Supporting Information

Exploiting the 1,4-Naphthoquinone and 3-Iodo-1,4-Naphthoquinone Motifs as Anion Binding Sites by Hydrogen or Halogen-Bonding Interactions

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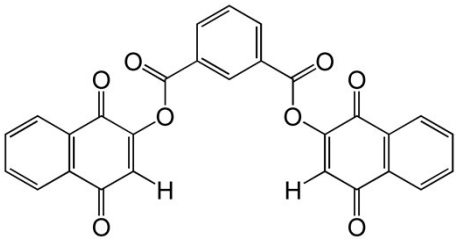
PART I: NMR Spectra.

bis(1,4-naphthoquinone-2-yl) isophthalate 4:



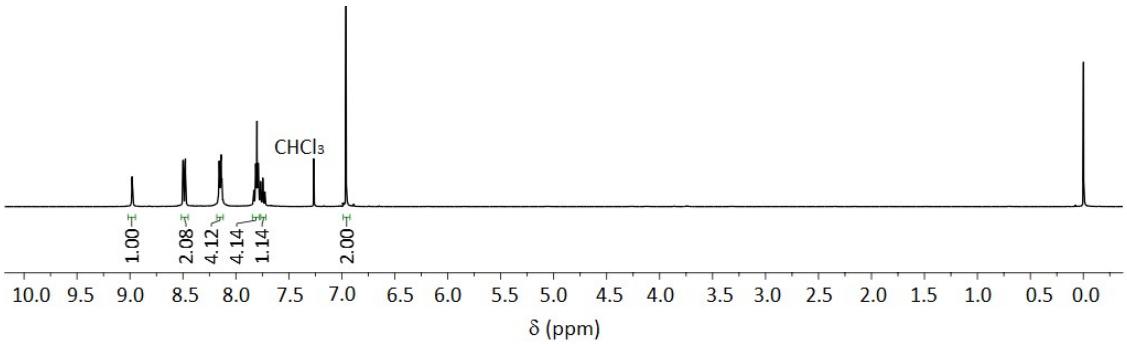


Figure S1. ^{1}H NMR spectra of bis(1,4-naphthoquinone-2-yl) isophthalate **4**.

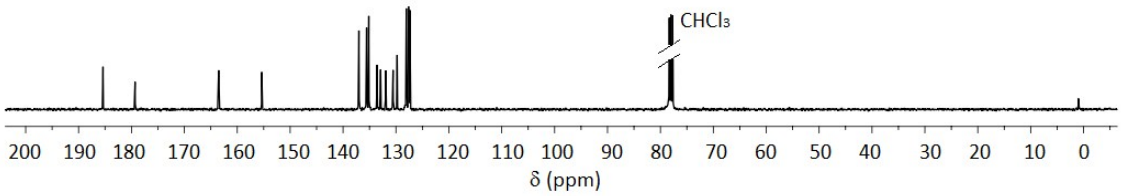


Figure S2. ^{13}C NMR spectra of bis(1,4-naphthoquinone-2-yl) isophthalate **4**.

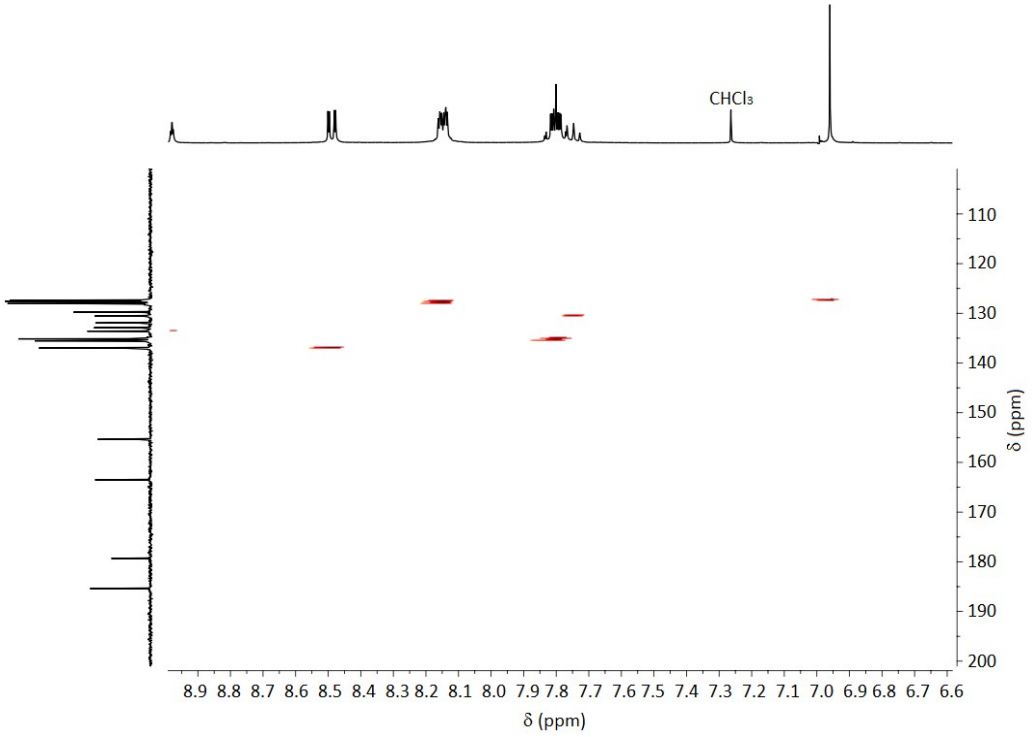


Figure S3. HSQC NMR spectra of bis(1,4-naphthoquinone-2-yl) isophthalate **4**.

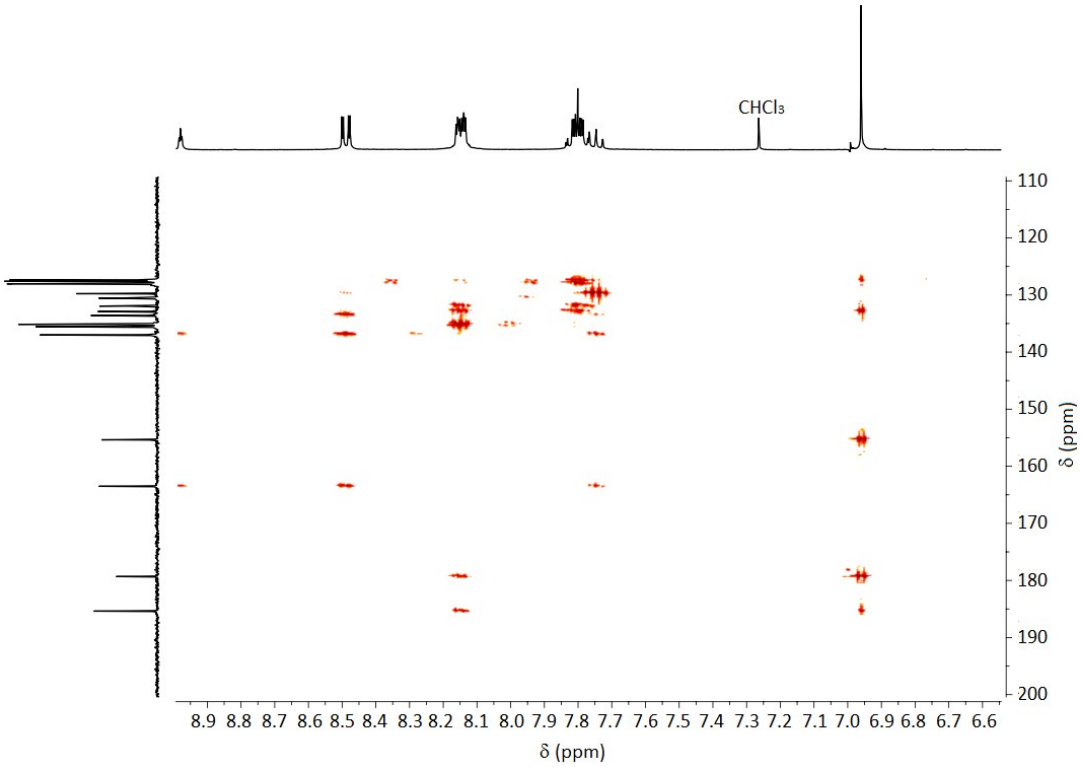


Figure S4. HMBC NMR spectra of bis(1,4-naphthoquinone-2-yl) isophthalate **4**.

bis(3-iodo-1,4-naphthoquinone-2-yl) isophthalate 5:

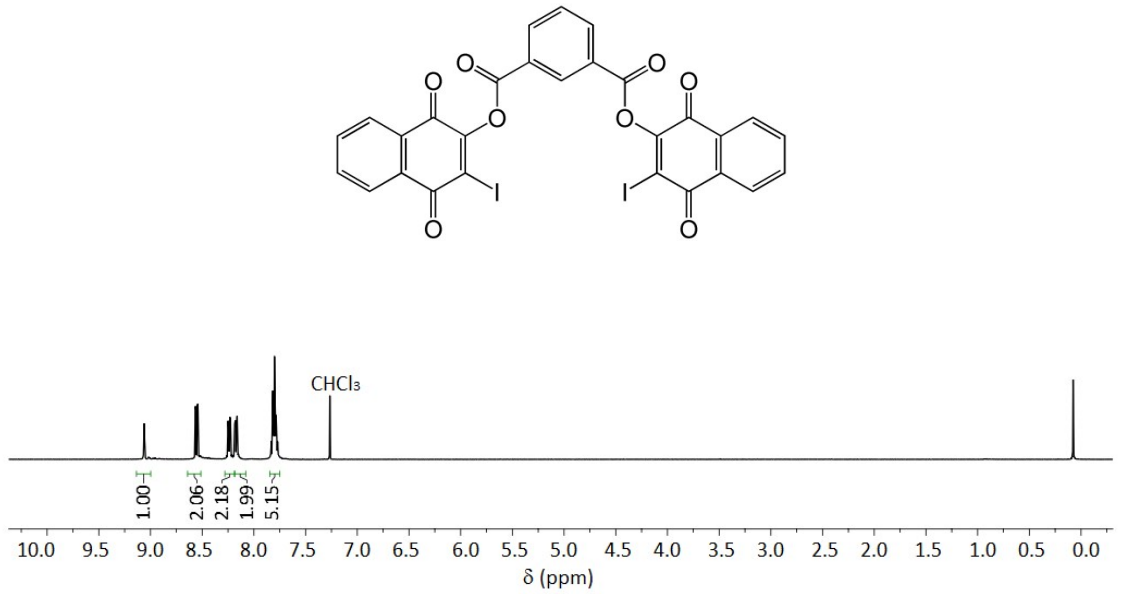


Figure S5. ^{1}H NMR spectra of bis(3-iodo-1,4-naphthoquinone-2-yl) isophthalate **5**.

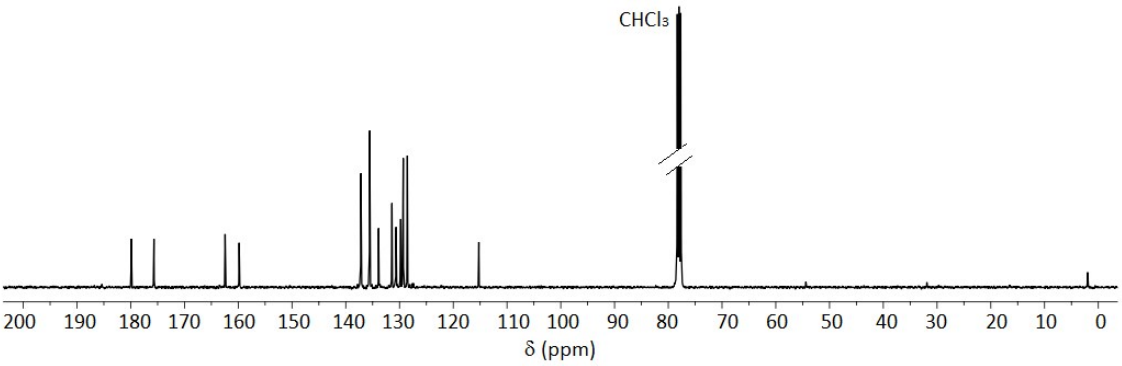


Figure S6. ^{13}C NMR spectra of bis(3-iodo-1,4-naphthoquinone-2-yl) isophthalate **5**.

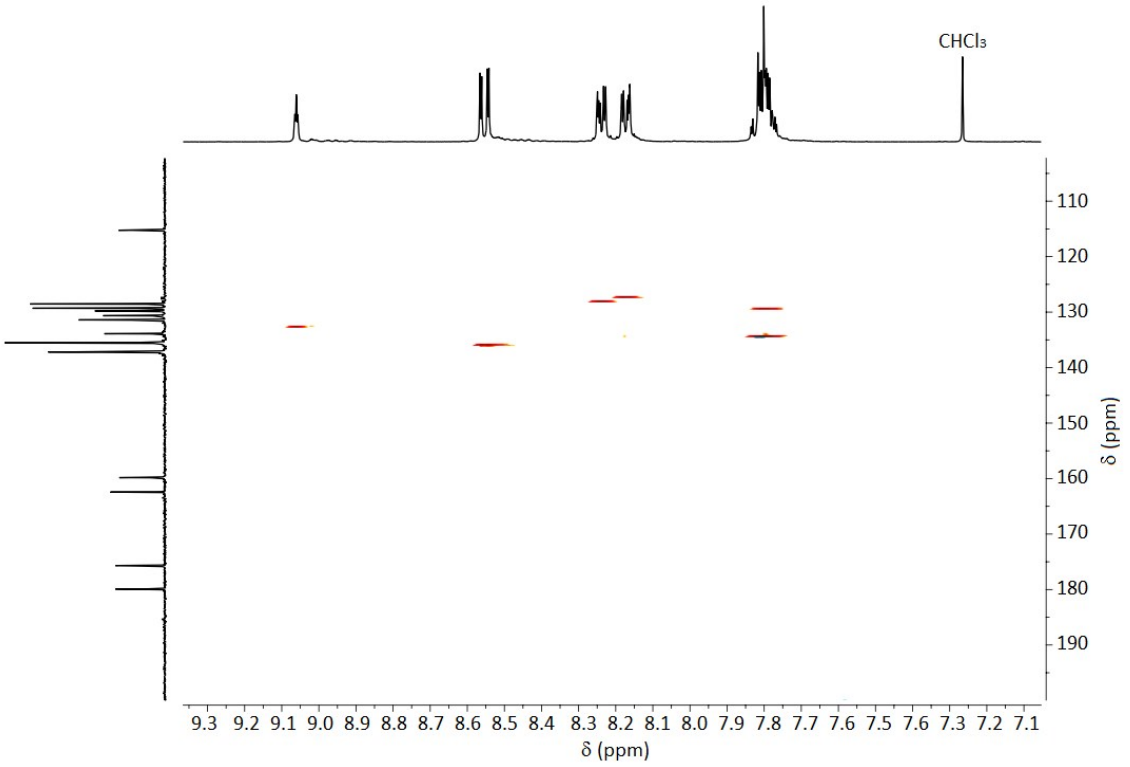


Figure S7. HSQC NMR spectra of bis(3-iodo-1,4-naphthoquinone-2-yl) isophthalate **5**.

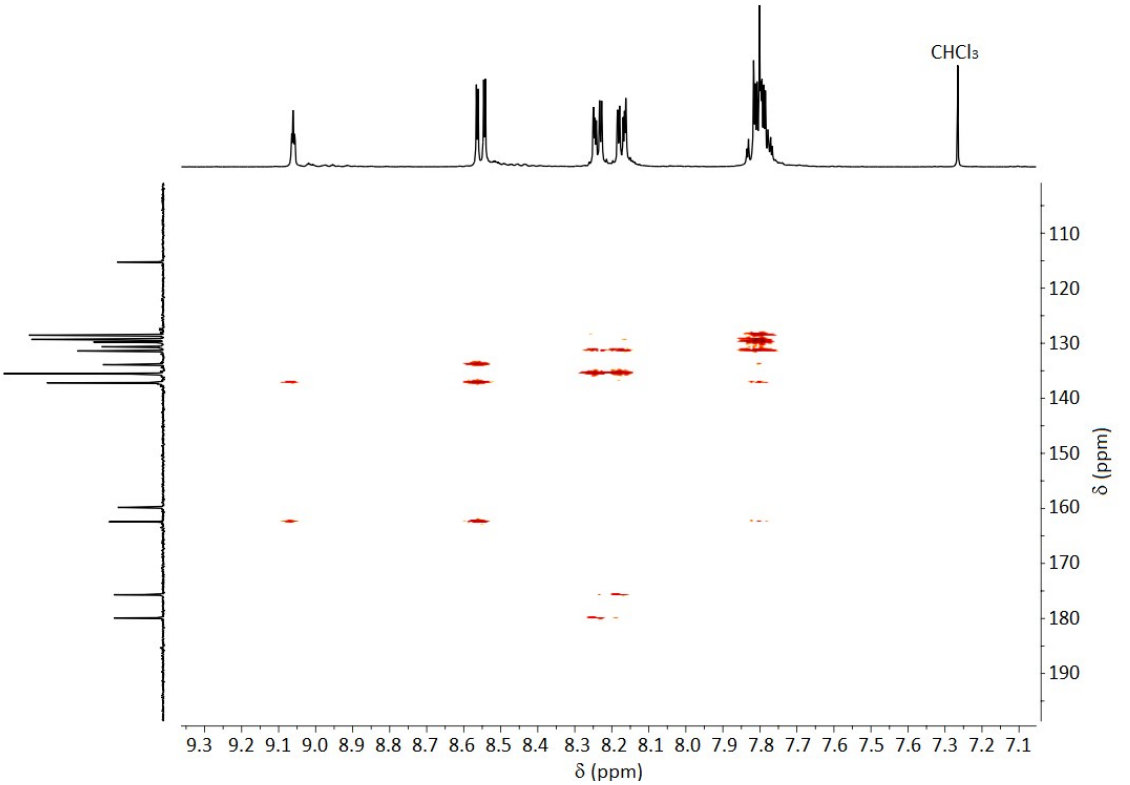


Figure S8. HMBC NMR spectra of bis(3-iodo-1,4-naphthoquinone-2-yl) isophthalate **5**.

