4.4967	2.2659	1.0392
4.0	0.09	10.5939	10.4012	10.0108	8.1766	8.0821	7.8406	7.6357	4.4827	2.2588	1.0209
8.0	0.19	broad	10.4826	10.0644	8.1504	8.0596	7.8687	7.6755	4.4675	2.2502	1.0021
12.0	0.28	broad	broad	broad	8.1229	8.0364	7.9006	7.7179	4.4528	2.2423	0.9827

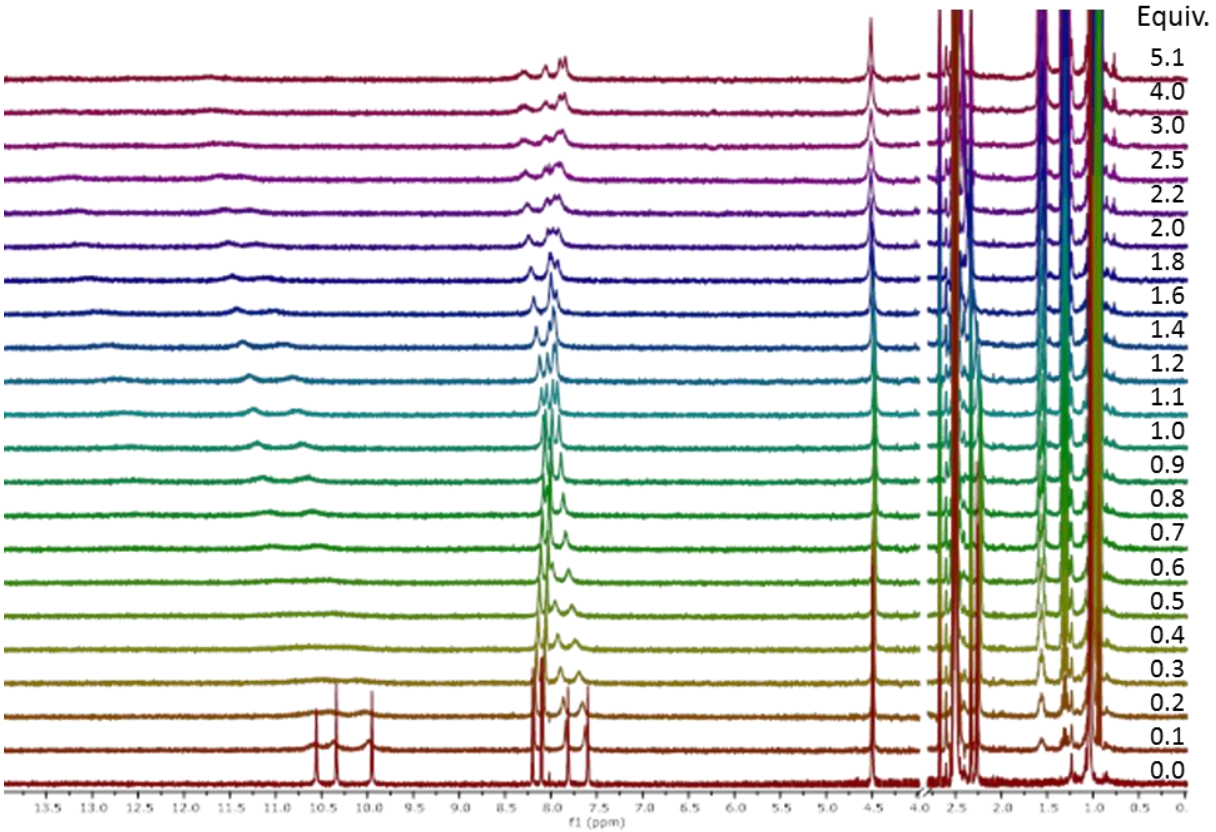
16.5	0.38	broad	broad	broad	8.0931	8.0104	7.9344	7.7659	4.4363	2.2344	0.9615
20.5	0.47	broad	broad	broad	8.0667	7.9878	7.9688	7.8090	4.4220	2.2279	0.9440
25.0.	0.57	13.3081	11.1945	10.6644	8.0372	7.9663	7.9951	7.8561	4.4064	2.2226	0.9246
29.5	0.67	13.2906	11.3144	10.7363	8.0128	7.9416	8.0213	7.9028	4.3918	2.2195	0.9052
34.0	0.76	13.3581	11.3978	10.8104	7.9874	7.9202	8.0563	7.9388	4.3770	2.2204	0.8869
38.5	0.86	13.4071	11.4609	10.8799	7.9678	7.9012	8.0810	7.9678	4.3644	2.2252	0.8716
43.0	0.95	13.4210	11.4792	10.8979	7.9583	7.8949	8.0890	7.9831	4.3599	2.2341	0.8665
47.5	1.05	13.4221	11.4799	10.8989	7.9582	7.8949	8.0894	7.9835	4.3602	2.2467	0.8669
52.0	1.14	13.4229	11.4801	10.8994	7.9577	7.8947	8.0903	7.9841	4.3608	2.2617	0.8678
62.0	1.33	13.4236	11.4808	10.9002	7.9556	7.8932	8.0935	7.9863	4.3629	2.2976	0.8710
71.5	1.52	13.4260	11.4830	10.9015	7.9528	7.8916	8.0970	7.9894	4.3652	overlap	0.8742
82.0	1.71	13.4251	11.4828	10.9016	7.9491	7.8898	8.1018	7.9933	4.3685	2.3588	0.8796
92.5	1.90	13.4300	11.4861	10.9039	7.9445	7.8875	8.1077	7.9964	4.3726	2.3811	0.8867
103.5	2.10	13.4330	11.4875	10.9075	7.9403	7.8859	8.1154	8.0037	4.3776	2.3980	0.8948
120.0	2.37	13.4370	11.4864	10.9027	7.9338	7.8828	8.1257	8.0123	4.3829	2.4139	overlap
150.0	2.85	13.4391	11.4984	10.9137	7.9241	7.8785	8.1481	8.0531	4.4087	2.4285	overlap
218.0	3.80	broad	broad	broad	7.9066	7.8711	8.1842	8.1842	4.5786	2.4420	overlap
300.0	4.75	broad	broad	broad	7.8957	7.8661	8.1733	8.2384	4.6312	2.4512	1.0160

c) Titration curves

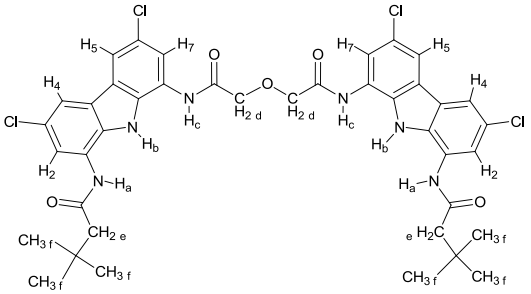


2.2.2. ^{1}H NMR titration of 0.001M solution of receptor **A** in DMSO-d_6 + 0.5% H_2O with 0.015M $TBAH_2PO_4$.

a) ^{1}H NMR spectra



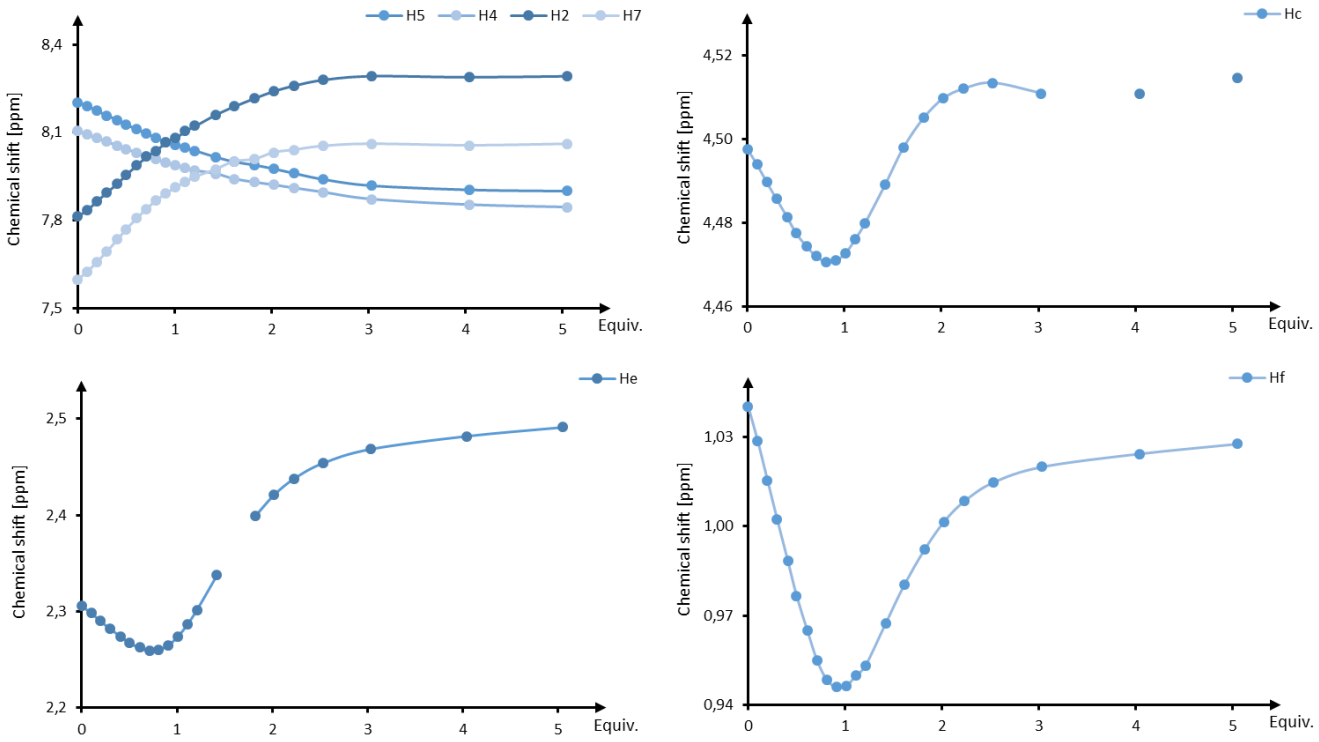
b) Raw data



Added volume of titrant solution [µl]	Equivalents of $TBAH_2PO_4$	Hb	Hc	Ha	H5	H4	H2	H7	Hc	He	Hf
0.0	0.00	10.5563	10.3387	9.9516	8.2029	8.1049	7.8127	7.5986	4.4976	2.2659	1.0403
4.0	0.10	10.5725	10.3724	9.9828	8.1891	8.0936	7.8366	7.6256	4.4939	2.2588	1.0285
8.0	0.20	broad	broad	10.0335	8.1734	8.0811	7.8655	7.6590	4.4897	2.2502	1.0154
12.0	0.30	broad	broad	broad	8.1578	8.0687	7.8959	7.6936	4.4857	2.2423	1.0023
16.5	0.41	broad	broad	broad	8.1419	8.0554	7.9256	7.7352	4.4814	2.2344	0.9883
20.5	0.50	broad	broad	broad	8.1262	8.0437	7.9565	7.7698	4.4776	2.2279	0.9767

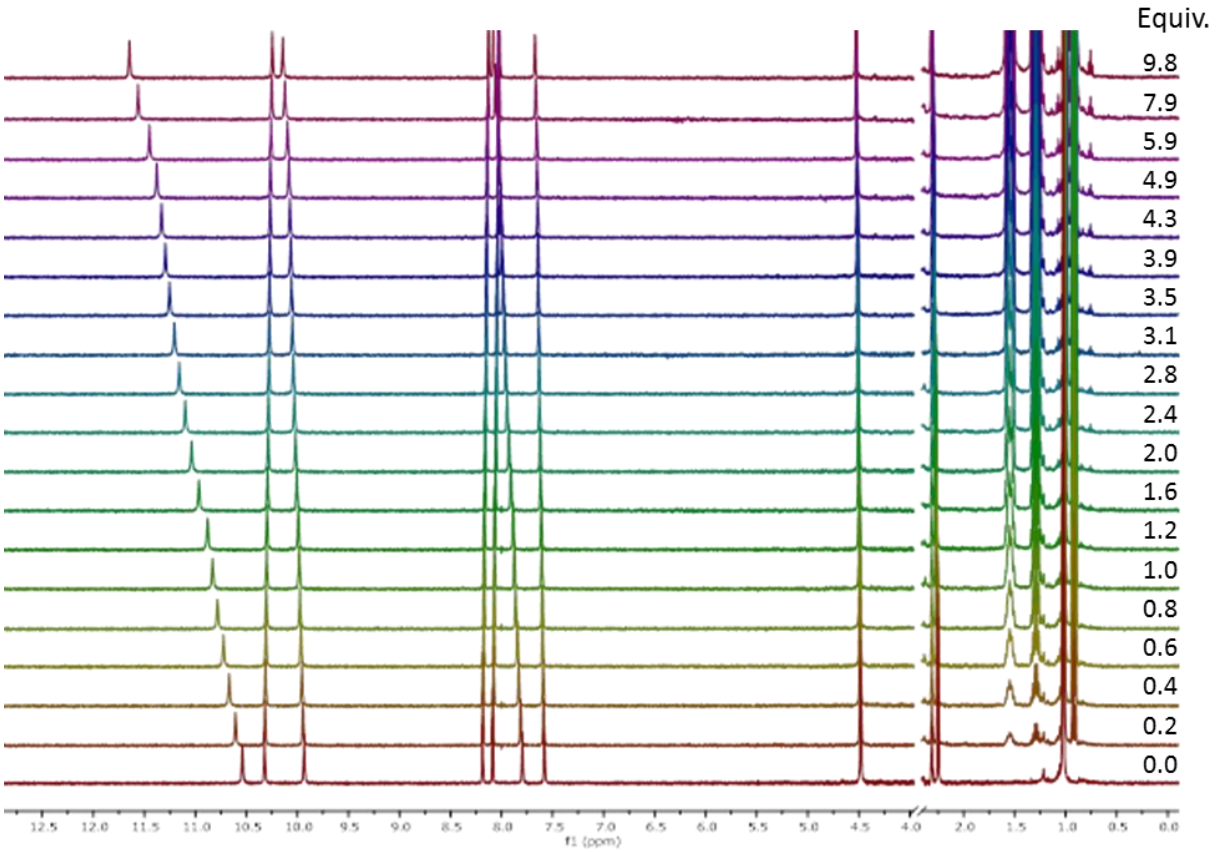
25.0	0.61	broad	broad	broad	8.1109	8.0307	7.9879	7.8071	4.4744	2.2226	0.9651
29.5	0.71	broad	broad	broad	8.0955	8.0179	8.0179	7.8390	4.4720	2.2195	0.9551
34.0	0.81	12.5146	11.1003	10.5971	8.0819	8.0083	8.0381	7.8681	4.4707	2.2204	0.9485
38.5	0.91	12.5653	11.1536	10.6588	8.0672	7.9970	8.0672	7.8913	4.4710	2.2252	0.9460
43.0	1.01	12.6010	11.1966	10.7092	8.0586	7.9882	8.0820	7.9123	4.4727	2.2341	0.9464
47.5	1.11	12.6560	11.2466	10.7637	8.0481	7.9801	8.1045	7.9305	4.4760	2.2467	0.9498
52.0	1.21	12.7249	11.2885	10.8138	8.0379	7.9705	8.1224	7.9480	4.4798	2.2617	0.9532
62.0	1.42	12.8330	11.3537	10.9257	8.0167	7.9598	8.1602	7.9737	4.4891	2.2976	0.9675
71.5	1.61	12.9461	11.4235	11.0304	8.0003	7.9417	8.1890	8.0003	4.4980	overlap	0.9803
82.0	1.82	13.0459	11.4727	11.1158	7.9894	7.9302	8.2169	8.0084	4.5051	2.3588	0.9922
92.5	2.02	13.1072	11.5174	11.198	7.9765	7.9210	8.2414	8.0312	4.5097	2.3811	1.0015
103.5	2.23	13.1680	11.5587	11.2789	7.9612	7.9105	8.2605	8.0401	4.5120	2.3980	1.0084
120.0	2.53	13.2238	11.6126	11.3740	7.9408	7.8961	8.2802	8.0532	4.5134	2.4139	1.0147
150.0.	3.03	broad	broad	broad	7.9193	7.8721	8.2934	8.0604	4.5109	2.4285	1.0199
218.0	4.04	13.3791	12.5914	11.7033	7.9050	7.8529	8.2899	8.0551	4.5109	2.4420	1.0243
300.0	5.05	13.3780	12.5533	11.7457	7.9006	7.8445	8.2933	8.0602	4.5146	2.4512	1.0276

c) Titration curves

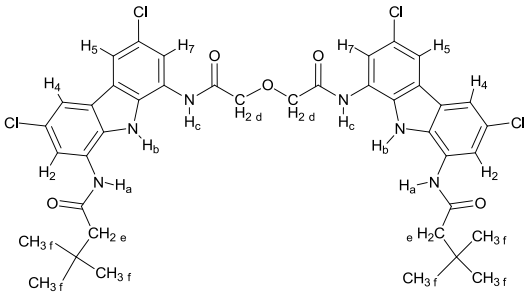


2.2.3. ^{1}H NMR titration of 0.001M solution of receptor **A** in DMSO-d_6 + 0.5% H_2O with 0.015M TBACl.

a) ^{1}H NMR spectra



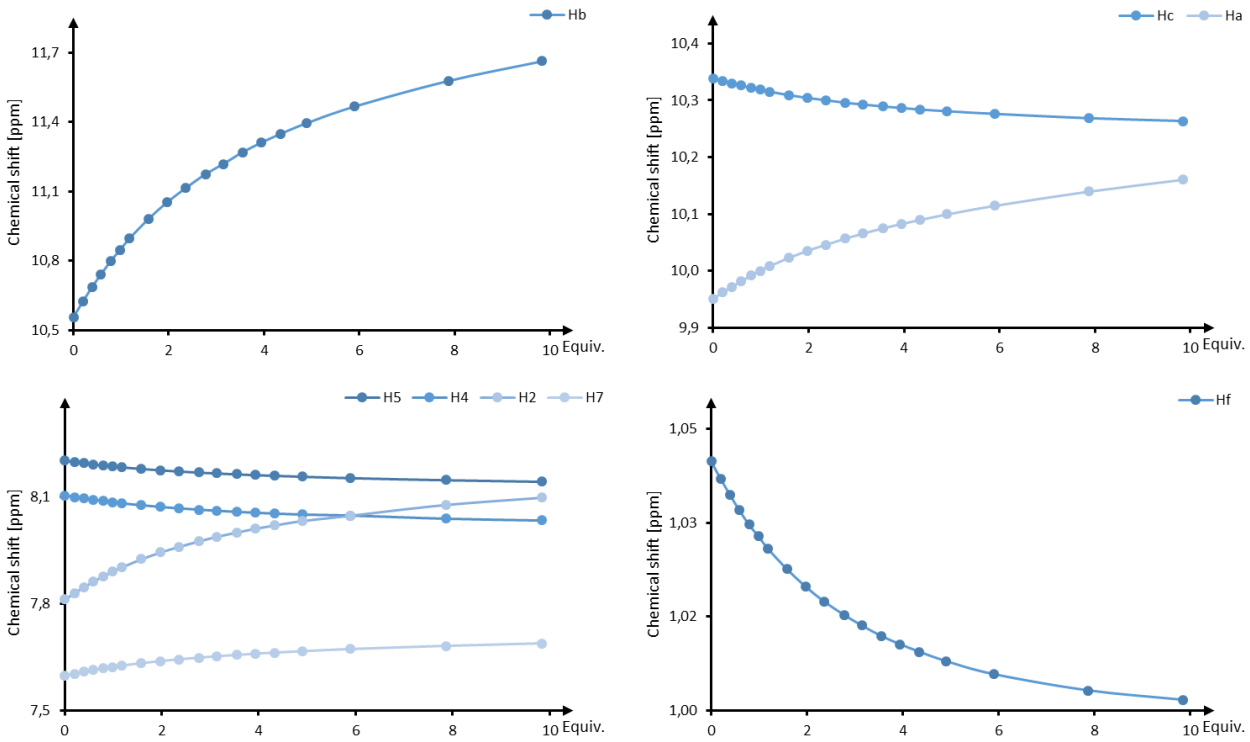
b) Raw data



Added volume of titrant solution [µl]	Equivalents of TBACl	Hb	Hc	Ha	H5	H4	H2	H7	Hc	He	Hf
0.0	0.00	10.5565	10.3390	9.9506	8.2026	8.1046	7.8125	7.5984	4.4972	2.2655	1.0398
4.0	0.20	10.6240	10.3344	9.9626	8.1990	8.1001	7.8306	7.6039	4.5002	2.2691	1.0370
8.0	0.39	10.6857	10.3298	9.9721	8.1956	8.0961	7.8471	7.6088	4.5030	2.2723	1.0345
12.0	0.58	10.7415	10.3261	9.9817	8.1927	8.0925	7.8619	7.6135	4.5054	2.2752	1.0321
16.5	0.79	10.8002	10.3220	9.9917	8.1895	8.0887	7.8776	7.6182	4.5078	2.2785	1.0297

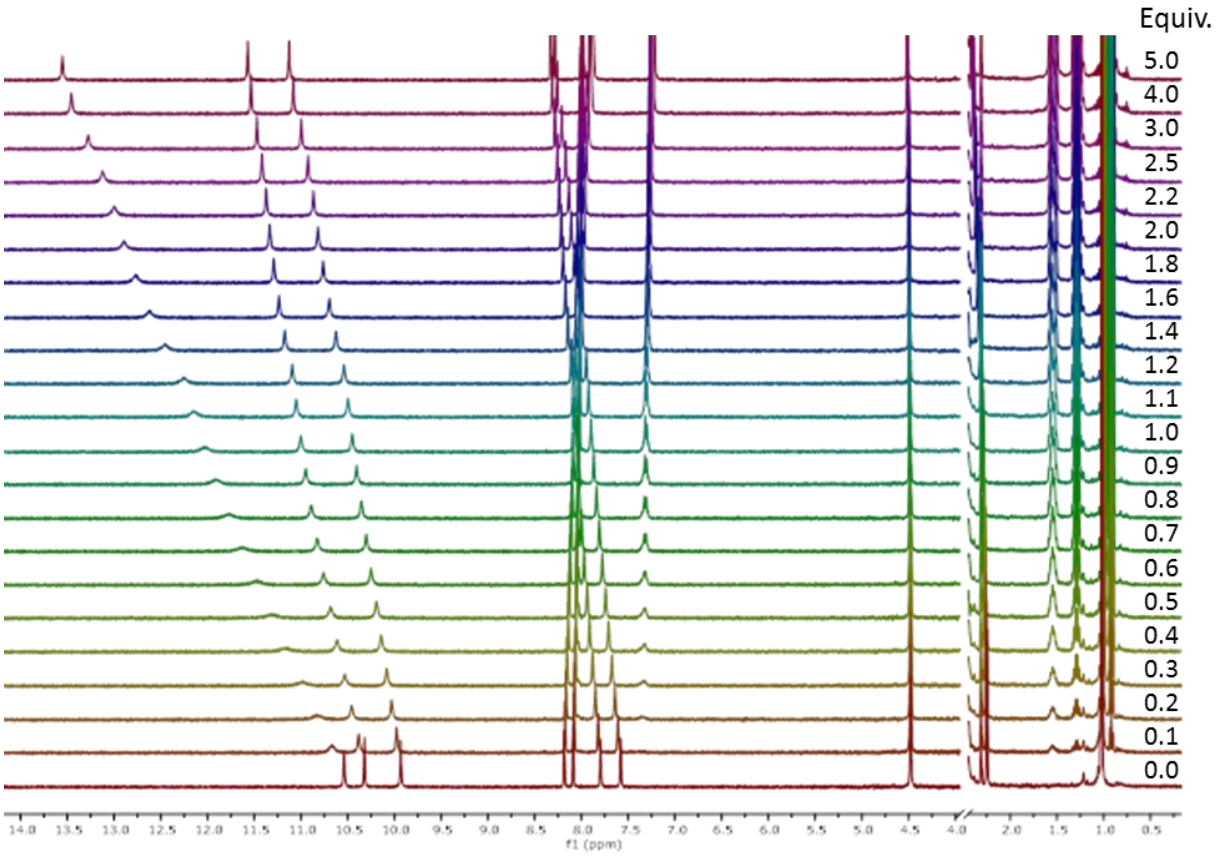
20.5	0.98	10.8474	10.3186	10.0000	8.1869	8.0857	7.8903	7.6220	4.5099	2.2811	1.0279
25.0	1.18	10.8969	10.3152	10.0084	8.1843	8.0824	7.9032	7.6261	4.5121	2.2838	1.0259
34.0	1.58	10.9819	10.3092	10.0229	8.1798	8.0771	7.9258	7.6330	4.5158	2.2885	1.0226
43.0	1.97	11.0536	10.3042	10.0355	8.1761	8.0725	7.9448	7.6387	4.5186	2.2926	1.0198
52.0	2.36	11.1150	10.3001	10.0462	8.1728	8.0685	7.9608	7.6439	4.5213	2.2960	1.0174
62.0	2.77	11.1744	10.2957	10.0571	8.1696	8.0648	7.9762	7.6486	4.5239	2.2996	1.0153
71.5	3.14	11.2181	10.2925	10.0659	8.1672	8.0618	7.9890	7.6527	4.5260	2.3024	1.0136
82.0	3.55	11.2696	10.2892	10.0750	8.1646	8.0588	8.0010	7.6563	4.5277	2.3053	1.0119
92.5	3.94	11.3106	10.2865	10.0827	8.1625	8.0562	8.0117	7.6598	4.5296	2.3079	1.0106
103.5	4.34	11.3482	10.2837	10.0900	8.1605	8.0539	8.0211	7.6629	4.5310	2.3102	1.0094
119.5	4.90	11.3955	10.2808	10.0996	8.1581	8.0512	8.0331	7.6668	4.5329	2.3135	1.0079
150.0	5.90	11.4671	10.2760	10.1147	8.1541	8.0484	8.0484	7.6728	4.5358	2.3182	1.0058
218.0	7.87	11.5779	10.2684	10.1397	8.1483	8.0396	8.0786	7.6819	4.5399	2.3267	1.0032
300.0	9.84	11.6631	10.2634	10.1605	8.1439	8.0346	8.0987	7.6890	4.5431	2.3337	1.0017

c) Titration curves

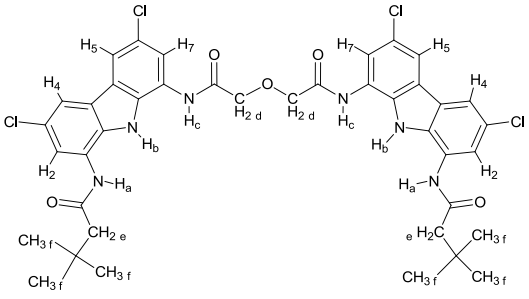


2.2.4. ^{1}H NMR titration of 0.001M solution of receptor **A** in DMSO-d_6 + 0.5% H_2O with 0.015M TBAPhCOO.

a) ^{1}H NMR spectra



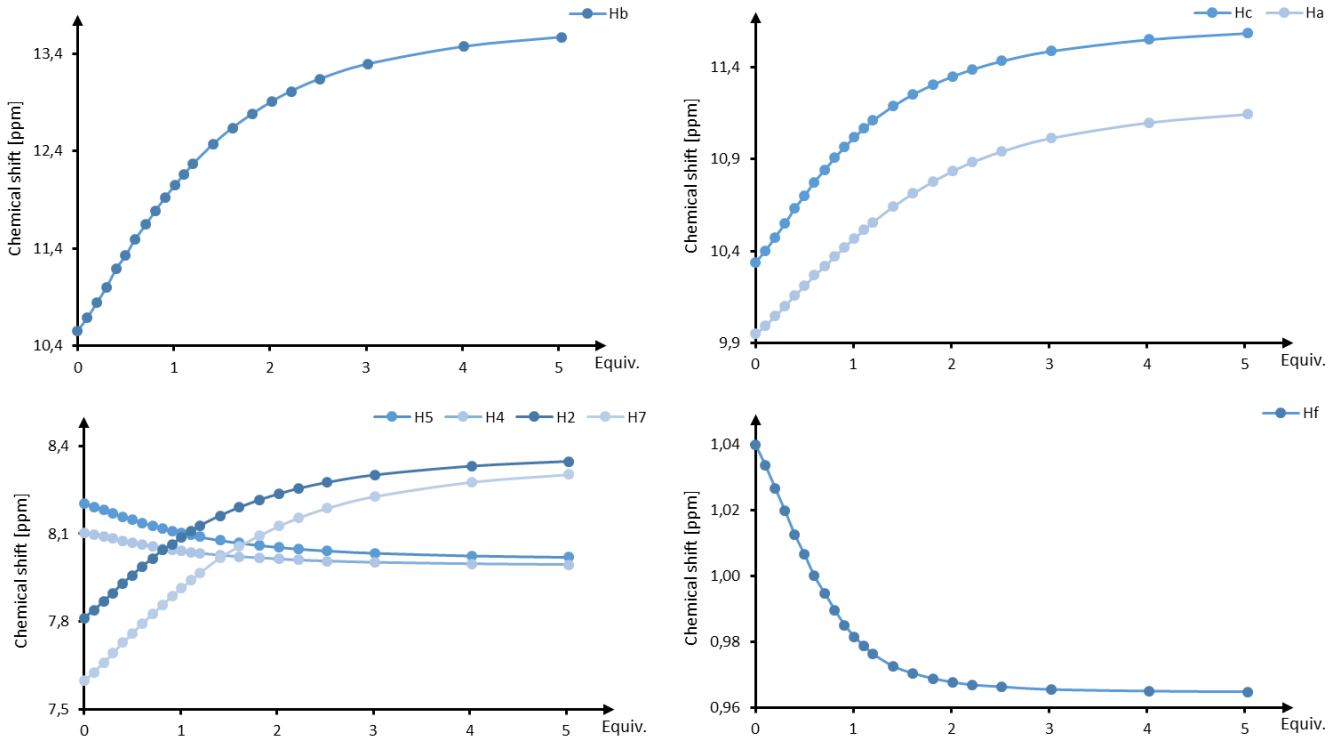
b) Raw data



Added volume of titrant solution [µl]	Equivalents of TBAPhCOO	Hb	Hc	Ha	H5	H4	H2	H7	Hc	He	Hf
0.0	0.00	10.5561	10.3388	9.9506	8.2024	8.1044	7.8122	7.5981	4.4972	2.2653	1.0397
4.0	0.10	10.6861	10.4007	9.9954	8.1923	8.0978	7.8382	7.6267	4.4971	2.2687	1.0335
8.0	0.20	10.8437	10.4753	10.0478	8.1814	8.0908	7.8681	7.6596	4.4978	2.2735	1.0266
12.0	0.30	10.9999	10.5494	10.1012	8.1706	8.0839	7.8977	7.6920	4.4981	2.2785	1.0197
16.5	0.40	11.1897	10.6317	10.1605	8.1587	8.0766	7.9308	7.7283	4.4987	2.2844	1.0125
20.5	0.50	11.3288	10.7004	10.2100	8.1486	8.0703	7.9577	7.7588	4.4992	2.2894	1.0064

25.0	0.60	11.4972	10.7762	10.2682	8.1378	8.0636	7.9883	7.7936	4.5001	2.2955	0.9999
29.5	0.71	11.6455	10.8437	10.3198	8.1282	8.0576	8.0152	7.8252	4.5008	2.3014	0.9945
34.0	0.81	11.7897	10.908	10.3721	8.1187	8.0498	8.0439	7.8567	4.5018	2.3078	0.9895
38.5	0.91	11.9225	10.9666	10.4224	8.1102	8.0462	8.0636	7.8867	4.5026	2.3144	0.9850
43.0	1.01	12.0479	11.0197	10.4703	8.1024	8.0418	8.0875	7.9146	4.5037	2.3216	0.9814
47.5	1.11	12.1637	11.0690	10.5157	8.0957	8.0376	8.1084	7.9411	4.5048	2.3270	0.9786
52.0	1.20	12.2685	11.1109	10.5579	8.0895	8.0341	8.1269	7.9658	4.5061	2.3340	0.9762
62.0	1.41	12.4725	11.1905	10.6441	8.0777	8.0271	8.1618	8.0181	4.5089	2.3481	0.9724
71.5	1.61	12.6390	11.2532	10.7145	8.0686	8.0221	8.1899	8.0574	4.5113	2.3604	0.9703
82.0	1.82	12.7853	11.3075	10.7805	8.0605	8.0182	8.2154	8.0937	4.5137	2.3722	0.9687
92.5	2.02	12.9095	11.3522	10.8366	8.0541	8.0143	8.2360	8.1259	4.5158	2.3824	0.9676
103.5	2.22	13.0148	11.3895	10.8847	8.0484	8.0106	8.2537	8.1534	4.5176	2.3914	0.9668
120.0	2.52	13.1414	11.4347	10.9426	8.0420	8.0071	8.2749	8.1867	4.5201	2.4023	0.9662
150.0	3.02	13.2940	11.4889	11.0146	8.0340	8.0027	8.3006	8.2275	4.5230	2.4159	0.9654
218.0	4.02	13.4740	11.5521	11.0991	8.0250	7.9978	8.3307	8.2762	4.5269	2.4322	0.9649
300.0	5.03	13.5702	11.5867	11.1450	8.0201	7.9950	8.3469	8.3023	4.5291	2.4411	0.9647

c) Titration curves

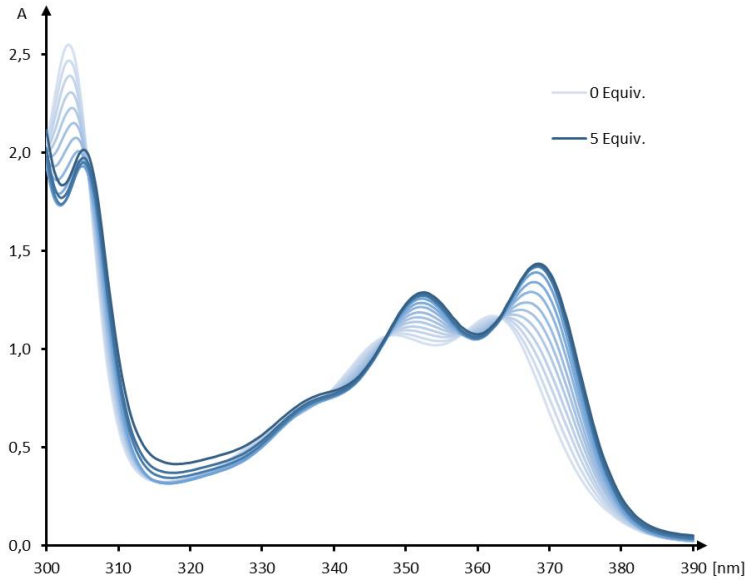


2.3. UV-Vis titration procedure.

To a solution of host (3 mL, $2 \cdot 10^{-5}$ - $1 \cdot 10^{-4}$M) in a septum-sealed screw-cap precision cell made of Quartz SUPRASIL (light path: 10 mm) appropriate aliquots of titrant (dissolved in the solution of host to avoid dilution) were added with a 25 µl gas-tight microsyringe. UV spectra were obtained on Thermo Scientific Evolution 300 spectrometer.[3] Association constants were calculated from absorbance changes at fixed wavelength. Nonlinear curve fit was carried out using the HypSpec software. Association constants $ß_{1:1}$ and $ß_{2:1}$ and molar absorption coefficients of receptor, both 1:1 and 2:1 complexes were set as free parameters for fitting.