PART II: Uv-Vis Anion Binding Studies.

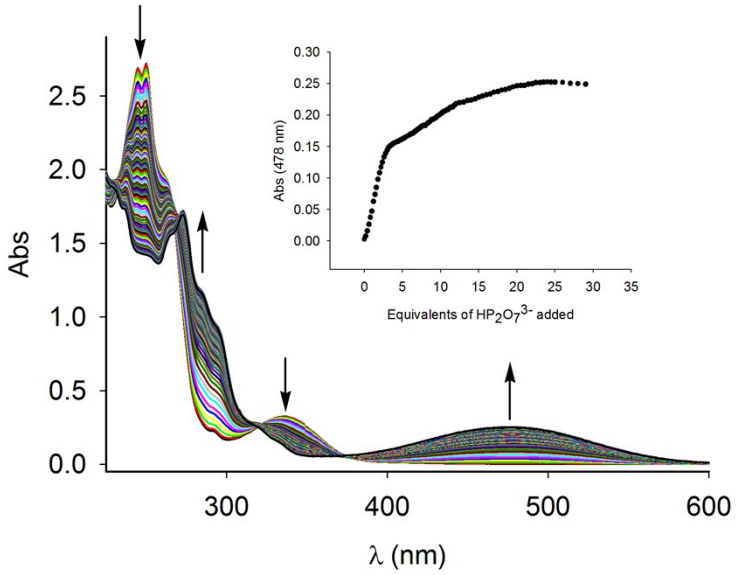


Figure S9. Changes in the absorption spectra of receptor **4** (c = 5 x 10^{-5} M in CH_3CN) upon addition of $HP_2O_7^{3-}$ anions at 20 °C.

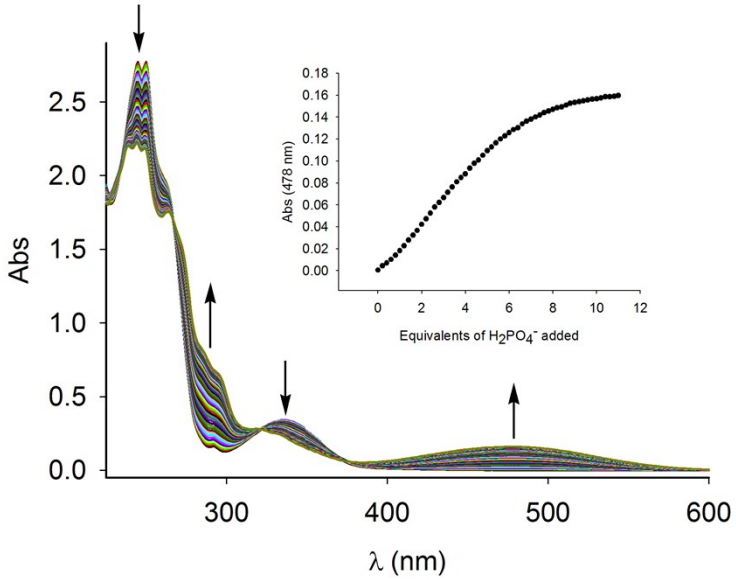


Figure S10. Changes in the absorption spectra of receptor **4** (c = 5 x 10^{-5} M in CH_3CN) upon addition of $H_2PO_4^-$ anions at 20 °C.

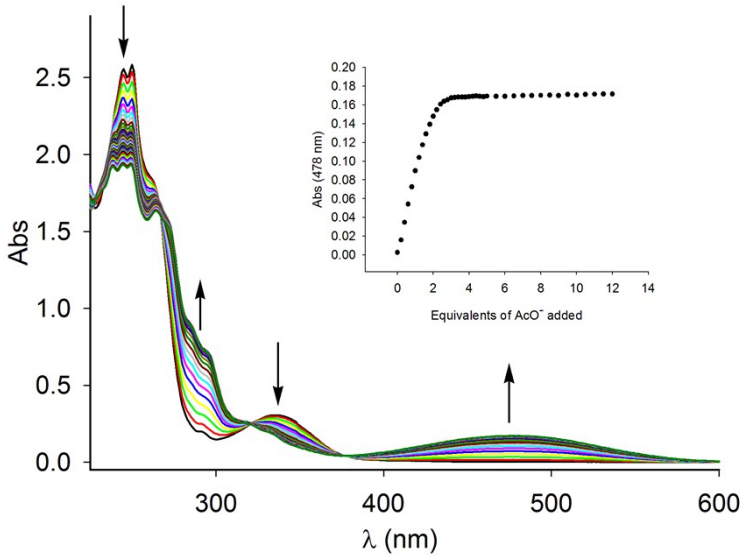


Figure S11. Changes in the absorption spectra of receptor **4** (c = 5 x 10^{-5} M in CH_3CN) upon addition of AcO^- anions at 20 °C.

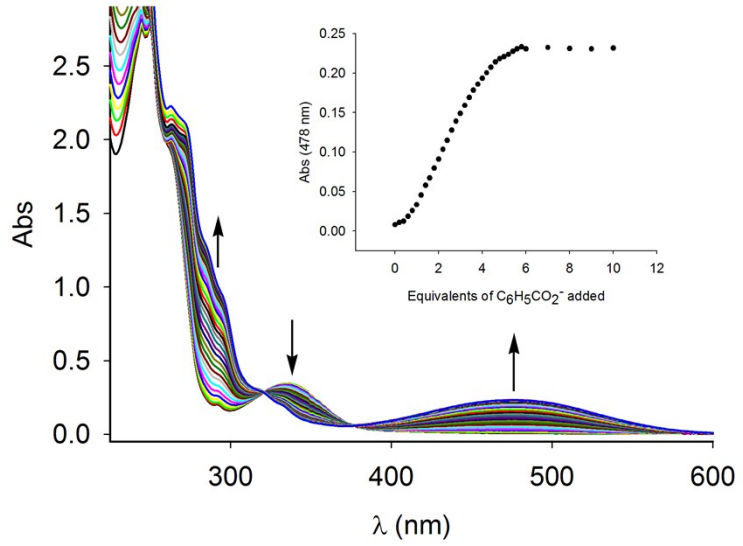


Figure S12. Changes in the absorption spectra of receptor **4** (c = 5 x 10^{-5} M in CH_3CN) upon addition of $C_6H_5CO_2^-$ anions at 20 °C.

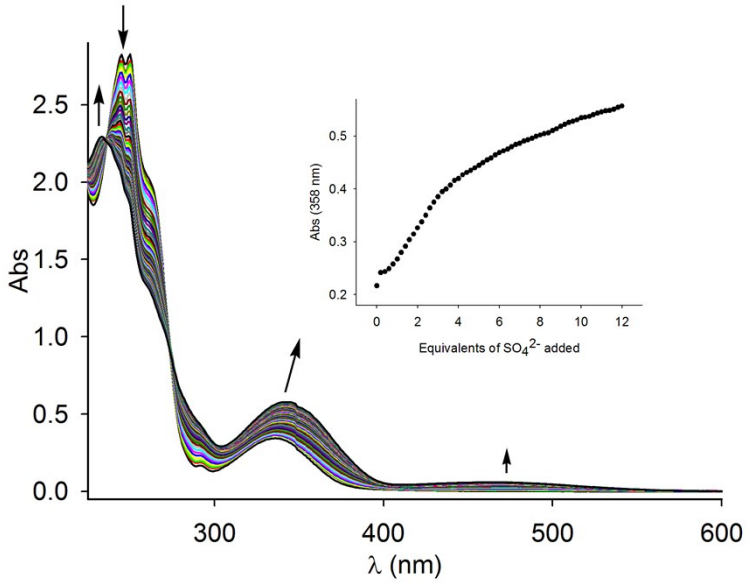


Figure S13. Changes in the absorption spectra of receptor **4** (c = 5 x 10^{-5} M in CH_3CN) upon addition of SO_4^{2-} anions at 20 °C.

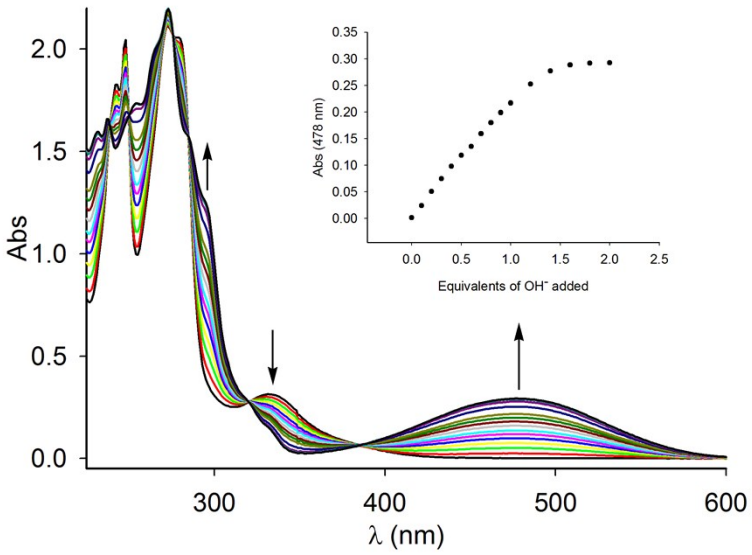


Figure S14. Changes in the absorption spectra of receptor 2-hydroxy-1,4-naphthoquinone (c = 5 x 10^{-5} M in CH_3CN) upon addition of OH^- anions at 20 °C.

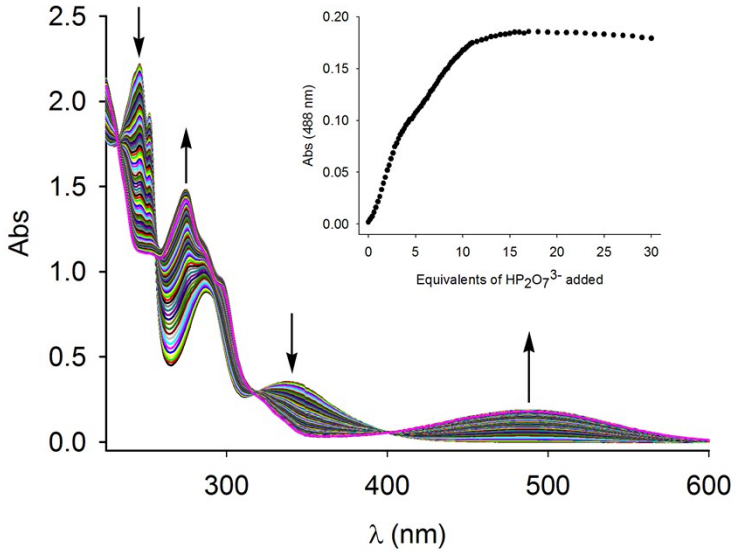


Figure S15. Changes in the absorption spectra of receptor **5** (c = 5 x 10^{-5} M in CH_3CN) upon addition of $HP_2O_7^{3-}$ anions at 20 °C.

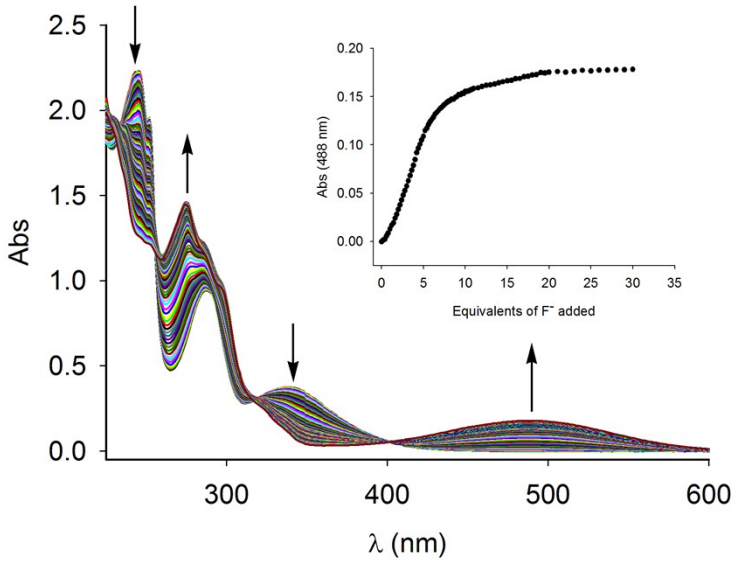


Figure S16. Changes in the absorption spectra of receptor **5** (c = 5 x 10^{-5} M in CH_3CN) upon addition of F^- anions at 20 °C.

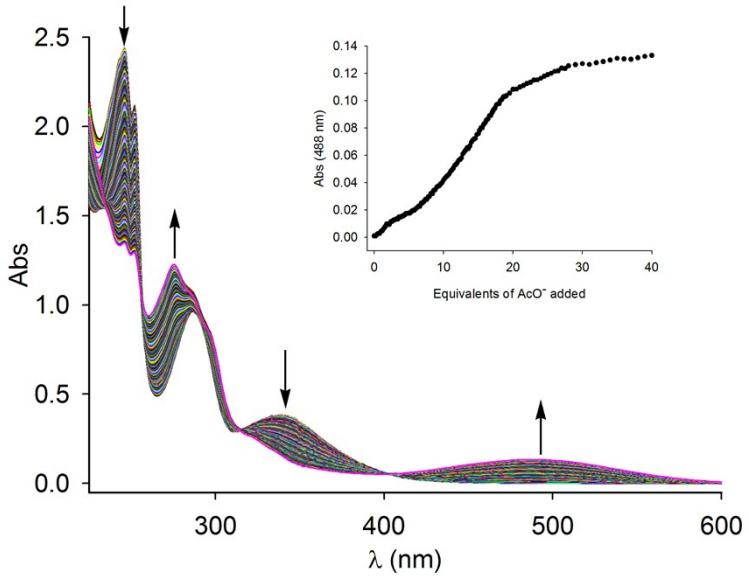


Figure S17. Changes in the absorption spectra of receptor **5** (c = 5 x 10^{-5} M in CH_3CN) upon addition of AcO^- anions at 20 °C.

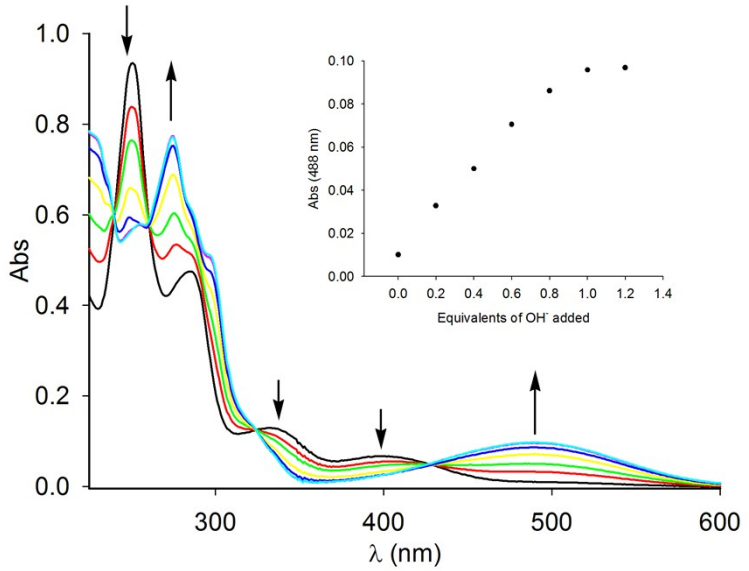


Figure S18. Changes in the absorption spectra of 2-hydroxy-3-iodo-1,4-naphthoquinone (c = 5 x 10^{-5} M in CH_3CN) upon addition of OH^- anions at 20 °C.

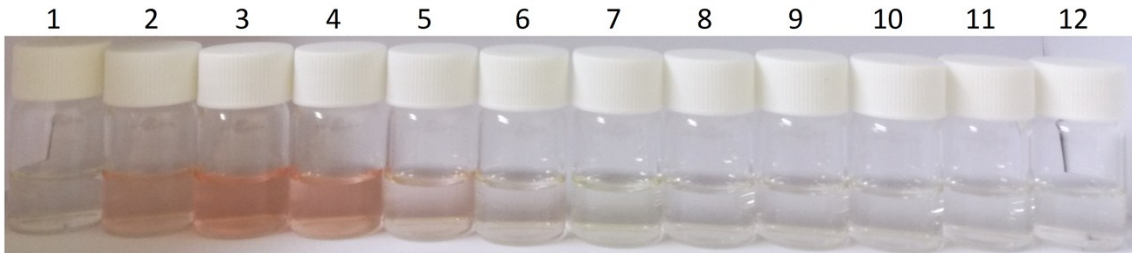


Figure S19. Changes in the colour of a solution of the receptor **5** (1) in CH_3CN upon addition of F^- (2), $HP_2O_7^{3-}$ (3), AcO^- (4), $H_2PO_4^-$ (5), $C_6H_5CO_2^-$ (6), SO_4^{2-} (7), HSO_4^- (8), NO_3^- (9), Cl^- (10), Br^- (11) and I^- (12).

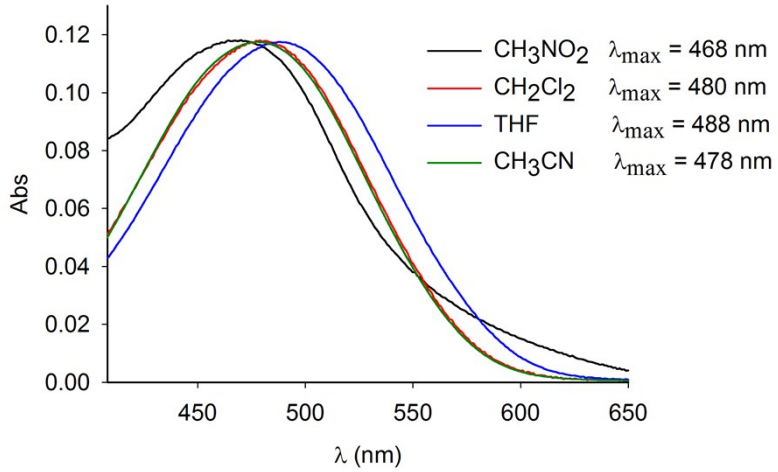


Figure S20. Changes in the absorption spectra of the Charge Transfer band of the complex **4·2AcO**$^-$ in different solvents.