2.3.1. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO + 0.5% H_2O with 0.0075 M solution of $(TBA)_2SO_4$ (dissolved in the solution of receptor **A**).

a) UV-Vis spectra



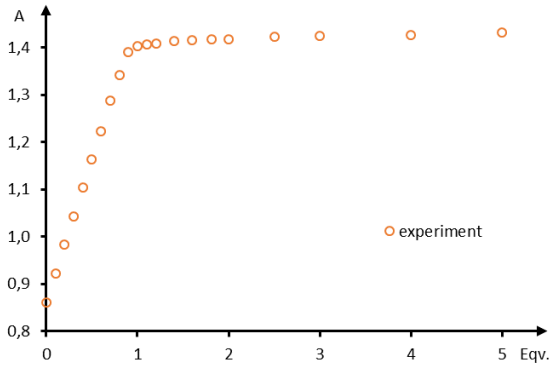
b) Raw data

Added volume of titrant solution [µL]	Equivalents of $(TBA)_2SO_4$	Wavelength [nm]									
		303	303.5	352.5	353	353.5	368	368.5	369	369.5	370
		Absorbance									
0.0	0.00	2.548	2.533	1.029	1.025	1.021	0.861	0.816	0.769	0.721	0.674
4.0	0.10	2.466	2.458	1.055	1.051	1.046	0.922	0.881	0.837	0.793	0.748
8.0	0.20	2.385	2.386	1.082	1.077	1.072	0.983	0.947	0.908	0.866	0.822
12.0	0.30	2.298	2.306	1.107	1.103	1.097	1.043	1.012	0.976	0.937	0.895
16.0	0.40	2.211	2.227	1.133	1.128	1.121	1.103	1.077	1.045	1.009	0.970
20.0	0.50	2.123	2.146	1.158	1.153	1.146	1.163	1.141	1.114	1.081	1.043
24.0	0.60	2.033	2.063	1.186	1.181	1.173	1.223	1.207	1.183	1.153	1.117
28.5	0.71	1.932	1.969	1.213	1.209	1.199	1.287	1.277	1.258	1.231	1.197
32.5	0.80	1.847	1.891	1.236	1.231	1.221	1.342	1.336	1.321	1.298	1.265
36.5	0.90	1.778	1.827	1.257	1.251	1.242	1.390	1.388	1.377	1.356	1.324

[3]P. Gans, A. Sabatini and A. Vacca, *Talanta*, 1996, **43**, 1739

40.5	1.00	1.764	1.813	1.262	1.258	1.248	1.402	1.402	1.391	1.372	1.341
44.5	1.10	1.763	1.812	1.264	1.259	1.250	1.407	1.406	1.396	1.377	1.347
49.0	1.21	1.764	1.814	1.266	1.261	1.251	1.409	1.409	1.400	1.381	1.351
57.0	1.40	1.766	1.814	1.267	1.263	1.253	1.413	1.413	1.404	1.385	1.356
65.5	1.60	1.770	1.819	1.269	1.264	1.254	1.415	1.416	1.407	1.389	1.360
74.0	1.81	1.776	1.824	1.271	1.267	1.258	1.418	1.419	1.411	1.392	1.363
82.0	2.00	1.779	1.827	1.272	1.268	1.258	1.418	1.420	1.412	1.394	1.364
103.5	2.50	1.793	1.839	1.275	1.271	1.261	1.422	1.423	1.415	1.398	1.369
125.0	3.00	1.806	1.852	1.278	1.274	1.265	1.425	1.426	1.419	1.402	1.375
169.0	4.00	1.833	1.876	1.282	1.278	1.269	1.427	1.429	1.423	1.407	1.380
214.5	5.00	1.859	1.900	1.289	1.286	1.277	1.432	1.435	1.430	1.416	1.390

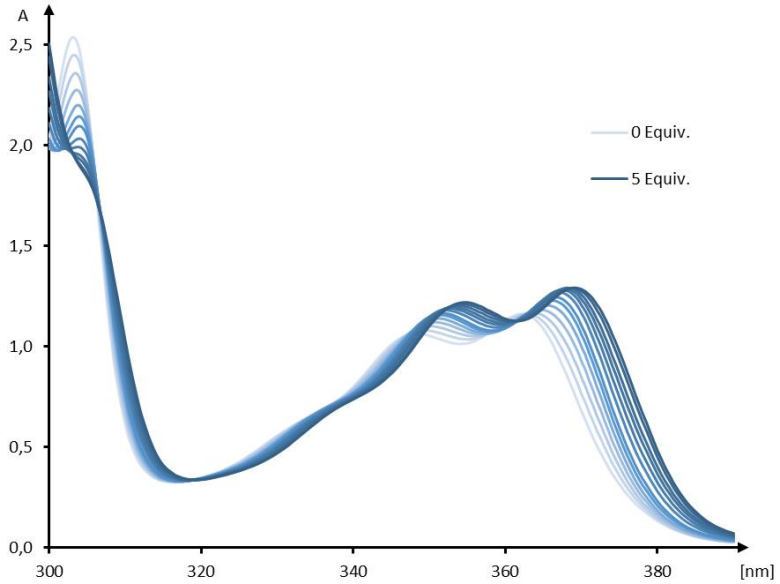
c) Titration curve at 368 nm



The curve is too sharp to be reliably reproduced by fitting software.

2.3.2. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO + 0.5% H_2O with 0.0075 M solution of $TBAH_2PO_4$ (dissolved in the solution of receptor **A**).

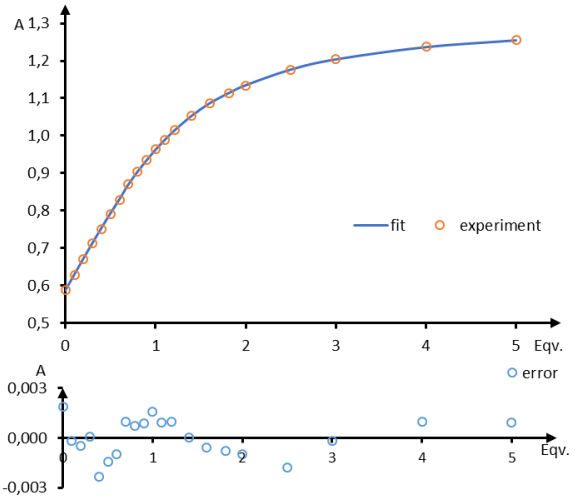
a) UV-Vis spectra



b) Raw data

Added volume of titrant solution [µL]	Equivalents of $TBAH_2PO_4$	Wavelength [nm]									
		303	303.5	354	354.5	369.5	370	370.5	371	371.5	372
		Absorbance									
0.0	0.00	2.535	2.526	1.013	1.013	0.722	0.676	0.633	0.588	0.546	0.506
4.0	0.10	2.487	2.488	1.025	1.024	0.768	0.717	0.676	0.629	0.587	0.544
8.0	0.20	2.440	2.444	1.038	1.036	0.812	0.761	0.720	0.671	0.628	0.582
12.0	0.30	2.392	2.401	1.051	1.047	0.855	0.805	0.763	0.713	0.669	0.621
16.0	0.40	2.343	2.358	1.064	1.059	0.894	0.844	0.802	0.751	0.707	0.656
20.0	0.50	2.295	2.315	1.074	1.068	0.934	0.884	0.842	0.791	0.743	0.693
24.0	0.60	2.250	2.273	1.086	1.079	0.973	0.924	0.883	0.829	0.782	0.729
28.5	0.71	2.203	2.229	1.097	1.089	1.012	0.965	0.923	0.871	0.822	0.769
32.5	0.80	2.165	2.195	1.107	1.099	1.044	0.998	0.957	0.904	0.856	0.801
36.5	0.90	2.133	2.162	1.117	1.107	1.073	1.028	0.987	0.935	0.886	0.831
40.5	1.00	2.104	2.134	1.126	1.117	1.100	1.056	1.016	0.964	0.916	0.860
44.5	1.10	2.082	2.110	1.133	1.124	1.123	1.078	1.040	0.989	0.941	0.885
49.0	1.21	2.059	2.086	1.141	1.132	1.144	1.102	1.064	1.015	0.965	0.914
57.0	1.40	2.031	2.053	1.154	1.145	1.175	1.136	1.100	1.053	1.007	0.954
65.5	1.60	2.010	2.026	1.164	1.156	1.198	1.164	1.129	1.086	1.040	0.990
74.0	1.81	1.994	2.005	1.173	1.166	1.218	1.186	1.155	1.113	1.071	1.022
82.0	2.00	1.983	1.988	1.179	1.173	1.232	1.202	1.173	1.134	1.094	1.047
103.5	2.50	1.966	1.96	1.192	1.188	1.257	1.233	1.209	1.175	1.14	1.097
125.0	3.00	1.961	1.944	1.201	1.199	1.272	1.254	1.233	1.204	1.173	1.134
169.0	4.00	1.962	1.931	1.211	1.211	1.285	1.274	1.259	1.238	1.213	1.180
214.5	5.00	1.969	1.93	1.216	1.218	1.289	1.283	1.272	1.256	1.235	1.207

c) Titration curve at 371 nm



Binding constants K derived from simultaneous fitting of 1:1 and 1:2 models to ten selected wavelengths using HypSpec:

$\log K_{1:1} = 5.354$
$\log K_{1:2} = 4.092$

Molar absorption coefficient derived from simultaneous fitting of 1:1 and 1:2 models to ten selected wavelengths using HypSpec:

	Wavelength [nm]									
	303	303.5	354	354.5	369.5	370	370.5	371	371.5	372
L [$M^{-1}cm^{-1}$]	25442	25370	10127	10131	7217	6726	6317	5861	5462	5054
L×$H_2PO_4^-$ [$M^{-1}cm^{-1}$]	19759	20328	11481	11330	11974	11460	11005	10390	9809	9152
L×$(H_2PO_4^-)_2$ [$M^{-1}cm^{-1}$]	19508	18889	12348	12404	13205	13237	13192	13120	12980	12767

d) Binding constants K derived from the experiment repeated according to the same methodology:

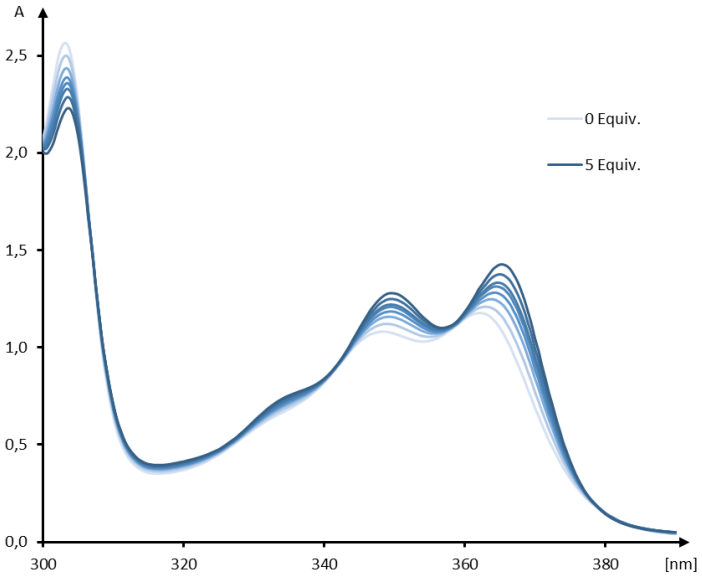
$\log K_{1:1} = 5.325$
$\log K_{1:2} = 3.988$

e) Binding constants averaged from the above two experiments:

$\log K_{1:1} = 5.340$
$\log K_{1:2} = 4.066$

2.3.3. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO + 0.5% H_2O with 0.0075 M solution of TBAPhCOO (dissolved in the solution of receptor **A**).

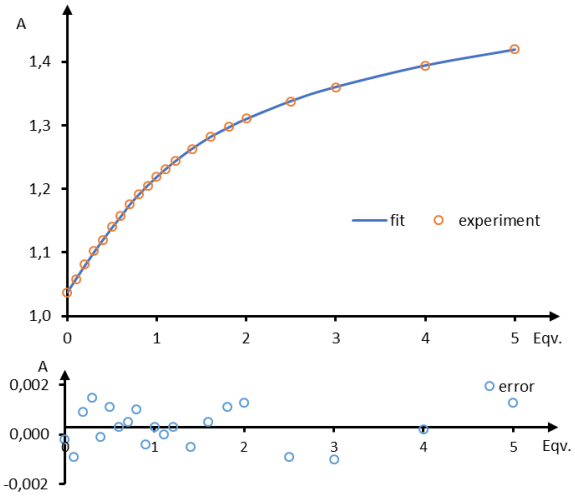
a) UV-Vis spectra



b) Raw data

Added volume of titrant solution [µL]	Equivalents of TBAPhCOO	Wavelength [nm]									
		303	303.5	349.5	350	350.5	365.5	366	366.5	367	367.5
		Absorbance									
0.0	0.00	2.566	2.557	1.076	1.071	1.065	1.072	1.037	1.002	0.959	0.919
4.0	0.10	2.551	2.546	1.086	1.081	1.076	1.091	1.058	1.024	0.982	0.943
8.0	0.20	2.536	2.529	1.098	1.094	1.088	1.113	1.081	1.048	1.007	0.968
12.0	0.30	2.515	2.512	1.109	1.105	1.1	1.132	1.102	1.07	1.03	0.991
16.0	0.40	2.495	2.495	1.12	1.116	1.11	1.15	1.12	1.09	1.051	1.012
20.0	0.50	2.477	2.478	1.13	1.126	1.121	1.167	1.14	1.11	1.072	1.034
24.0	0.60	2.46	2.462	1.139	1.135	1.13	1.183	1.157	1.128	1.091	1.052
28.5	0.70	2.443	2.447	1.148	1.145	1.14	1.2	1.176	1.148	1.111	1.074
32.5	0.80	2.428	2.433	1.157	1.154	1.148	1.215	1.192	1.164	1.129	1.091
36.5	0.90	2.413	2.42	1.164	1.162	1.156	1.228	1.205	1.179	1.143	1.106
40.5	1.00	2.403	2.411	1.172	1.169	1.164	1.24	1.219	1.193	1.158	1.121
44.5	1.10	2.391	2.4	1.179	1.176	1.171	1.252	1.231	1.206	1.171	1.135
49.0	1.21	2.378	2.388	1.186	1.184	1.178	1.264	1.244	1.22	1.185	1.15
57.0	1.40	2.36	2.371	1.196	1.194	1.188	1.281	1.263	1.239	1.206	1.169
65.5	1.60	2.343	2.357	1.207	1.205	1.199	1.3	1.282	1.26	1.226	1.192
74.0	1.81	2.328	2.342	1.216	1.214	1.209	1.315	1.298	1.276	1.244	1.208
82.0	2.00	2.316	2.331	1.222	1.22	1.215	1.326	1.311	1.289	1.258	1.222
103.5	2.50	2.288	2.305	1.237	1.235	1.23	1.351	1.337	1.318	1.286	1.253
125.0	3.00	2.265	2.285	1.248	1.247	1.242	1.371	1.359	1.34	1.31	1.275
169.0	4.00	2.235	2.255	1.267	1.266	1.261	1.404	1.394	1.375	1.348	1.312
214.5	5.00	2.21	2.232	1.281	1.28	1.275	1.428	1.42	1.403	1.374	1.341

c) Titration curve at 366 nm



Binding constants K derived from simultaneous fitting of 1:1 and 1:2 models to ten selected wavelengths using HypSpec:

$\log K_{1:1} = 4.779$
$\log K_{1:2} = 3.379$

Molar absorption coefficients derived from simultaneous fitting of 1:1 and 1:2 models to ten selected wavelengths using HypSpec:

	Wavelength [nm]									
	303	303.5	349.5	350	350.5	365.5	366	366.5	367	367.5
L [$M^{-1}cm^{-1}$]	25712	25624	10751	10701	10646	10724	10375	10023	9596	9195
L×PhCOO [$M^{-1}cm^{-1}$]	20444	20759	13725	13726	13685	15839	15859	15747	15519	15197
L×$(PhCOO)_2$ [$M^{-1}cm^{-1}$]	23334	23490	12124	12108	12052	13103	12943	12729	12411	12060

d) Binding constants K derived from the experiment repeated according to the same methodology:

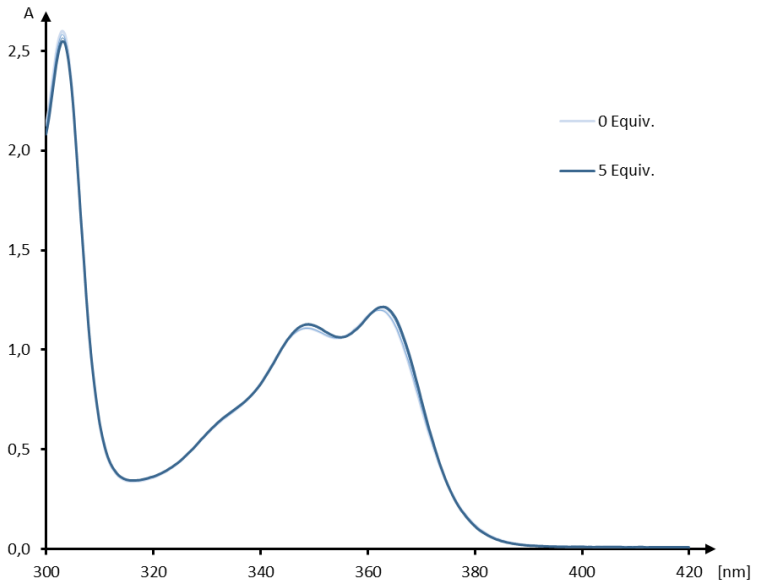
$\log K_{1:1} = 4.783$
$\log K_{1:2} = 3.489$

e) Binding constants averaged from the above two experiments:

$\log K_{1:1} = 4.781$
$\log K_{1:2} = 3.434$

2.3.4. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO + 0.5% H_2O with 0.015 M solution of TBACl (dissolved in the solution of receptor **A**).

a) UV-Vis spectra



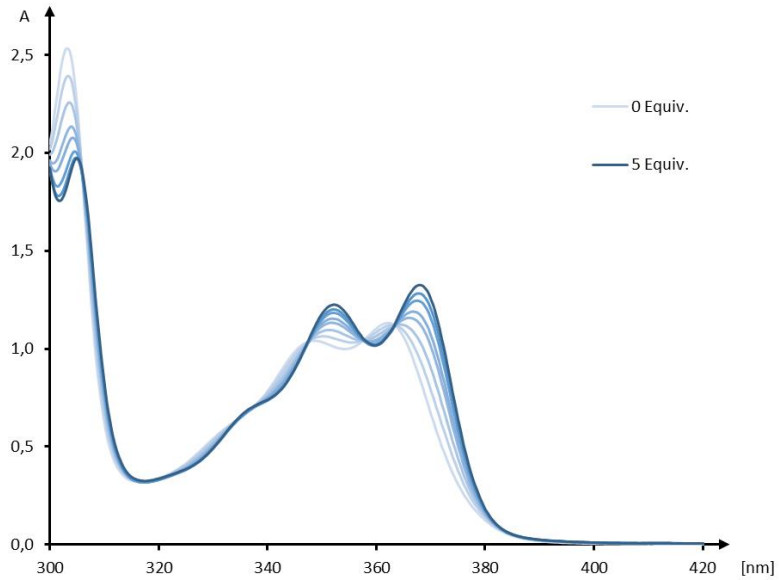
b) Raw data

Added volume of titrant solution [µL]	Equivalents of TBACl	Wavelength [nm]									
		303	303.5	349	349.5	350	364	364.5	365	365.5	366
		Absorbance									
0.0	0.00	2.599	2.583	1.107	1.105	1.100	1.171	1.153	1.128	1.100	1.066
4.0	0.10	2.596	2.578	1.107	1.105	1.100	1.171	1.151	1.128	1.098	1.066
8.0	0.20	2.592	2.574	1.107	1.105	1.101	1.171	1.152	1.129	1.100	1.067
12.0	0.30	2.584	2.568	1.108	1.106	1.102	1.171	1.153	1.130	1.101	1.068
16.0	0.40	2.584	2.566	1.109	1.107	1.103	1.173	1.155	1.132	1.104	1.071
20.0	0.50	2.585	2.569	1.111	1.109	1.104	1.177	1.159	1.137	1.108	1.077
24.0	0.60	2.582	2.567	1.112	1.110	1.106	1.178	1.16	1.138	1.111	1.079
28.5	0.71	2.574	2.561	1.119	1.117	1.112	1.188	1.170	1.149	1.121	1.091
32.5	0.80	2.565	2.553	1.124	1.122	1.118	1.193	1.178	1.157	1.130	1.099
36.5	0.90	2.551	2.542	1.126	1.124	1.120	1.199	1.184	1.165	1.139	1.109
40.5	1.00	2.546	2.537	1.129	1.127	1.123	1.203	1.190	1.171	1.147	1.117

Changes are too small to fit any model.

2.3.5. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO/10% H_2O with 0.0075 M solution of $(TBA)_2SO_4$ (dissolved in the solution of receptor **A**).

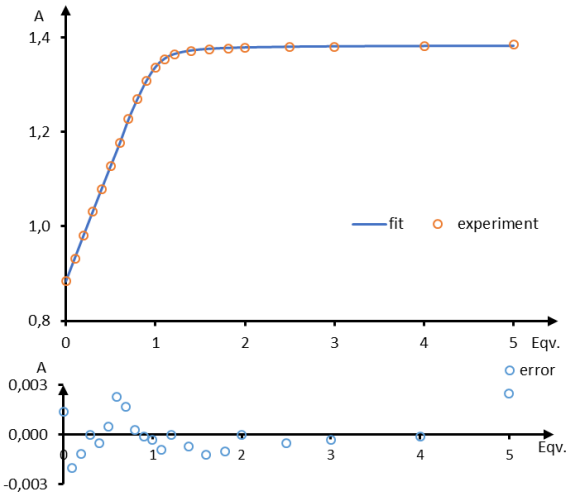
a) UV-Vis spectra



b) Raw data

Added volume of titrant solution [µL]	Equivalents of $(TBA)_2SO_4$	Wavelength [nm]									
		303	303.5	352	352.5	353	368	368.5	369	369.5	370
		Absorbance									
0.0	0.00	2.659	2.646	1.068	1.063	1.059	0.885	0.839	0.792	0.744	0.698
4.0	0.10	2.587	2.583	1.087	1.082	1.078	0.931	0.889	0.845	0.799	0.754
8.0	0.20	2.516	2.517	1.107	1.103	1.099	0.981	0.943	0.902	0.858	0.814
12.0	0.30	2.440	2.450	1.128	1.124	1.120	1.031	0.997	0.959	0.917	0.874
16.0	0.40	2.365	2.381	1.149	1.145	1.140	1.079	1.049	1.014	0.975	0.934
20.0	0.50	2.289	2.312	1.169	1.166	1.161	1.128	1.102	1.070	1.034	0.992
24.0	0.60	2.215	2.244	1.190	1.188	1.182	1.177	1.154	1.126	1.091	1.052
28.5	0.71	2.131	2.167	1.211	1.209	1.204	1.228	1.211	1.184	1.153	1.115
32.5	0.80	2.063	2.104	1.229	1.227	1.221	1.270	1.255	1.233	1.203	1.166
36.5	0.90	2.002	2.048	1.246	1.244	1.239	1.308	1.297	1.277	1.249	1.213
40.5	1.00	1.956	2.006	1.258	1.256	1.250	1.337	1.328	1.310	1.283	1.248
44.5	1.10	1.928	1.979	1.265	1.264	1.258	1.354	1.347	1.330	1.304	1.270
49.0	1.21	1.912	1.963	1.270	1.269	1.263	1.365	1.358	1.342	1.317	1.283
57.0	1.40	1.900	1.953	1.272	1.272	1.266	1.372	1.366	1.351	1.326	1.292
65.5	1.60	1.896	1.950	1.274	1.273	1.268	1.375	1.369	1.354	1.329	1.296
74.0	1.81	1.894	1.947	1.275	1.274	1.269	1.377	1.371	1.356	1.332	1.298
82.0	2.00	1.893	1.946	1.276	1.275	1.270	1.379	1.373	1.358	1.335	1.300
103.5	2.50	1.891	1.944	1.276	1.275	1.270	1.380	1.374	1.360	1.336	1.302
125.0	3.00	1.891	1.944	1.277	1.276	1.270	1.381	1.375	1.361	1.337	1.304
169.0	4.00	1.889	1.942	1.277	1.277	1.271	1.382	1.377	1.363	1.339	1.306
214.5	5.00	1.889	1.944	1.279	1.278	1.273	1.385	1.380	1.366	1.343	1.309

c) Titration curve at 368 nm



Binding constant K derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

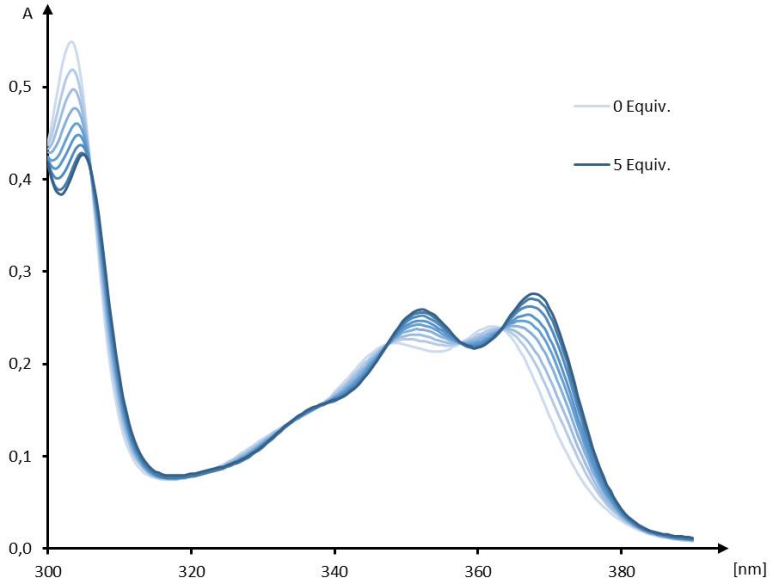
$\log K_{1:1} = 6.029$

Molar absorption coefficients derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

	Wavelength [nm]									
	303	303.5	352	352.5	353	368	368.5	369	369.5	370
L [$M^{-1}cm^{-1}$]	26667	26564	10664	10612	10571	8835	8376	7899	7413	6948
$LxSO_4^{2-}$ [$M^{-1}cm^{-1}$]	18855	19401	12776	12768	12711	13836	13783	13638	13398	13061

2.3.6. UV-Vis titration of $2x10^{-5}$ M solution of receptor **A** in DMSO/10% H_2O with 0.0015 M solution of $(TBA)_2SO_4$ (dissolved in the solution of receptor **A**).

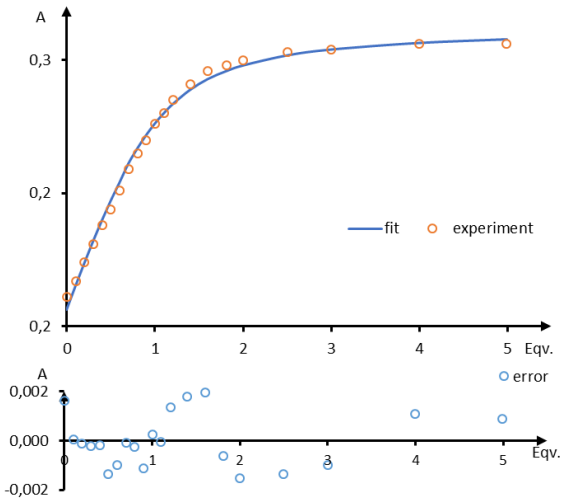
a) UV-Vis spectra



b) Raw data

Added volume of titrant solution [µL]	Equivalents of $(TBA)_2SO_4$	Wavelength [nm]									
		303	303.5	352	352.5	353	367.5	368	368.5	369	369.5
		Absorbance									
0.0	0.00	0.548	0.549	0.217	0.216	0.215	0.19	0.181	0.173	0.163	0.154
4.0	0.10	0.538	0.540	0.220	0.218	0.218	0.195	0.187	0.179	0.169	0.161
8.0	0.20	0.528	0.529	0.222	0.222	0.221	0.201	0.194	0.186	0.177	0.169
12.0	0.30	0.516	0.519	0.225	0.225	0.224	0.208	0.201	0.194	0.185	0.177
16.0	0.40	0.505	0.509	0.229	0.228	0.227	0.214	0.208	0.201	0.193	0.186
20.0	0.50	0.493	0.498	0.232	0.231	0.230	0.220	0.214	0.209	0.201	0.194
24.0	0.60	0.483	0.487	0.234	0.234	0.233	0.226	0.221	0.216	0.209	0.202
28.5	0.71	0.470	0.476	0.237	0.237	0.236	0.233	0.229	0.224	0.217	0.211
32.5	0.80	0.461	0.467	0.24	0.240	0.239	0.239	0.235	0.231	0.224	0.218
36.5	0.90	0.451	0.458	0.243	0.242	0.241	0.244	0.240	0.237	0.231	0.225
40.5	1.00	0.443	0.450	0.245	0.245	0.243	0.248	0.246	0.242	0.237	0.231
44.5	1.10	0.435	0.443	0.247	0.247	0.246	0.253	0.250	0.247	0.242	0.237
49.0	1.21	0.427	0.436	0.249	0.249	0.248	0.257	0.255	0.252	0.248	0.242
57.0	1.40	0.418	0.427	0.252	0.252	0.250	0.262	0.261	0.259	0.255	0.250
65.5	1.60	0.411	0.420	0.254	0.254	0.253	0.267	0.266	0.264	0.260	0.255
74.0	1.81	0.405	0.415	0.255	0.255	0.253	0.269	0.268	0.267	0.263	0.259
82.0	2.00	0.403	0.413	0.256	0.256	0.255	0.271	0.270	0.269	0.265	0.261
103.5	2.50	0.399	0.409	0.257	0.257	0.255	0.273	0.273	0.272	0.268	0.264
125.0	3.00	0.398	0.408	0.258	0.258	0.257	0.274	0.274	0.273	0.270	0.265
169.0	4.00	0.397	0.407	0.259	0.259	0.257	0.276	0.276	0.275	0.272	0.267
214.5	4.99	0.397	0.407	0.259	0.259	0.257	0.276	0.276	0.275	0.272	0.268

c) Titration curve at 368 nm



Binding constant K derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

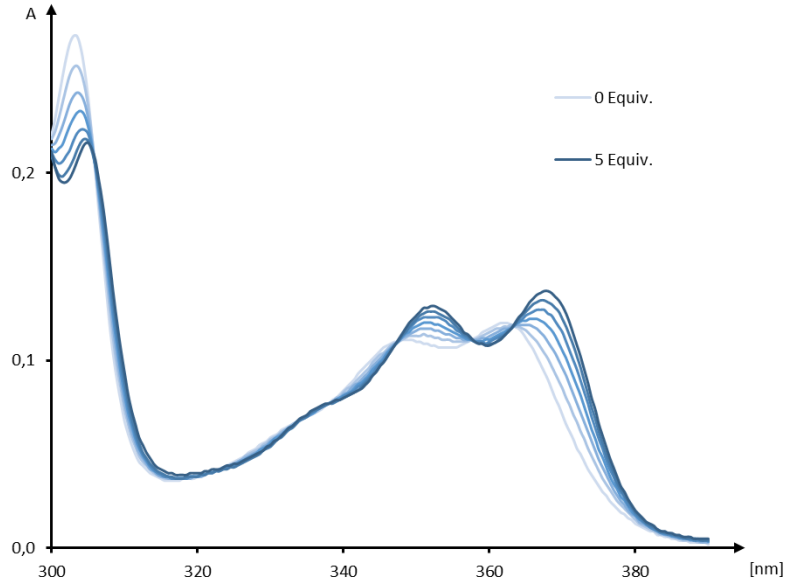
$\log K_{1:1} = 5.456$

Molar absorption coefficients derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

	Wavelength [nm]									
	303	303.5	352	352.5	353	367.5	368	368.5	369	369.5
L [$M^{-1}cm^{-1}$]	27766	27790	10732	10683	10655	8815	8371	7842	7402	6889
$LxSO_4^{2-}$ [$M^{-1}cm^{-1}$]	19208	19756	13067	13076	12991	14116	14098	13962	13762	13403

2.3.7. UV-Vis titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with 0.00075 M solution of $(TBA)_2SO_4$ (dissolved in the solution of receptor **A**).