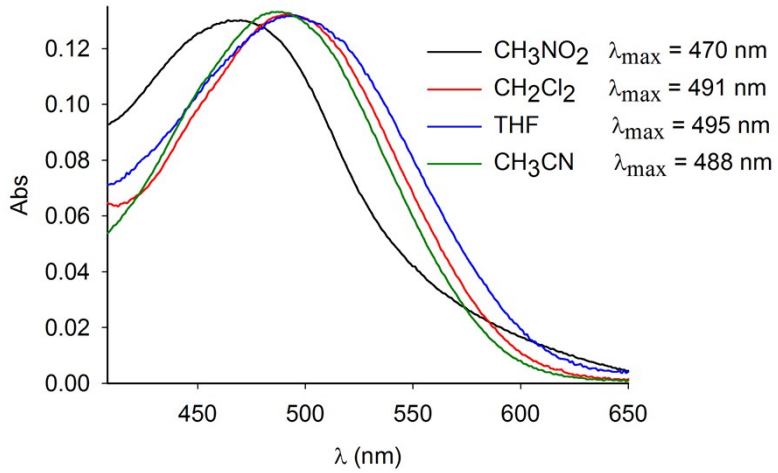


Figure S21. Changes in the absorption spectra of the Charge Transfer band of the complex **5·2AcO**$^-$ in different solvents.

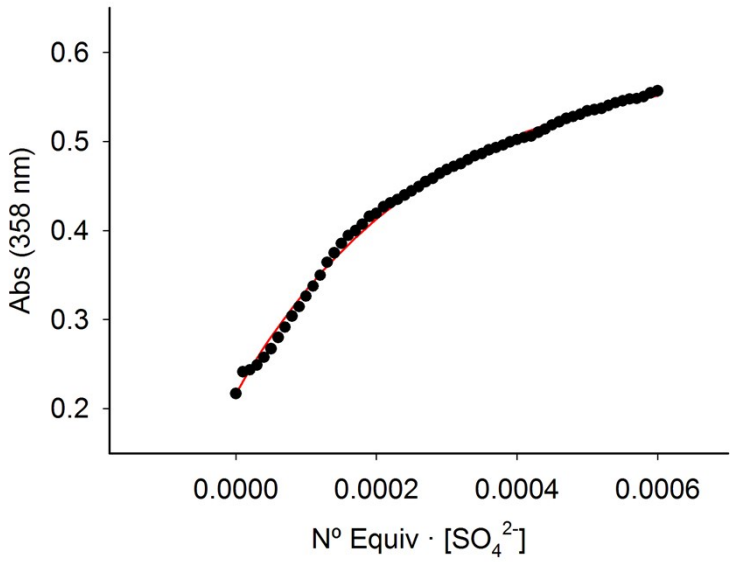


Figure S22. Changes in the absorption spectra at λ = 358 nm of the receptor **4** (*c* = 5 x 10^{-5} M in CH_3CN) upon addition of increasing amounts of SO_4^{2-} anions. Data points represent experimental data, continuous lines represent calculated curves.

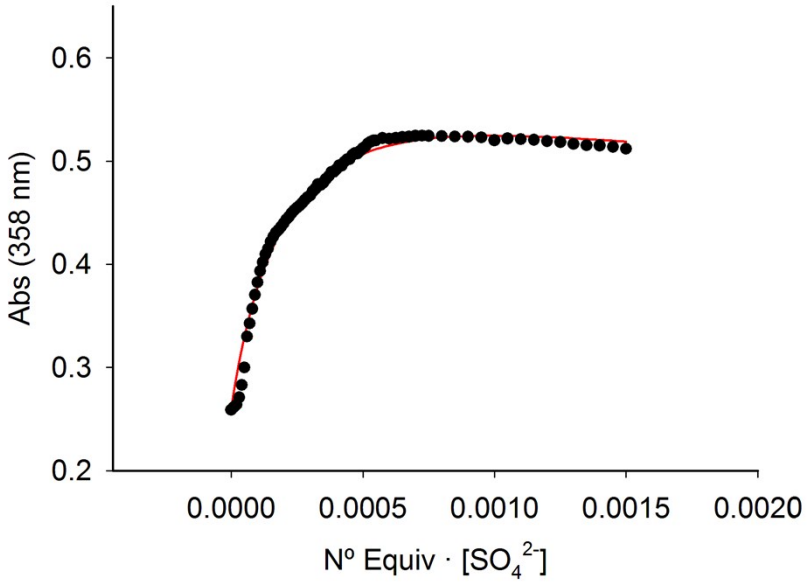


Figure S23. Changes in the absorption spectra at λ = 358 nm of the receptor **5** (*c* = 5 x 10^{-5} M in CH_3CN) upon addition of increasing amounts of SO_4^{2-} anions. Data points represent experimental data, continuous lines represent calculated curves.

PART III: Mass Spectrometry Studies.

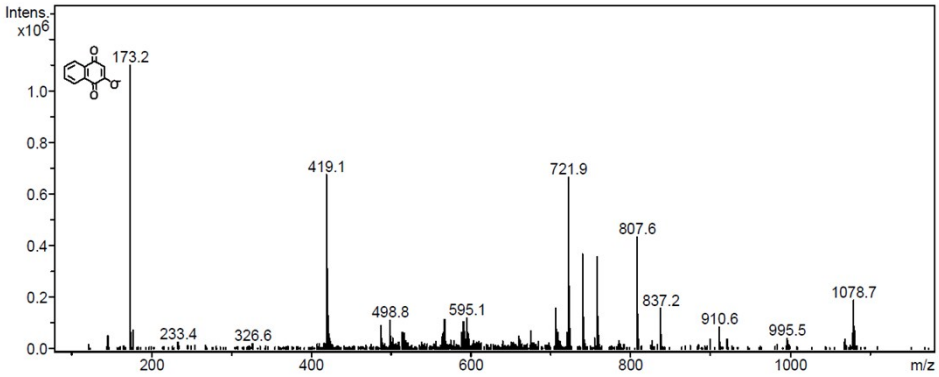


Figure S24. Mass spectrum of the solution of **4** (2.5 x 10^{-3} M in CH_3CN) after the addition of 2 equivalents of $HP_2O_7^{3-}$ ions, indicating the disruption of the ester group.

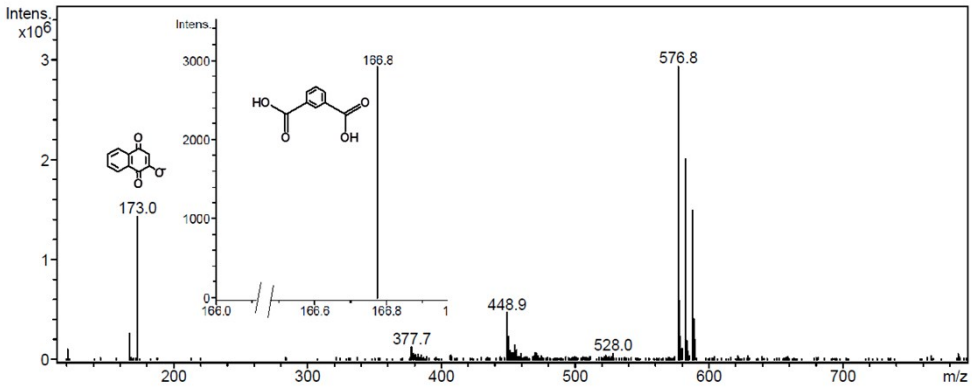


Figure S25. Mass spectrum of the solution of **4** (2.5 x 10^{-3} M in CH_3CN) after the addition of 2 equivalents of F^- ions, indicating the disruption of the ester group.

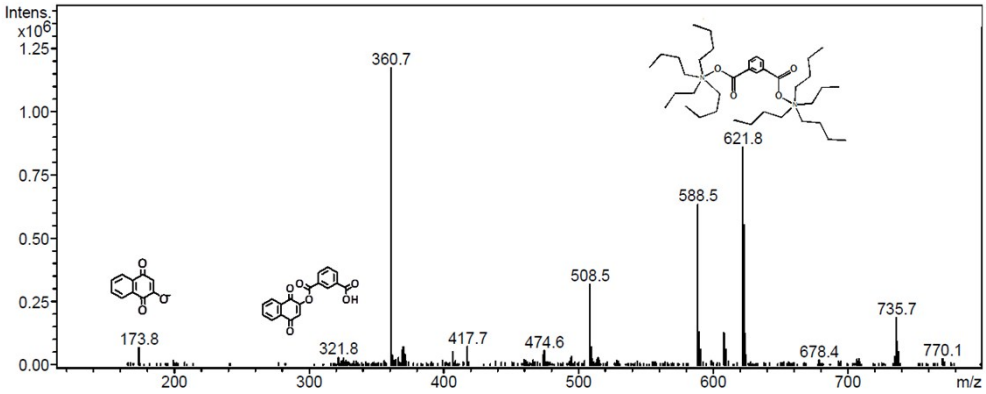


Figure S26. Mass spectrum of the solution of **4** (2.5 x 10^{-3} M in CH_3CN) after the addition of 2 equivalents of AcO^- ions, indicating the disruption of the ester group.

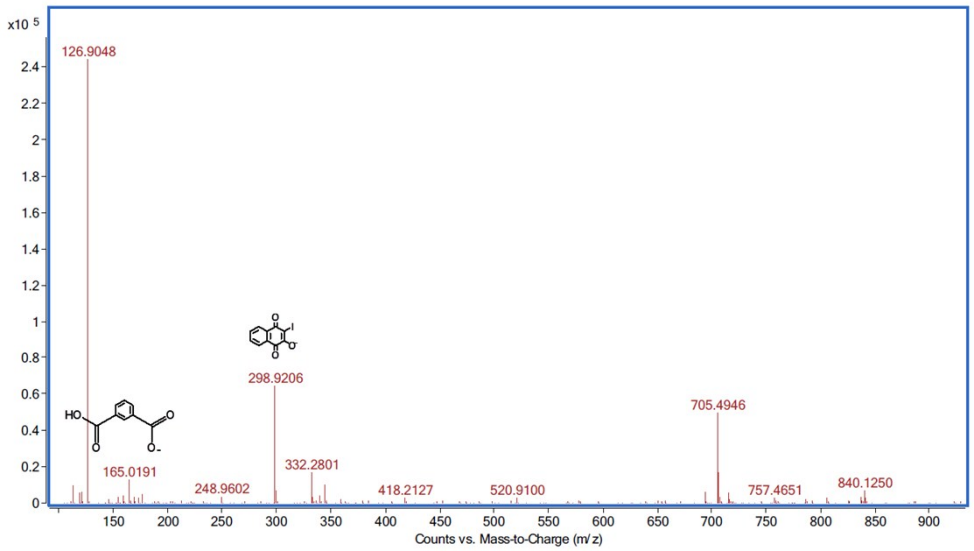


Figure S27. Mass spectrum of the solution of **5** (2.5 x 10^{-3} M in CH_3CN) after the addition of 2 equivalents of $HP_2O_7^{3-}$ ions, indicating the disruption of the ester group.

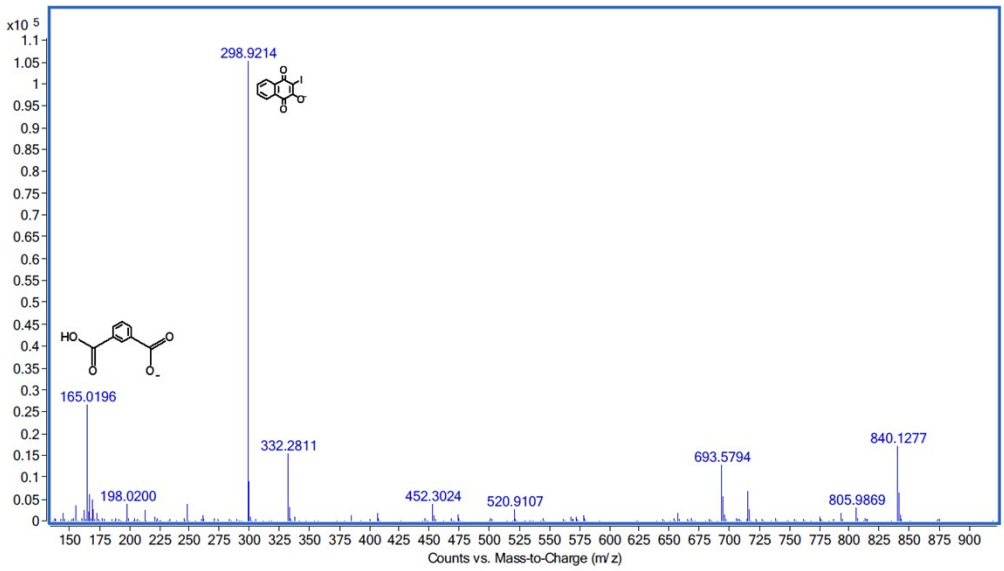


Figure S28. Mass spectrum of the solution of **5** (2.5 x 10^{-3} M in CH_3CN) after the addition of 2 equivalents of F^- ions, indicating the disruption of the ester group.

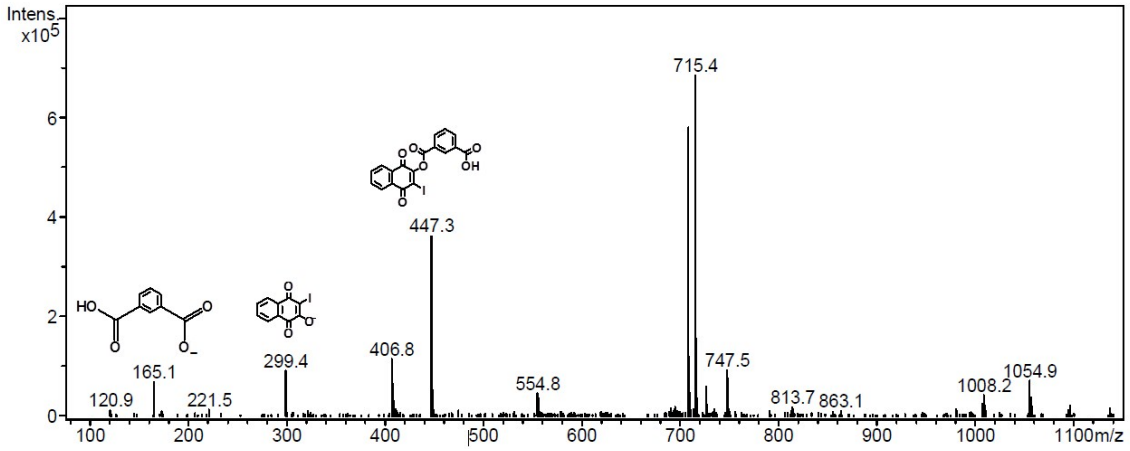


Figure S29. Mass spectrum of the solution of **5** (2.5 x 10^{-3} M in CH_3CN) after the addition of 2 equivalents of AcO^- ions, indicating the disruption of the ester group.

PART IV: Fluorescence Anion Binding Studies.

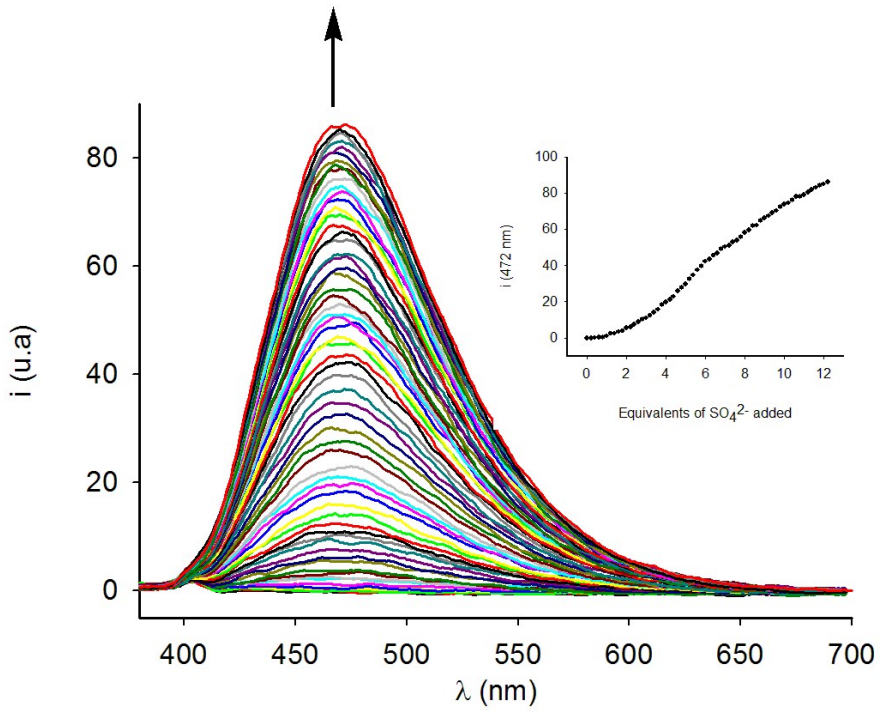


Figure S30. Changes in the fluorescence spectra of receptor **5** (c = 5 x 10^{-5} M in CH_3CN) upon addition increasing amounts of SO_4^{2-} anions.

PART V: ^{1}H-NMR Anion Binding Studies.