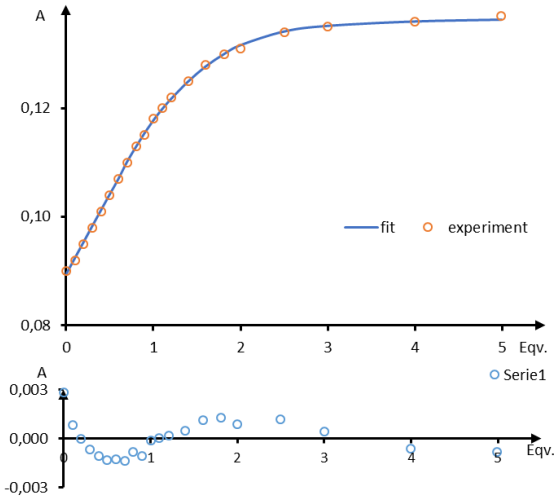
a) UV-Vis spectra



b) Raw data

Added volume of titrant solution [µL]	Equivalents of $(TBA)_2SO_4$	Wavelength [nm]									
		303	303.5	352	352.5	353	367.5	368	368.5	369	369.5
		Absorbance									
0.0	0.00	0.273	0.273	0.108	0.108	0.107	0.094	0.090	0.085	0.080	0.076
4.0	0.10	0.270	0.270	0.109	0.109	0.108	0.097	0.092	0.088	0.083	0.079
8.0	0.20	0.265	0.266	0.110	0.110	0.109	0.099	0.095	0.091	0.086	0.082
12.0	0.30	0.261	0.262	0.112	0.111	0.110	0.102	0.098	0.094	0.090	0.086
16.0	0.40	0.256	0.257	0.113	0.112	0.112	0.104	0.101	0.097	0.093	0.089
20.0	0.50	0.251	0.252	0.114	0.114	0.113	0.107	0.104	0.101	0.097	0.093
24.0	0.60	0.246	0.248	0.115	0.115	0.115	0.110	0.107	0.104	0.100	0.096
28.5	0.71	0.241	0.243	0.117	0.116	0.116	0.113	0.110	0.107	0.104	0.100
32.5	0.80	0.237	0.239	0.118	0.118	0.117	0.115	0.113	0.110	0.107	0.103
36.5	0.90	0.232	0.235	0.119	0.118	0.118	0.117	0.115	0.113	0.110	0.106
40.5	1.00	0.229	0.232	0.120	0.119	0.119	0.120	0.118	0.116	0.113	0.109
44.5	1.10	0.225	0.229	0.121	0.121	0.120	0.122	0.120	0.118	0.115	0.112
49.0	1.21	0.221	0.225	0.122	0.122	0.121	0.123	0.122	0.121	0.118	0.115
57.0	1.40	0.217	0.221	0.123	0.123	0.123	0.127	0.125	0.124	0.121	0.118
65.5	1.60	0.212	0.217	0.124	0.124	0.124	0.129	0.128	0.127	0.124	0.122
74.0	1.81	0.209	0.214	0.126	0.126	0.125	0.131	0.130	0.129	0.127	0.124
82.0	2.00	0.207	0.212	0.126	0.126	0.125	0.132	0.131	0.130	0.128	0.126
103.5	2.50	0.204	0.209	0.127	0.127	0.127	0.134	0.134	0.133	0.131	0.129
125.0	3.00	0.202	0.207	0.128	0.128	0.127	0.135	0.135	0.134	0.132	0.130
169.0	4.00	0.201	0.206	0.128	0.128	0.128	0.136	0.136	0.136	0.134	0.132
214.5	4.99	0.201	0.206	0.129	0.129	0.128	0.137	0.137	0.136	0.134	0.132

c) Titration curve at 368 nm



Binding constant K derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

$\log K_{1:1} = 5.477$

Molar absorption coefficients derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

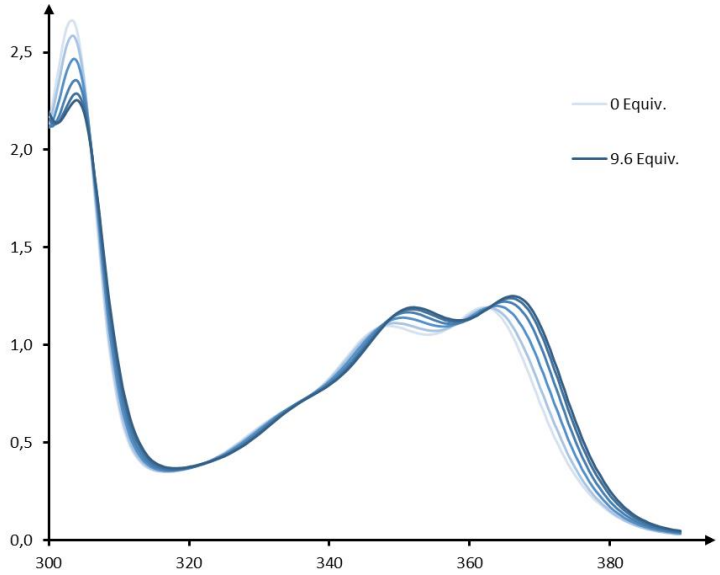
	Wavelength [nm]									
	303	303.5	352	352.5	353	367.5	368	368.5	369	369.5
L [$M^{-1}cm^{-1}$]	27737	27697	10676	10631	10555	8715	8234	7727	7260	6781
$LxSO_4^{2-}$ [$M^{-1}cm^{-1}$]	19081	19681	13072	13067	13027	14196	14200	14047	13850	13502

Binding constant averaged from two experiments at different concentrations:

$\log K_{1:1} = 5.467$

2.3.8. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO/10% H_2O with 0.0075 M solution of $TBAH_2PO_4$ (dissolved in the solution of receptor **A**).

a) UV-Vis spectra

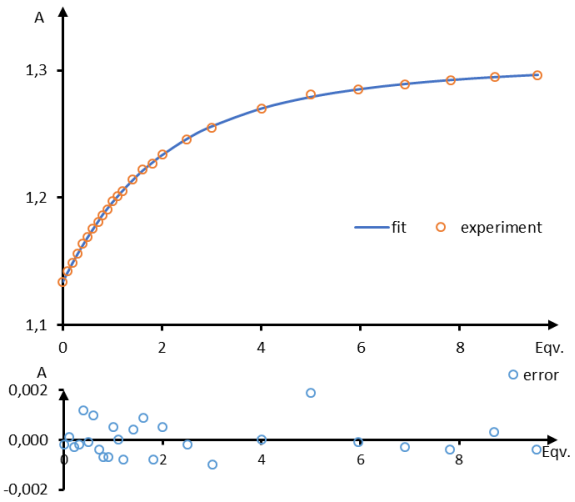


b) Raw data

Added volume of titrant solution [µL]	Equivalents of $TBAH_2PO_4$	Wavelength [nm]									
		303	303.5	351.5	352	352.5	365.5	366	366.5	367	367.5
		Absorbance									
0.0	0.00	2.659	2.658	1.070	1.064	1.059	1.084	1.048	1.014	0.970	0.930
4.0	0.10	2.644	2.644	1.076	1.070	1.065	1.092	1.058	1.024	0.982	0.943
8.0	0.20	2.629	2.630	1.081	1.075	1.070	1.099	1.067	1.034	0.994	0.956
12.0	0.30	2.616	2.618	1.086	1.080	1.075	1.106	1.076	1.044	1.005	0.967
16.0	0.40	2.601	2.606	1.090	1.085	1.080	1.114	1.083	1.054	1.014	0.979
20.0	0.50	2.586	2.593	1.095	1.090	1.084	1.119	1.091	1.061	1.024	0.989
24.0	0.60	2.574	2.583	1.099	1.094	1.088	1.126	1.098	1.070	1.034	0.999
28.5	0.71	2.558	2.569	1.102	1.097	1.091	1.131	1.105	1.077	1.043	1.008
32.5	0.80	2.546	2.557	1.106	1.101	1.095	1.136	1.111	1.084	1.051	1.018
36.5	0.90	2.535	2.547	1.109	1.104	1.099	1.141	1.118	1.091	1.059	1.026
40.5	1.00	2.524	2.536	1.114	1.108	1.103	1.147	1.124	1.099	1.067	1.036
44.5	1.10	2.512	2.525	1.117	1.112	1.107	1.151	1.130	1.105	1.075	1.043
49.0	1.21	2.501	2.517	1.119	1.114	1.109	1.155	1.134	1.112	1.081	1.051
57.0	1.40	2.482	2.499	1.126	1.121	1.116	1.164	1.146	1.123	1.096	1.066
65.5	1.60	2.463	2.481	1.130	1.126	1.121	1.172	1.153	1.134	1.106	1.079
74.0	1.81	2.445	2.467	1.135	1.131	1.126	1.177	1.162	1.143	1.116	1.091
82.0	2.00	2.431	2.453	1.140	1.136	1.130	1.184	1.168	1.151	1.126	1.101
103.5	2.50	2.397	2.422	1.148	1.145	1.140	1.196	1.184	1.169	1.147	1.124
125.0	3.00	2.370	2.396	1.155	1.152	1.147	1.205	1.196	1.182	1.164	1.141
169.0	4.00	2.328	2.354	1.167	1.165	1.160	1.220	1.215	1.205	1.190	1.169
214.5	5.00	2.296	2.324	1.175	1.174	1.170	1.231	1.229	1.221	1.209	1.192
259.0	5.96	2.270	2.299	1.179	1.178	1.175	1.235	1.234	1.228	1.217	1.203

304.0	6.90	2.255	2.282	1.182	1.182	1.18	1.239	1.239	1.235	1.225	1.213
349.0	7.82	2.241	2.266	1.185	1.185	1.183	1.242	1.243	1.240	1.232	1.220
394.0	8.71	2.231	2.256	1.189	1.189	1.188	1.245	1.247	1.245	1.238	1.228
439.0	9.57	2.223	2.246	1.191	1.192	1.190	1.246	1.250	1.248	1.243	1.232

c) Titration curve at 365.5 nm



Binding constants K derived from simultaneous fitting of 1:1 and 1:2 models to ten selected wavelengths using HypSpec:

$\log K_{1:1} = 3.936$
$\log K_{1:2} = 3.224$

Molar absorption coefficients derived from simultaneous fitting of 1:1 and 1:2 models to ten selected wavelengths using HypSpec:

	Wavelength [nm]									
	303	303.5	351.5	352	352.5	365.5	366	366.5	367	367.5
L [$M^{-1}cm^{-1}$]	26616	26588	10709	10649	10600	10842	10488	10138	9705	9306
L×$H_2PO_4^-$ [$M^{-1}cm^{-1}$]	21192	21314	12063	12113	12147	12571	12680	12752	12789	12784
L× $(H_2PO_4^-)_2$ [$M^{-1}cm^{-1}$]	22971	23427	11850	11810	11734	12552	12534	12447	12310	12118

d) Binding constants K derived from the experiment repeated according to the same methodology:

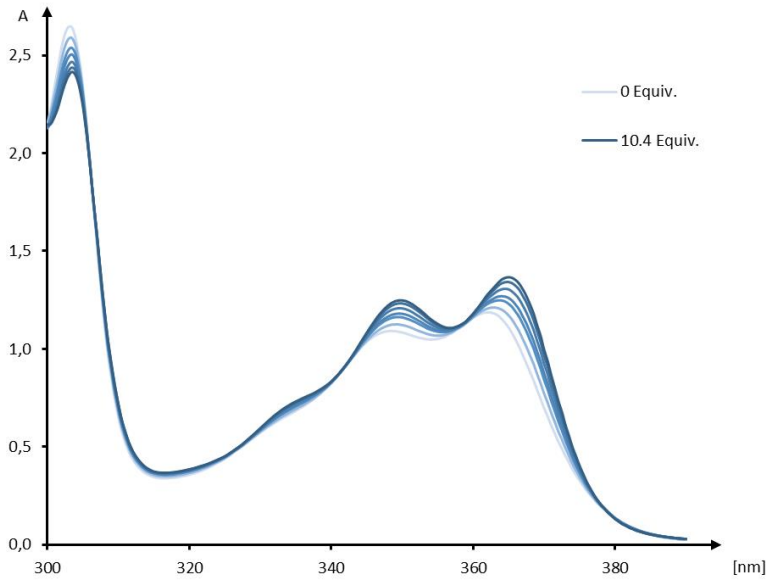
$\log K_{1:1} = 4.037$
$\log K_{1:2} = 3.334$

d) Binding constants averaged from the two experiments:

$\log K_{1:1} = 3.987$
$\log K_{1:2} = 3.279$

2.3.9. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO/10% H_2O with 0.0075 M solution of TBAPhCOO (dissolved in the solution of receptor **A**).

a) UV-Vis spectra

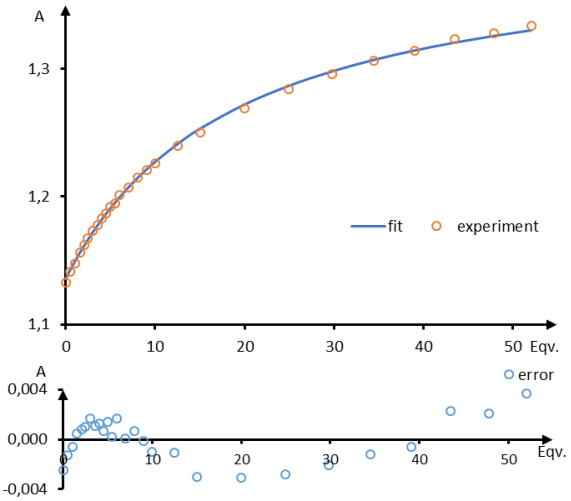


b) Raw data

Added volume of titrant solution [µL]	Equivalents of TBAPhCOO	Wavelength [nm]									
		303	303.5	349	349.5	350	364	364.5	365	365.5	366
		Absorbance									
0.0	0.00	2.645	2.642	1.090	1.087	1.083	1.153	1.133	1.109	1.079	1.045
4.0	0.50	2.638	2.636	1.097	1.094	1.090	1.161	1.143	1.119	1.092	1.057
8.0	1.00	2.631	2.629	1.102	1.100	1.096	1.168	1.152	1.129	1.102	1.069
12.5	1.56	2.624	2.621	1.108	1.106	1.102	1.176	1.160	1.138	1.113	1.080
16.5	2.05	2.615	2.614	1.112	1.111	1.107	1.182	1.167	1.146	1.121	1.090
20.0	2.48	2.607	2.608	1.116	1.114	1.111	1.187	1.172	1.153	1.128	1.098
24.0	2.98	2.602	2.603	1.120	1.118	1.116	1.193	1.178	1.159	1.135	1.105
28.5	3.53	2.594	2.596	1.124	1.123	1.120	1.198	1.185	1.167	1.144	1.115
32.5	4.02	2.585	2.589	1.127	1.127	1.124	1.203	1.191	1.173	1.151	1.122
36.5	4.51	2.580	2.583	1.131	1.130	1.128	1.207	1.196	1.179	1.157	1.129
40.5	5.00	2.575	2.579	1.134	1.134	1.131	1.212	1.201	1.184	1.163	1.135
44.5	5.48	2.569	2.573	1.138	1.137	1.135	1.215	1.206	1.189	1.169	1.141
49.0	6.03	2.564	2.569	1.142	1.141	1.138	1.221	1.211	1.196	1.176	1.148
57.0	6.99	2.551	2.557	1.146	1.146	1.144	1.227	1.219	1.205	1.186	1.160
65.5	8.01	2.543	2.549	1.151	1.152	1.150	1.235	1.227	1.214	1.196	1.171
74.0	9.03	2.532	2.542	1.157	1.157	1.155	1.241	1.234	1.222	1.205	1.181
82.0	9.98	2.526	2.536	1.161	1.161	1.160	1.246	1.241	1.229	1.213	1.188
103.5	12.51	2.507	2.519	1.171	1.172	1.171	1.260	1.256	1.247	1.232	1.210
125.0	15.00	2.493	2.506	1.179	1.181	1.180	1.270	1.268	1.261	1.247	1.226
169.0	20.00	2.469	2.484	1.194	1.196	1.194	1.289	1.290	1.285	1.273	1.254
214.0	24.97	2.451	2.467	1.205	1.208	1.207	1.304	1.307	1.304	1.293	1.276

259.0	29.80	2.438	2.455	1.215	1.217	1.217	1.316	1.320	1.319	1.311	1.295
304.0	34.50	2.427	2.445	1.222	1.225	1.225	1.326	1.332	1.331	1.324	1.309
349.0	39.08	2.418	2.436	1.228	1.232	1.232	1.334	1.340	1.341	1.335	1.321
394.0	43.53	2.410	2.429	1.235	1.239	1.239	1.343	1.351	1.352	1.348	1.334
439.0	47.87	2.403	2.421	1.239	1.243	1.243	1.348	1.357	1.359	1.355	1.343
484.0	52.10	2.396	2.416	1.244	1.248	1.248	1.354	1.363	1.367	1.363	1.352

c) Titration curve at 364 nm



Binding constant K derived from simultaneous fitting of 1:1 to ten selected wavelengths using HypSpec:

$\log K_{1:1} = 2.742$

Molar absorption coefficients derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

	Wavelength [nm]									
	303.0	303.5	349.0	349.5	350.0	364.0	364.5	365.0	365.5	366.0
L [$M^{-1}cm^{-1}$]	26458	26429	10918	10891	10853	11555	11366	11123	10841	10496
L×PhCOO [$M^{-1}cm^{-1}$]	23075	23367	12930	12995	13013	14189	14380	14508	14555	14514

d) Binding constant K derived from the experiment repeated according to the same methodology:

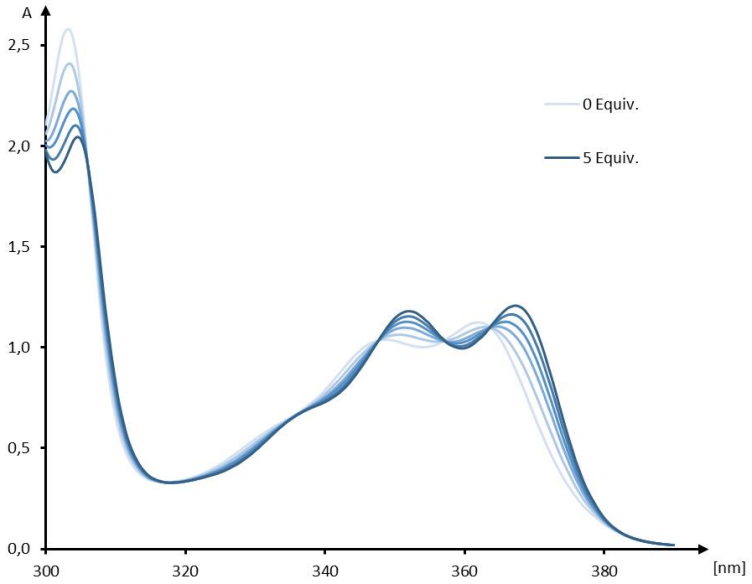
$\log K_{1:1} = 3.037$

e) Binding constant averaged from the two experiments:

$\log K_{1:1} = 2.890$

2.3.10. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO/20% H_2O with 0.0075 M solution of $(TBA)_2SO_4$ (dissolved in the solution of receptor **A**).

a) UV-Vis spectra

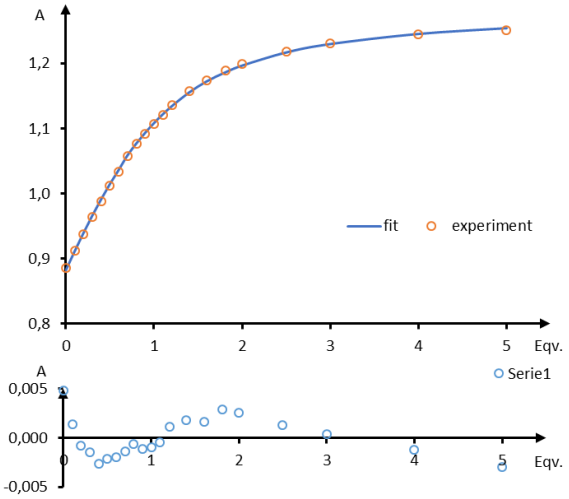


b) Raw data

Added volume of titrant solution [µL]	Equivalents of $(TBA)_2SO_4$	Wavelength [nm]									
		303	303.5	352	352.5	353	367.5	368	368.5	369	369.5
		Absorbance									
0.0	0.00	2.577	2.572	1.013	1.009	1.005	0.877	0.836	0.794	0.751	0.706
4.0	0.10	2.534	2.530	1.025	1.020	1.017	0.90	0.862	0.822	0.779	0.736
8.0	0.20	2.488	2.490	1.036	1.031	1.028	0.924	0.888	0.850	0.809	0.768
12.0	0.30	2.443	2.448	1.047	1.043	1.039	0.947	0.914	0.877	0.839	0.798
16.0	0.40	2.401	2.410	1.059	1.055	1.050	0.969	0.938	0.905	0.867	0.827
20.0	0.50	2.359	2.372	1.069	1.066	1.061	0.991	0.962	0.930	0.894	0.856
24.0	0.60	2.323	2.339	1.079	1.075	1.071	1.011	0.984	0.954	0.919	0.881
28.5	0.71	2.283	2.302	1.089	1.086	1.081	1.032	1.007	0.979	0.945	0.909
32.5	0.80	2.251	2.273	1.097	1.095	1.089	1.049	1.026	0.999	0.967	0.931
36.5	0.90	2.221	2.244	1.106	1.102	1.097	1.064	1.042	1.018	0.986	0.951
40.5	1.00	2.195	2.221	1.112	1.109	1.104	1.077	1.057	1.032	1.003	0.968
44.5	1.10	2.171	2.199	1.119	1.116	1.111	1.089	1.071	1.048	1.019	0.986
49.0	1.21	2.146	2.174	1.126	1.123	1.118	1.103	1.086	1.064	1.037	1.003
57.0	1.40	2.111	2.142	1.136	1.133	1.128	1.122	1.107	1.087	1.060	1.028
65.5	1.60	2.082	2.115	1.144	1.142	1.136	1.137	1.124	1.105	1.080	1.048
74.0	1.81	2.058	2.094	1.151	1.149	1.143	1.151	1.139	1.121	1.097	1.066
82.0	2.00	2.041	2.077	1.156	1.154	1.148	1.160	1.149	1.132	1.109	1.078
103.5	2.50	2.007	2.046	1.165	1.163	1.158	1.177	1.168	1.153	1.130	1.101

125.0	3.00	1.987	2.028	1.171	1.168	1.163	1.188	1.180	1.166	1.144	1.115
169.0	4.00	1.962	2.004	1.176	1.175	1.169	1.200	1.194	1.181	1.160	1.133
214.5	5.00	1.948	1.990	1.180	1.178	1.173	1.207	1.201	1.189	1.169	1.142

c) Titration curve at 368 nm



Binding constant K derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

$\log K_{1:1} = 4.466$

Molar absorption coefficients derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

	Wavelength [nm]									
	303	303.5	352	352.5	353	367.5	368	368.5	369	369.5
L [$M^{-1}cm^{-1}$]	25851	25798	10095	10047	10011	8312	7886	7442	6995	6551
$LxSO_4^{2-}$ [$M^{-1}cm^{-1}$]	18905	19387	11951	11935	11875	12354	12257	12076	11814	11466

d) Binding constant K derived from the experiment repeated according to the same methodology:

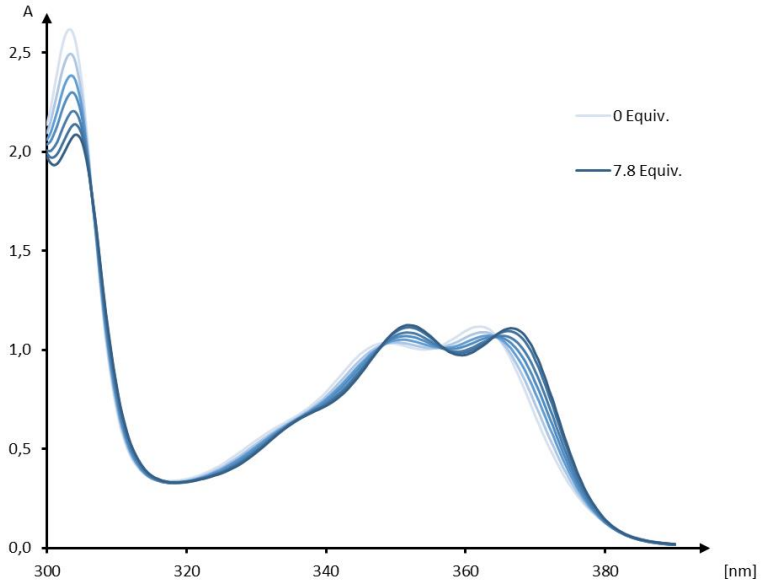
$\log K_{1:1} = 4.361$

e) Binding constant averaged from the two experiments:

$\log K_{1:1} = 4.414$

2.3.11. UV-Vis titration of 10^{-4} M solution of receptor **A** in DMSO/25% H_2O with 0.0075 M solution of $(TBA)_2SO_4$ (dissolved in the solution of receptor **A**).

a) UV-Vis spectra

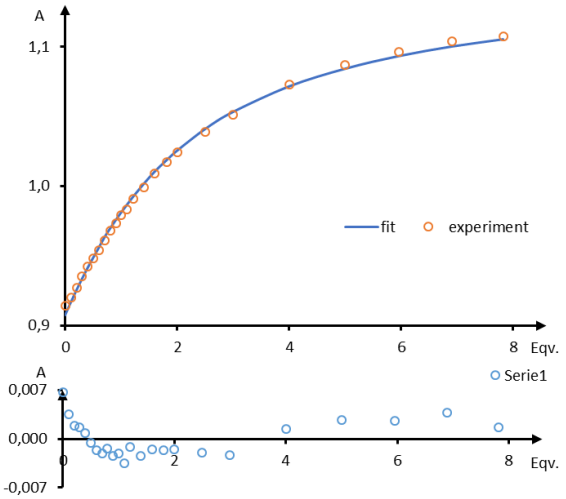


b) Raw data

Added volume of titrant solution [µL]	Equivalents of $(TBA)_2SO_4$	Wavelength [nm]									
		303	303.5	352	352.5	353	367	367.5	368	368.5	369
		Absorbance									
0.0	0.00	2.613	2.613	1.012	1.008	1.005	0.914	0.877	0.836	0.796	0.752
4.0	0.10	2.581	2.584	1.015	1.011	1.007	0.920	0.884	0.845	0.806	0.762
8.0	0.20	2.556	2.56	1.019	1.015	1.011	0.927	0.894	0.855	0.818	0.775
12.0	0.30	2.531	2.538	1.022	1.018	1.015	0.935	0.902	0.865	0.828	0.785
16.0	0.40	2.506	2.512	1.025	1.022	1.018	0.942	0.910	0.874	0.838	0.797
20.0	0.50	2.484	2.493	1.029	1.025	1.021	0.948	0.917	0.882	0.847	0.807
24.0	0.60	2.463	2.471	1.032	1.028	1.024	0.954	0.925	0.891	0.856	0.816
28.5	0.71	2.440	2.450	1.036	1.033	1.028	0.961	0.934	0.900	0.867	0.827
32.5	0.80	2.422	2.434	1.039	1.036	1.032	0.968	0.940	0.908	0.875	0.837
36.5	0.90	2.404	2.418	1.043	1.039	1.035	0.973	0.947	0.915	0.883	0.845
40.5	1.00	2.387	2.401	1.046	1.042	1.038	0.979	0.954	0.923	0.892	0.854
44.5	1.10	2.37	2.384	1.048	1.044	1.040	0.983	0.958	0.929	0.898	0.860
49.0	1.21	2.353	2.369	1.053	1.050	1.045	0.991	0.967	0.938	0.908	0.871
57.0	1.40	2.326	2.343	1.057	1.054	1.049	0.999	0.977	0.949	0.920	0.884
65.5	1.60	2.302	2.320	1.063	1.060	1.056	1.009	0.987	0.961	0.933	0.899
74.0	1.81	2.277	2.297	1.068	1.065	1.061	1.017	0.997	0.972	0.945	0.911
82.0	2.00	2.254	2.275	1.072	1.069	1.064	1.024	1.005	0.981	0.955	0.922
103.5	2.50	2.213	2.236	1.082	1.079	1.074	1.039	1.024	1.001	0.977	0.945
125.0	3.00	2.175	2.201	1.088	1.086	1.081	1.051	1.036	1.016	0.992	0.963
169.0	4.00	2.130	2.159	1.103	1.101	1.096	1.073	1.062	1.044	1.024	0.994
214.5	5.00	2.094	2.124	1.113	1.110	1.105	1.087	1.077	1.062	1.042	1.015
259.0	5.96	2.069	2.100	1.118	1.115	1.110	1.096	1.087	1.073	1.055	1.029

304.0	6.90	2.049	2.082	1.123	1.121	1.115	1.104	1.097	1.084	1.066	1.041
349.0	7.82	2.033	2.065	1.124	1.122	1.117	1.107	1.101	1.089	1.072	1.046

c) Titration curve at 367 nm



Binding constant K derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

$\log K_{1:1} = 3.780$

Molar absorption coefficients derived from simultaneous fitting of 1:1 model to ten selected wavelengths using HypSpec:

	Wavelength [nm]									
	303	303.5	352	352.5	353	367.5	368	368.5	369	369.5
L [$M^{-1}cm^{-1}$]	26037	26052	10050	10009	9973	8705	8293	7895	7447	7023
LxSO_4^{2-} [$M^{-1}cm^{-1}$]	18971	19381	11484	11466	11408	11513	11454	11336	11128	10876

d) Binding constant K derived from the experiment repeated according to the same methodology:

$\log K_{1:1} = 3.685$

e) Binding constant averaged from the two experiments:

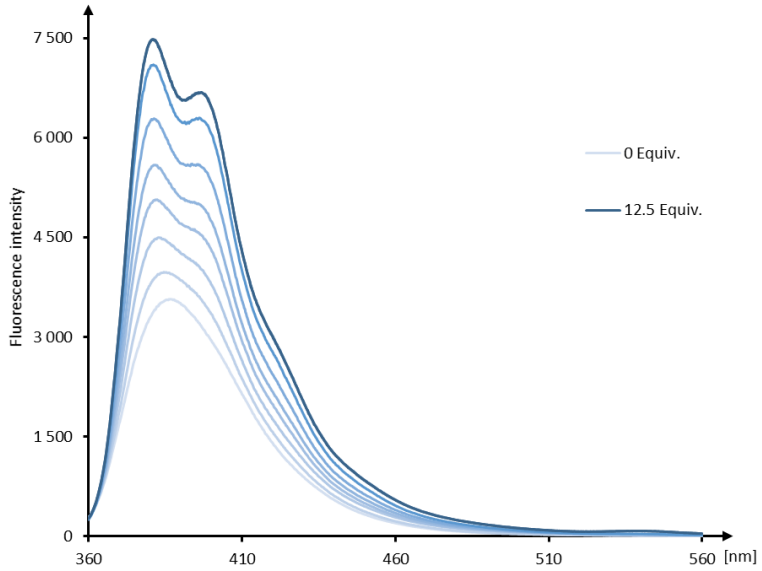
$\log K_{1:1} = 3.733$

2.4. Fluorescence titrations procedure.

To a solution of a host (2 mL, 10^{-5} M) in a fluorescence cuvette with screw-cap made of Quartz SUPRASIL (light path: 10 mm) appropriate aliquot of titrant (dissolved in water) followed by appropriate aliquot of the solution of receptor in DMSO to avoid dilution was added with a 100 µl gas-tight microsyringe. Fluorescence spectra were obtained on Hitachi F-7000. Excitation wavelength: 348 nm, scan speed: 240 nm/min, temperature: 25°C.