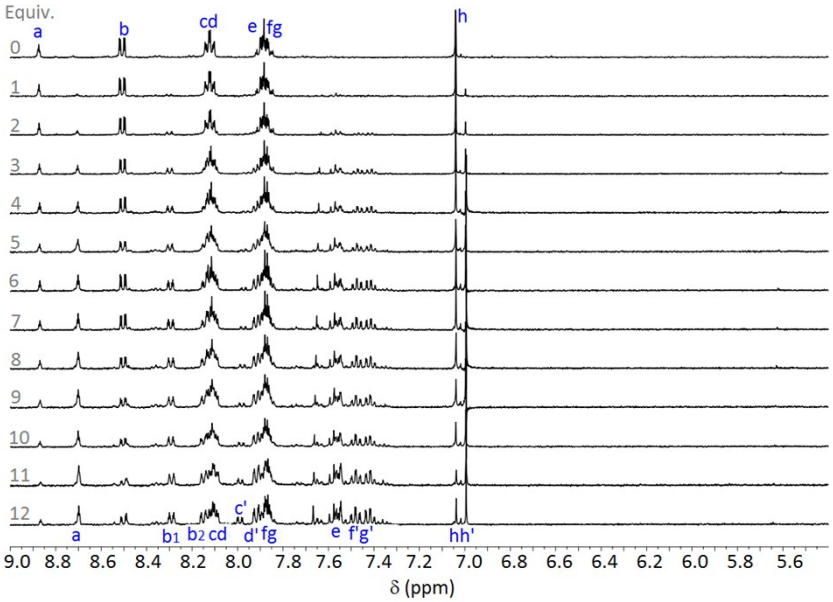


Figure S31. ^{1}H NMR spectral changes observed in the receptor **4** in CD_3CN/MeOD (9:1) during the addition of SO_4^{2-} anion.

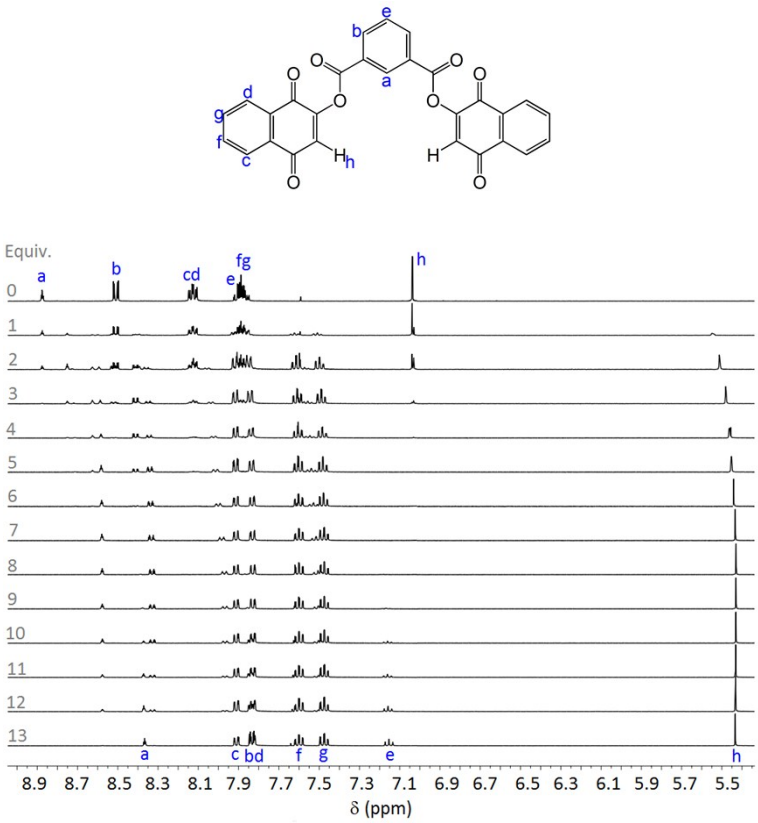


Figure S32. ^{1}H NMR spectral changes observed in the receptor **4** in CD_3CN during the addition of F^- anion.

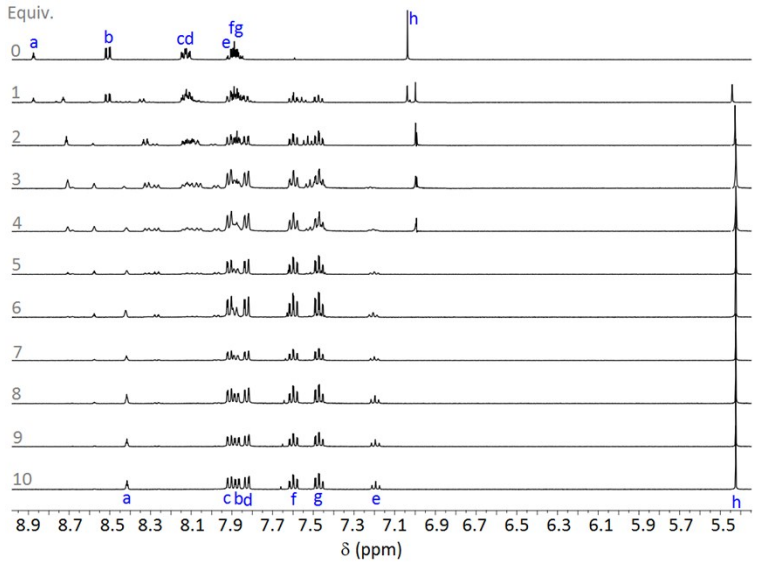


Figure S33. ^{1}H NMR spectral changes observed in the receptor **4** in CD_3CN during the addition of AcO^{-} anion.

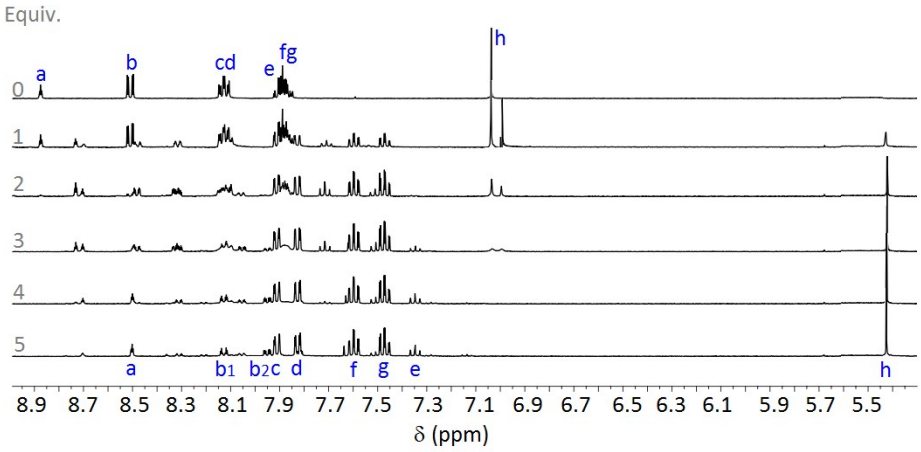


Figure S34. ^{1}H NMR spectral changes observed in the receptor **4** in CD_3CN during the addition of $HP_2O_7^{3-}$ anion.

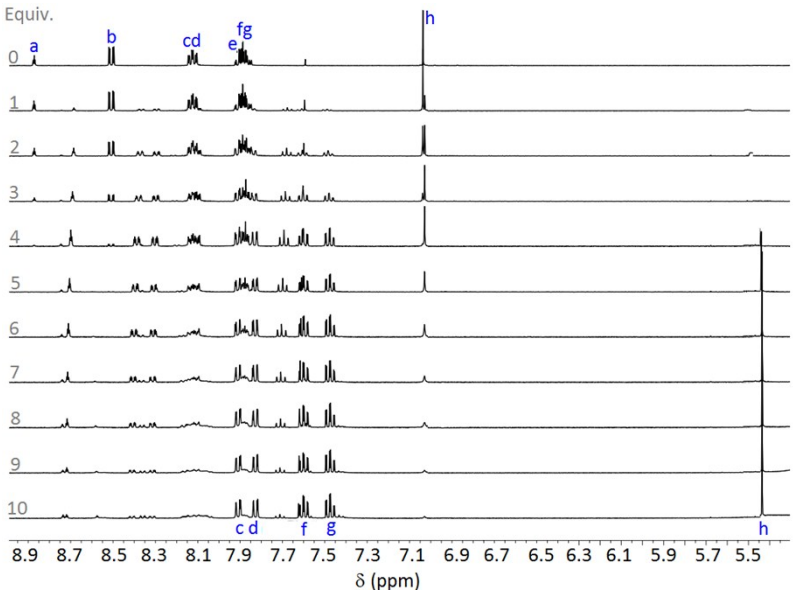


Figure S35. ^{1}H NMR spectral changes observed in the receptor **4** in CD_3CN during the addition of $H_2PO_4^-$ anion.