2.4.1. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with Na_2SO_4 (dissolved in water) and the solution of receptor in DMSO.

a) Fluorescence spectra

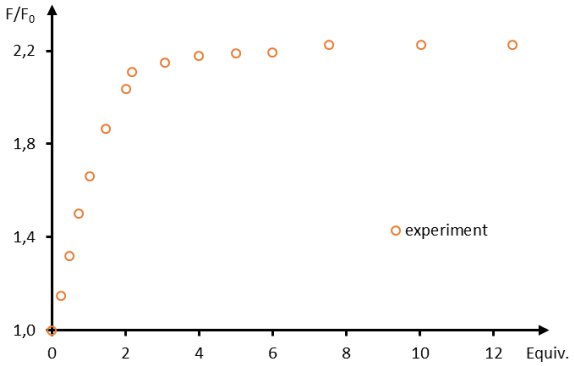


b) Raw data

Added volume of titrant solution [µL]	Equivalents of Na_2SO_4	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]										
			375	378	381	384	387	390	393	396	399	402	405
			Fluorescence intensity										
0.0	0.00	0.0	2647	3065	3360	3514	3561	3504	3364	3206	3015	2807	2569
2.0	0.25	18.0	3045	3563	3856	3962	3939	3849	3739	3607	3417	3180	2890
4.0	0.49	36.0	3531	4143	4431	4465	4374	4257	4172	4061	3875	3607	3249
6.0	0.73	54.0	4011	4731	5041	5005	4864	4707	4640	4564	4405	4110	3679
8.5	1.02	76.5	4448	5258	5579	5505	5285	5106	5046	5006	4864	4521	4035
12.5	1.47	112.5	5012	5960	6272	6135	5826	5610	5580	5580	5443	5075	4514
17.5	2.01	157.5	5464	6514	6843	6640	6273	6028	6008	6006	5895	5495	4884
22.0	2.18	198.0	5642	6703	7083	6857	6494	6242	6238	6292	6172	5764	5122
28.0	3.07	252.0	5773	6893	7224	6980	6571	6311	6305	6333	6231	5813	5174
38.0	3.99	342.0	5836	6967	7322	7081	6681	6432	6431	6491	6392	5969	5306
50.0	5.00	450.0	5873	6999	7361	7092	6696	6455	6455	6504	6403	5973	5314
63.0	5.99	567.0	5861	7002	7367	7124	6736	6495	6499	6584	6474	6051	5388

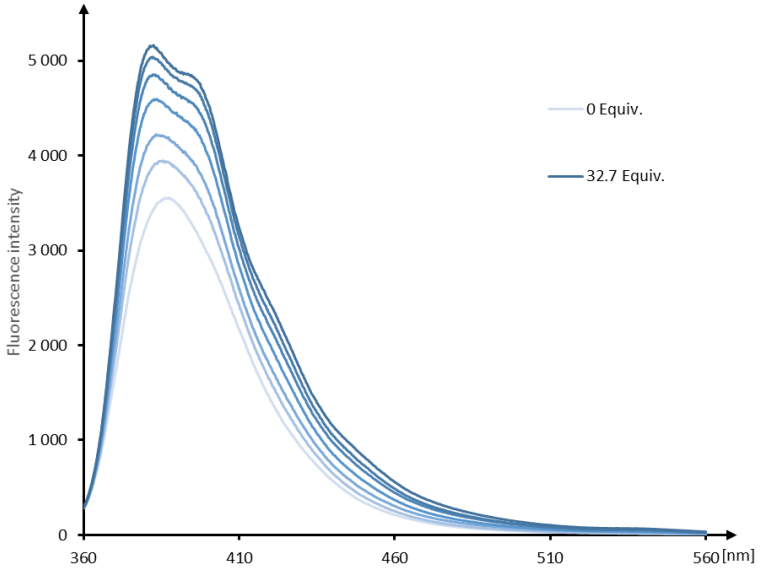
86.0	7.52	774.0	5928	7104	7477	7228	6833	6571	6582	6672	6572	6156	5467
134.0	10.03	1206.0	5926	7092	7478	7230	6831	6585	6599	6667	6590	6144	5478
200.0	12.50	1800.0	5945	7113	7473	7232	6848	6575	6604	6678	6561	6150	5486

c) Titration curve at 381 nm



2.4.2. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with NaH_2PO_4 (dissolved in water) and the solution of receptor in DMSO.

a) Fluorescence spectra

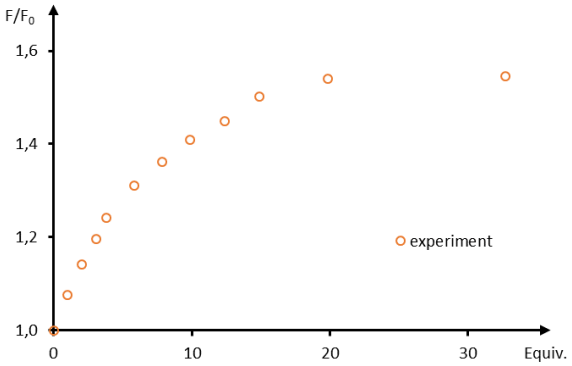


b) Raw data

Added volume of titrant solution [µL]	Equivalents of NaH_2PO_4	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]										
			375	378	381	384	387	390	393	396	399	402	405
			Fluorescence intensity										
0.0	0.00	0.0	2626	3056	3338	3504	3553	3492	3360	3199	3012	2814	2578
4.0	0.98	36.0	2847	3322	3590	3750	3753	3695	3578	3432	3246	3012	2758
8.5	2.04	76.5	3041	3537	3809	3932	3929	3857	3758	3624	3432	3191	2912
13.0	3.05	117.0	3201	3710	3993	4100	4082	4007	3906	3787	3594	3341	3031
16.5	3.80	157.5	3323	3868	4144	4216	4191	4113	4005	3897	3709	3453	3128

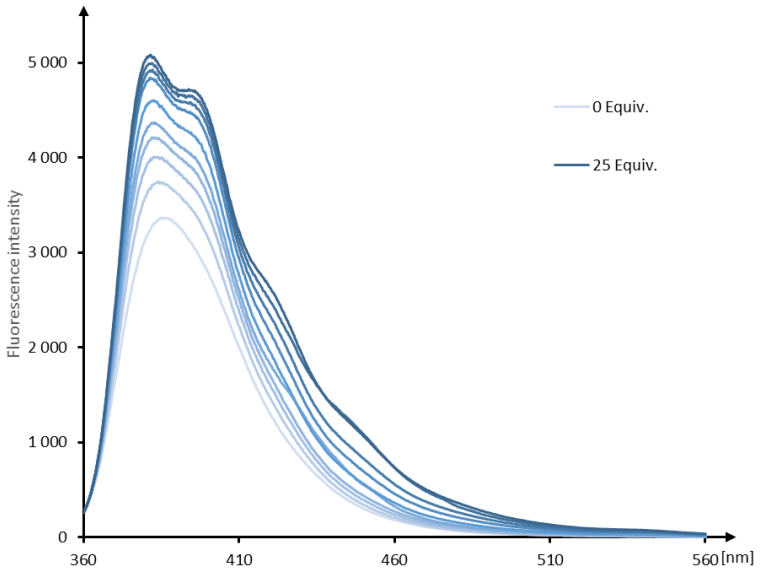
26.5	5.83	247.5	3530	4099	4373	4418	4375	4304	4217	4105	3928	3651	3297
37.5	7.87	346.5	3682	4283	4546	4573	4513	4422	4351	4273	4075	3792	3434
49.5	9.88	454.5	3835	4438	4703	4726	4640	4550	4495	4414	4221	3925	3553
66.0	12.36	603.0	3933	4567	4836	4832	4739	4643	4598	4514	4347	4044	3652
85.0	14.87	774.0	4080	4745	5010	4994	4884	4813	4759	4697	4518	4202	3792
132.5	19.87	1201.5	4210	4876	5142	5105	4981	4891	4858	4807	4631	4316	3895
266.0	32.71	1800.0	4229	4902	5156	5115	4969	4882	4838	4803	4645	4325	3909

c) Titration curve at 381 nm



2.4.3. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with NaH_2PO_4 (dissolved in water) and the solution of receptor in DMSO.

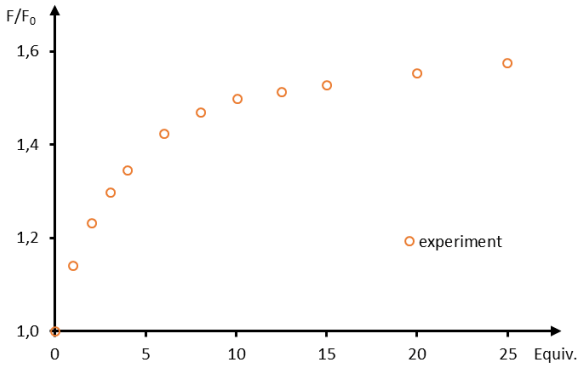
a) Fluorescence spectra



b) Raw data

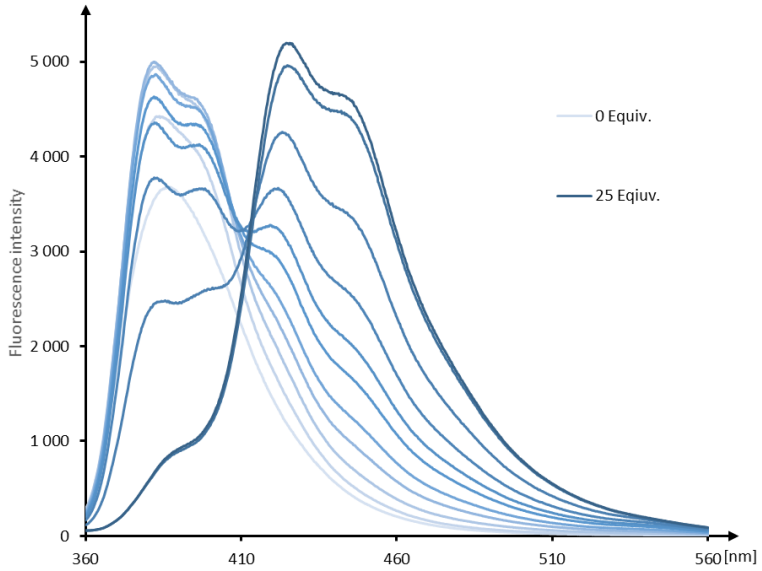
Added volume of titrant solution [µL]	Equivalents of NaH_2PO_4	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]										
			375	378	381	384	387	390	393	396	399	402	405
			Fluorescence intensity										
0.0	0.00	0.0	2547	2960	3216	3345	3364	3295	3178	3030	2860	2647	2413
4.0	0.98	36.0	2921	3403	3664	3738	3713	3623	3532	3397	3221	2997	2716
8.5	2.04	76.5	3171	3694	3958	4007	3953	3861	3773	3653	3488	3234	2928
13.0	3.05	117.0	3354	3905	4173	4202	4126	4032	3949	3844	3684	3422	3070
17.5	4.02	157.5	3494	4078	4326	4342	4250	4153	4073	3992	3821	3538	3194
27.5	6.04	247.5	3714	4318	4577	4563	4456	4356	4287	4212	4059	3760	3379
38.5	8.07	346.5	3837	4478	4726	4681	4565	4455	4393	4331	4184	3888	3496
50.5	10.08	454.5	3940	4576	4816	4767	4635	4537	4490	4428	4272	3977	3583
67.0	12.55	603.0	3965	4614	4863	4815	4673	4567	4534	4484	4340	4040	3641
86.0	15.04	774.0	4005	4665	4909	4859	4708	4601	4581	4549	4384	4105	3704
133.5	20.02	1201.5	4082	4741	4992	4911	4766	4687	4636	4622	4469	4183	3776
200.0	25.00	1800.0	4158	4831	5062	4989	4823	4718	4708	4690	4550	4253	3845

c) Titration curve at 381 nm



2.4.4. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with Na_2HPO_4 (dissolved in water) and the solution of receptor in DMSO.

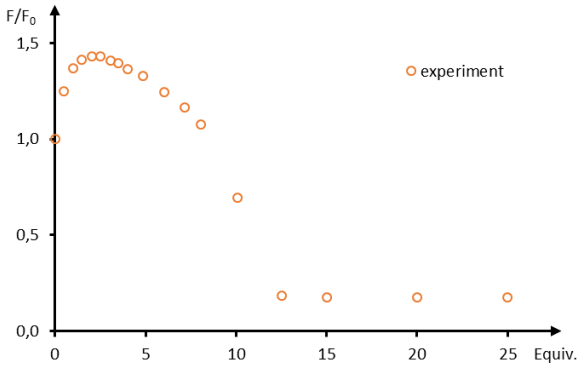
a) Fluorescence spectra



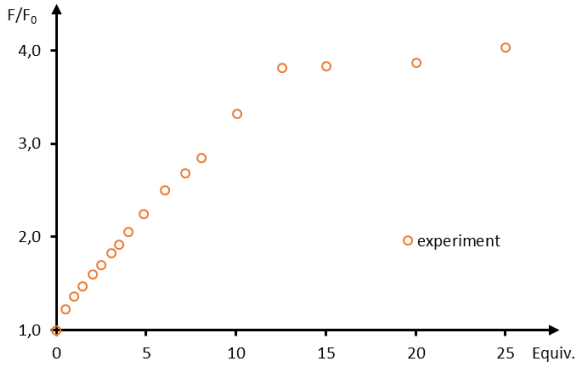
b) Raw data

Added volume of titrant solution [µL]	Equivalents of Na_2HPO_4	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]										
			375	381	385	390	400	410	420	425	430	440	450
			Fluorescence intensity										
0.0	0.00	0.0	2738	3471	3663	3614	3054	2227	1457	1165	932.7	568.1	338.6
2.0	0.50	18.0	3455	4344	4409	4264	3767	2650	1768	1438	1141	696.3	428.8
4.0	0.98	36.0	3785	4747	4743	4531	4104	2847	1947	1599	1282	791.3	513.2
6.0	1.46	54.0	3929	4911	4883	4653	4262	2974	2083	1741	1403	890.5	600.4
8.5	2.04	76.5	3964	4972	4917	4709	4347	3045	2236	1906	1560	1030	734.7
10.5	2.49	94.5	3962	4965	4912	4699	4347	3104	2370	2045	1691	1155	848.6
13.0	3.05	117.0	3900	4889	4840	4622	4326	3129	2501	2203	1841	1298	991.5
15.0	3.49	135.0	3837	4838	4777	4568	4292	3162	2610	2321	1963	1421	1104
17.5	4.02	157.5	3750	4741	4672	4478	4238	3185	2749	2489	2125	1585	1266
21.5	4.85	193.5	3635	4607	4542	4347	4170	3232	2976	2758	2382	1833	1501
27.5	6.04	247.5	3389	4329	4274	4099	4009	3258	3261	3098	2737	2181	1835
33.5	7.17	301.5	3148	4049	4009	3867	3828	3244	3467	3331	2975	2430	2087
38.5	8.06	349.5	2897	3741	3724	3602	3603	3220	3643	3570	3212	2689	2332
50.5	10.08	454.5	1783	2412	2472	2453	2596	2931	4133	4230	3936	3470	3133
67.0	12.55	603.0	365.8	648.4	814.7	929.6	1205	2442	4594	4938	4751	4451	4086
86.0	15.04	774.0	334.8	605.6	773.5	895.2	1162	2424	4587	4961	4794	4485	4129
133.5	20.02	1201.5	344.3	612.6	788.6	906	1181	2446	4645	4999	4821	4519	4161
200.0	25	1800.0	336.4	615	792.9	919.3	1209	2545	4833	5195	4997	4671	4300

c) Titration curve at 381 nm

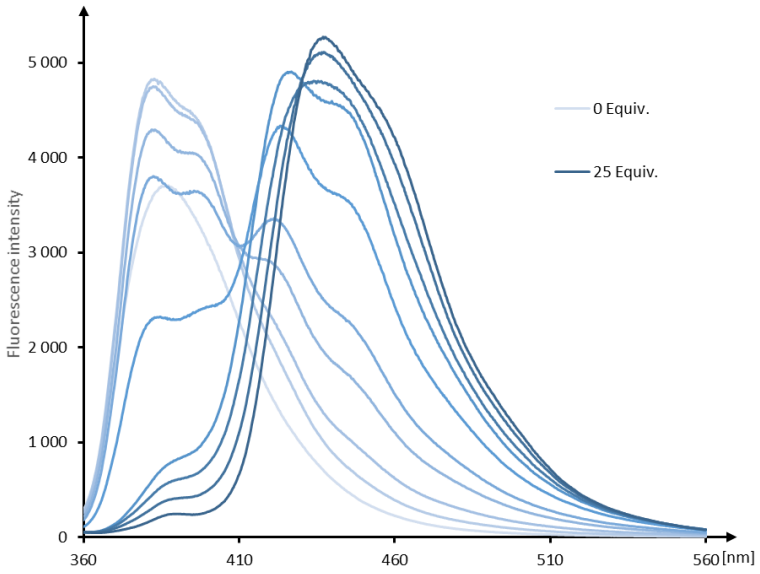


Titration curve at 423 nm



2.4.5. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with Na_3PO_4 (dissolved in water) and the solution of receptor in DMSO.

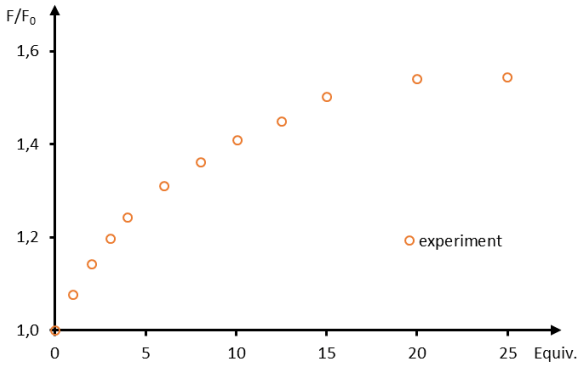
a) Fluorescencet spectra



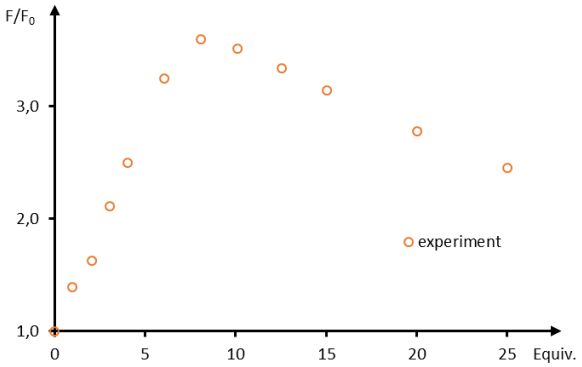
b) Raw data

Added volume of titrant solution [µL]	Equivalents of Na_3PO_4	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]										
			375	381	387	393	400	406	415	425	435	445	460
			Fluorescence intensity										
0.0	0.00	0.0	2769	3510	3703	3516	3082	2632	1861	1218	778	475.5	226.2
4.0	0.98	36.0	3812	4782	4706	4508	4174	3456	2421	1724	1110	737.3	391.3
8.5	2.04	76.5	3745	4707	4604	4435	4156	3470	2614	2048	1412	1041	620.1
13.0	3.05	117.0	3365	4266	4164	4051	3890	3371	2946	2710	2061	1708	1105
17.5	4.02	158.0	2937	3773	3687	3627	3561	3198	3184	3251	2598	2277	1510
27.5	6.04	248.0	1694	2258	2296	2321	2424	2536	3547	4312	3766	3549	2434
38.5	8.06	349.5	294.1	548.6	764.1	862.1	1075	1598	3422	4890	4640	4475	3178
50.5	10.08	454.5	275.1	511.5	713.2	807.3	1008	1508	3266	4818	4696	4533	3264
67.0	12.55	603.0	230	410	569.1	627.6	772.6	1153	2628	4439	4798	4619	3513
86.0	15.04	774.0	164.3	278.7	392	418.4	495.6	739.2	1906	4100	5087	4874	3934
133.5	20.02	1201.5	98.26	164.4	239.7	241.3	268.8	410.3	1349	3776	5220	4995	4212
200.0	25.00	1800.0	98.26	164.4	239.7	241.3	268.8	410.3	1349	3776	5220	4995	4212

c) Titration curve at 381 nm

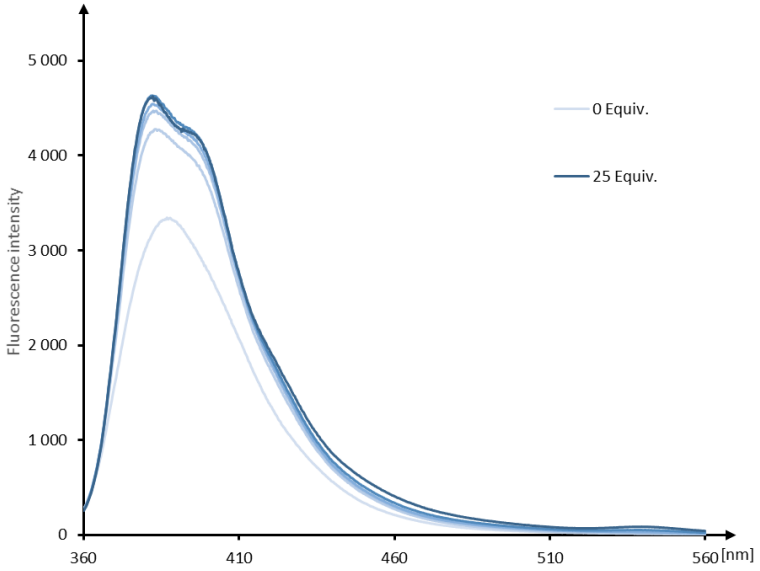


Titration curve at 423 nm



2.4.6. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with $NaHCO_3$ (dissolved in water) and the solution of receptor in DMSO.

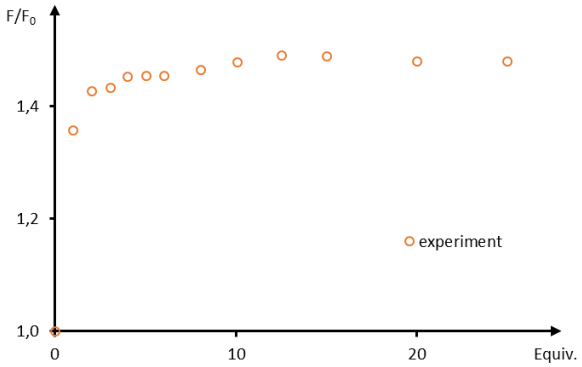
a) Fluorescent spectra



b) Raw data

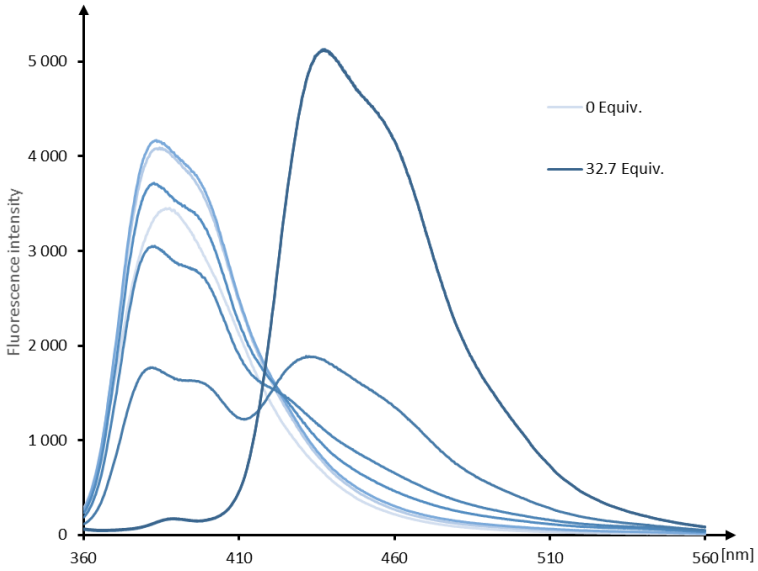
Added volume of titrant solution [µL]	Equivalents of $NaHCO_3$	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]									
			375	378	381	385	389	393	397	400	404	408
			Fluorescence intensity									
0.0	0.00	0.0	2447	2841	3111	3304	3313	3167	2954	2782	2509	2205
4.0	0.98	36.0	3359	3933	4222	4263	4138	4033	3900	3691	3295	2818
8.5	2.04	76.5	3544	4139	4436	4428	4297	4187	4051	3858	3435	2916
13.0	3.05	117.0	3572	4172	4458	4459	4287	4207	4081	3887	3461	2933
17.5	4.02	157.5	3593	4227	4515	4483	4331	4241	4116	3924	3482	2944
22.5	5.05	202.5	3619	4249	4522	4501	4342	4252	4131	3939	3495	2960
27.5	6.04	247.5	3627	4247	4520	4502	4337	4234	4131	3925	3486	2953
38.5	8.07	346.5	3658	4280	4555	4522	4347	4267	4160	3963	3511	2976
50.5	10.08	454.5	3698	4333	4595	4547	4391	4299	4192	3991	3541	2987
67.0	12.55	603.0	3727	4357	4635	4571	4400	4308	4208	4006	3549	2988
86.0	15.04	774.0	3717	4371	4630	4563	4394	4303	4206	4005	3550	3008
133.5	20.02	1201.5	3696	4342	4602	4530	4343	4245	4184	3979	3536	2984
200.0	25.00	1800.0	3712	4348	4601	4522	4337	4269	4177	3996	3546	2983

c) Titration curve at 381 nm



2.4.7. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with Na_2CO_3 (dissolved in water) and the solution of receptor in DMSO.

a) Fluorescent spectra

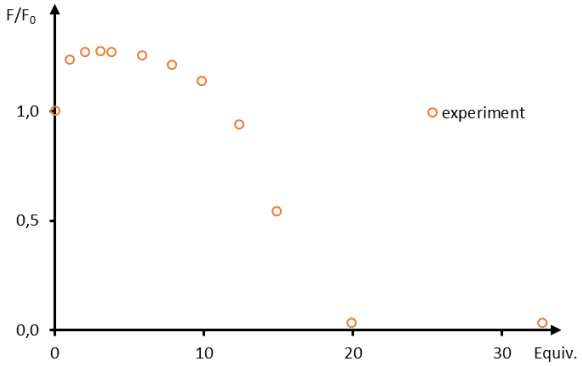


b) Raw data

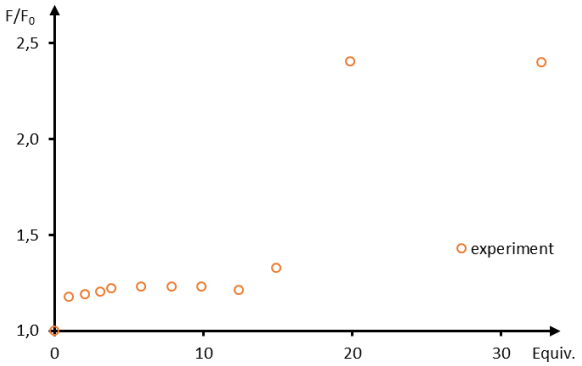
Added volume of titrant solution [µL]	Equivalents of Na_2CO_3	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]										
			375	381	388	397	406	413	423	431	439	449	460
			Fluorescence intensity										
0.0	0.00	0.0	2538	3235	3437	3056	2429	1884	1237	874,5	602	368,4	218,9
4.0	0.98	36.0	3183	3996	4018	3676	2889	2166	1457	1019	692,1	434,9	266,5
8.5	2.04	76.5	3264	4114	4077	3743	2936	2188	1475	1040	704,4	447,4	279,1
13.0	3.05	117.0	3284	4123	4087	3758	2932	2189	1488	1051	716,3	460,3	291,5
16.5	3.80	157.5	3277	4110	4067	3761	2946	2207	1510	1078	741,2	482,6	311,2
26.5	5.83	247.5	3225	4055	3987	3712	2900	2173	1522	1100	774,1	515,9	342,1
37.5	7.87	346.5	3139	3925	3839	3577	2804	2117	1521	1129	818,1	565,8	388,7
49.5	9.85	454.5	2942	3685	3583	3349	2640	2000	1524	1187	890,1	648,1	468,1
66.0	12.36	603.0	2429	3040	2921	2770	2207	1740	1500	1294	1073	850,8	656,3
85.0	14.87	774.0	1413	1762	1674	1622	1351	1232	1643	1872	1809	1601	1349

132.5	19.87	1202.0	61,78	104	169,9	149	257,3	764,3	2976	4705	5101	4656	4163
266.0	32.71	1800.0	63,6	104,3	170,6	146,8	255,5	759,9	2969	4709	5094	4670	4167

c) Titration curve at 381 nm

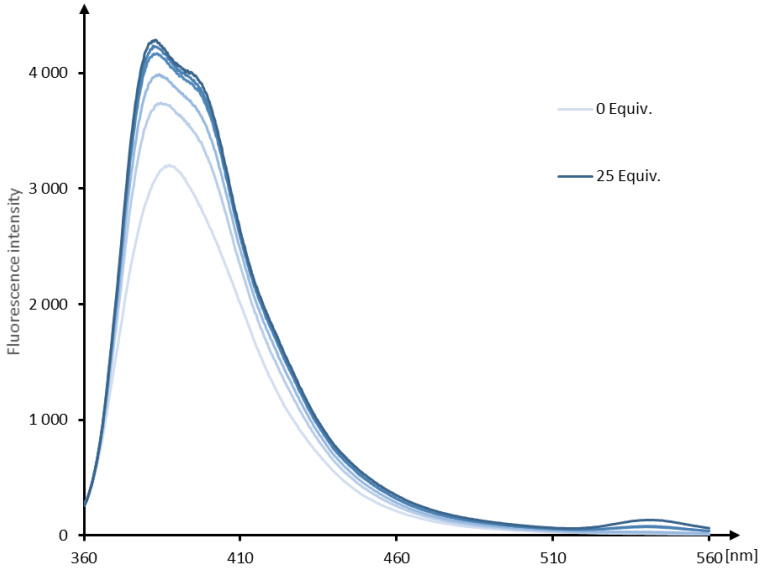


Titration curve at 423 nm



2.4.8. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with PhCOONa (dissolved in water) and the solution of receptor in DMSO.

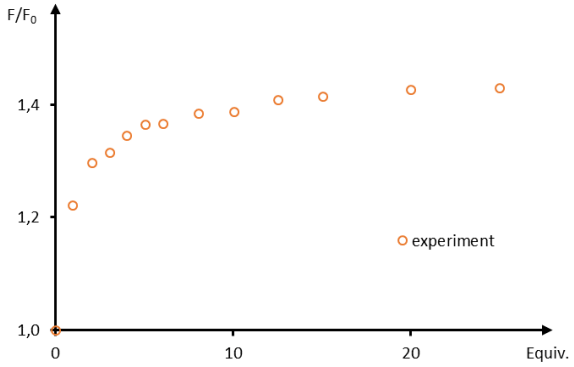
a) Fluorescent spectra



b) Raw data

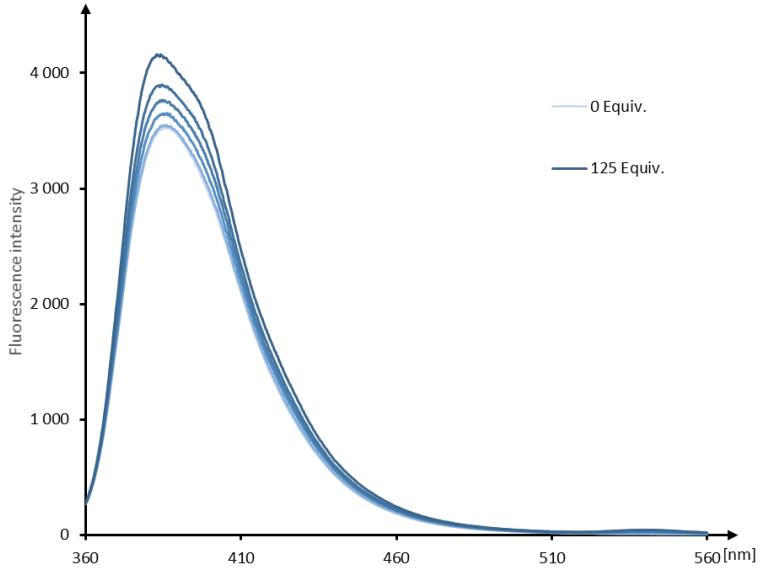
Added volume of titrant solution [µL]	Equivalents of PhCOONa	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]										
			375	378	381	385	390	395	400	405	410	415	420
			Fluorescence intensity										
0.0	0.00	0.0	2349	2715	2984	3171	3154	2947	2665	2347	1998	1635	1335
4.0	0.98	36.0	2893	3374	3642	3727	3644	3487	3227	2804	2321	1912	1565
8.5	2.04	76.5	3083	3596	3868	3924	3812	3666	3410	2948	2414	1989	1649
13.0	3.05	117.0	3135	3652	3923	3965	3847	3719	3468	3001	2460	2010	1684
17.5	4.02	157.5	3214	3749	4015	4063	3919	3804	3543	3060	2511	2055	1716
22.5	5.05	202.5	3266	3802	4071	4102	3955	3836	3590	3097	2536	2081	1739
27.5	6.04	247.5	3276	3822	4075	4102	3964	3852	3592	3097	2535	2088	1748
38.5	8.07	346.5	3322	3879	4129	4141	3973	3876	3631	3132	2563	2102	1765
50.5	10.08	454.5	3314	3870	4140	4136	3998	3891	3649	3155	2567	2104	1773
67.0	12.55	603.0	3379	3941	4204	4198	4022	3944	3695	3181	2599	2131	1797
86.0	15.04	774.0	3406	3981	4222	4211	4045	3949	3704	3183	2605	2139	1799
133.5	20.02	1201.5	3431	4011	4254	4228	4058	3985	3743	3218	2638	2160	1821
200.0	25.00	1800.0	3454	4024	4263	4223	4075	3990	3757	3214	2623	2156	1822

c) Titration curve at 381 nm



2.4.9. Fluorescent titration of 10^{-5} M solution of receptor **A** in DMSO/10% H_2O with NaCl (dissolved in water) and the solution of receptor in DMSO.

a) Fluorescent spectra



b) Raw data

Added volume of titrant solution [µL]	Equivalents of NaCl	Added volume of receptor solution in DMSO [µL]	Wavelength [nm]										
			375	378	381	384	387	390	393	396	399	402	405
			Fluorescence intensity										
0.0	0.00	0.0	2682	3122	3389	3513	3524	3455	3331	3184	3003	2791	2541
4.0	4.90	36.5	2687	3114	3395	3507	3517	3439	3330	3180	3015	2792	2545
8.5	10.19	77.5	2709	3136	3402	3527	3532	3460	3346	3202	3021	2810	2552
13.0	15.25	118.0	2712	3145	3416	3541	3538	3471	3355	3221	3039	2830	2574
17.5	20.12	157.5	2722	3159	3422	3538	3537	3474	3358	3217	3045	2838	2574
27.5	30.22	247.5	2784	3233	3498	3607	3600	3534	3418	3294	3107	2885	2633
38.5	40.36	346.5	2817	3272	3523	3647	3651	3556	3460	3317	3139	2922	2648
50.5	50.40	454.5	2835	3304	3564	3673	3657	3585	3476	3337	3157	2939	2676
85.5	74.76	773.5	2932	3404	3665	3758	3750	3670	3559	3428	3252	3021	2747
133.0	99.73	1201.0	3053	3543	3810	3882	3858	3776	3677	3551	3384	3142	2836
200.0	125	1800.0	3306	3843	4103	4148	4091	3985	3890	3769	3594	3346	3017

c) Titration curve at 381 nm