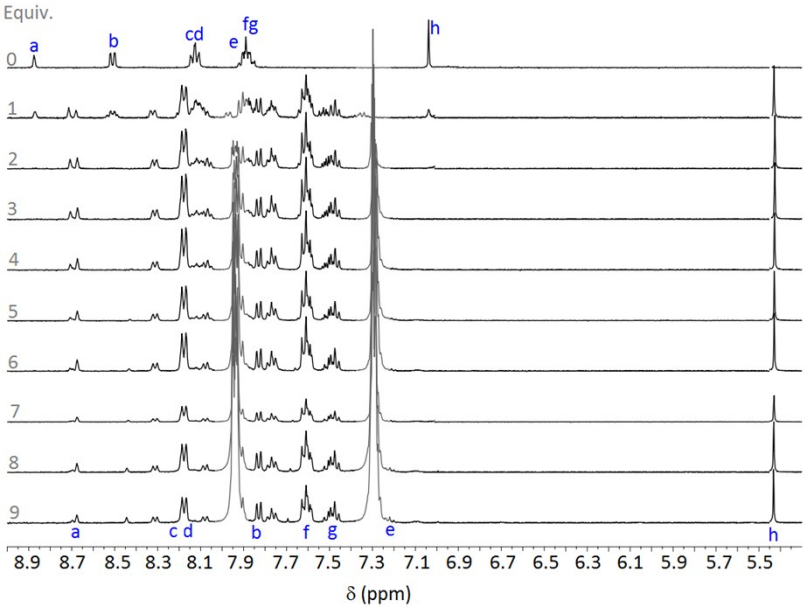


Figure S36. ^{1}H NMR spectral changes observed in the receptor **4** in CD_3CN during the addition of $C_6H_5CO_2^-$ anion.

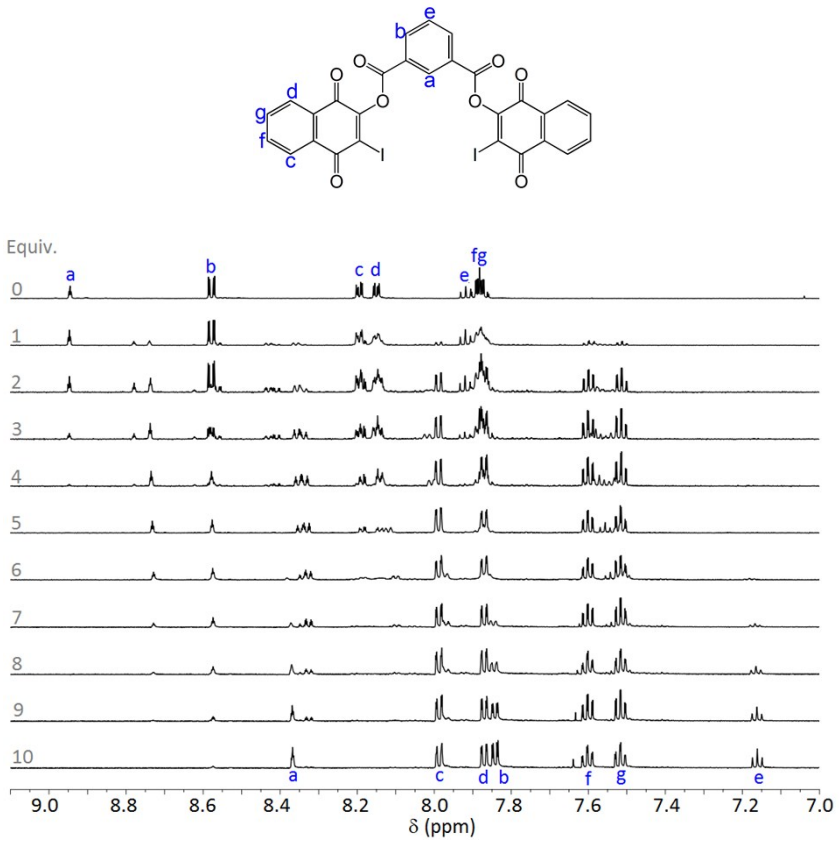


Figure S37. ^{1}H NMR spectral changes observed in the receptor **5** in CD_3CN during the addition of F^- anion.

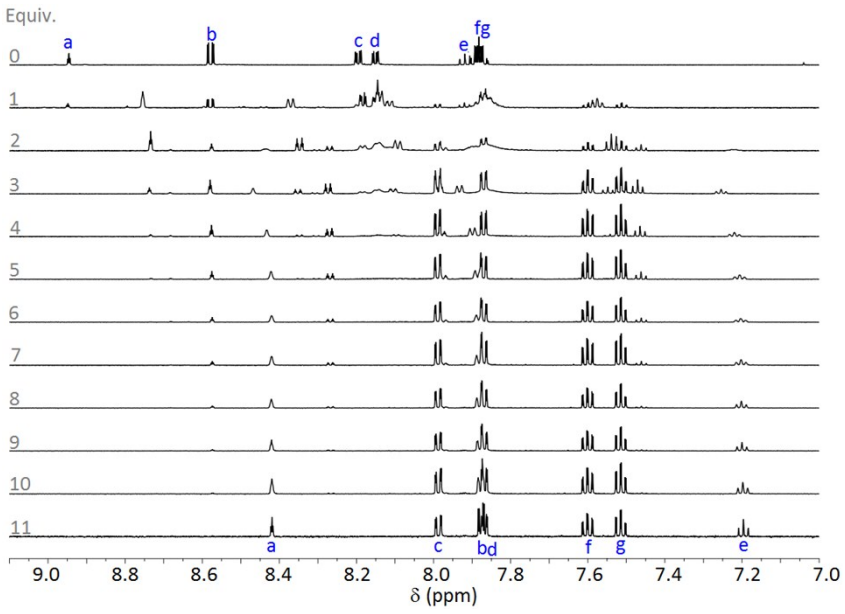


Figure S38. ^{1}H NMR spectral changes observed in the receptor **5** in CD_3CN during the addition of AcO^- anion.

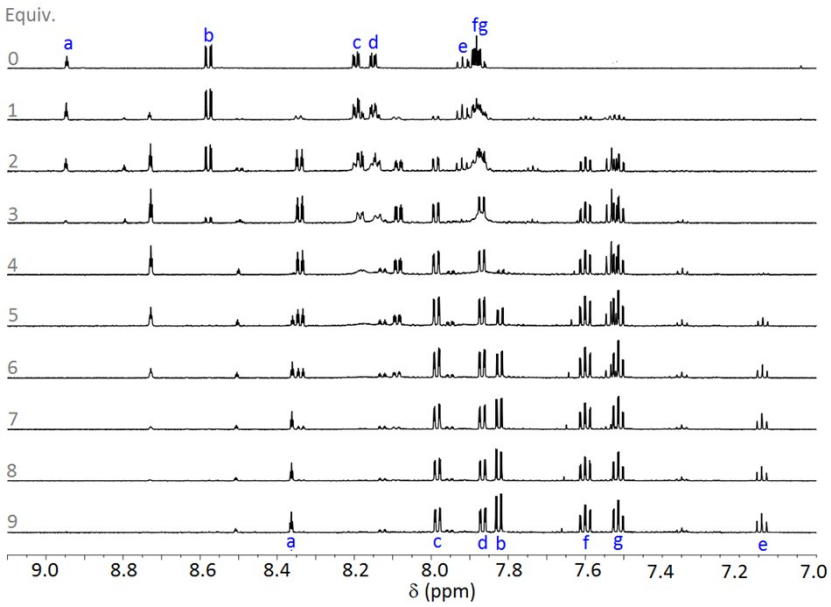


Figure S39. ^{1}H NMR spectral changes observed in the receptor **5** in CD_3CN during the addition of $HP_2O_7^{3-}$ anion.

PART VI: Computational Results.

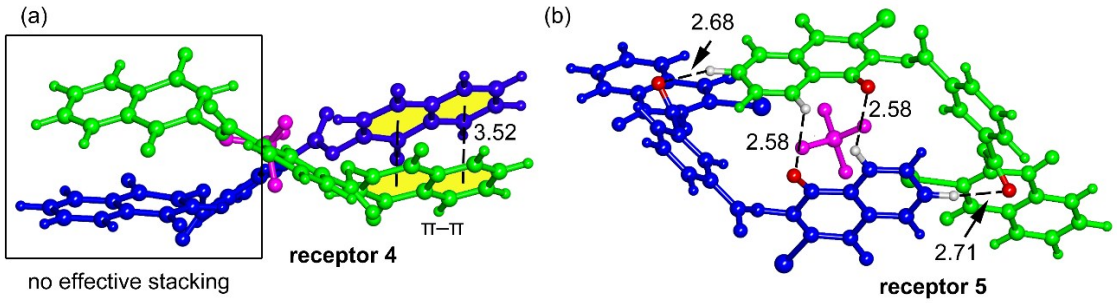


Figure S40. (a) Optimized 2:1 complex of receptor **4** (one molecule in blue and other in green) with sulfate (represented in pink). (b) Optimized 2:1 complex of receptor **5** (one molecule in blue and other in green) with sulfate (represented in pink). Interaction represented as dashed lines. Distances in Å

Cartesian coordinates of the optimized receptors and complexes

Receptor 4, planar conformation

C	1.2116523	0.0007831	-0.0856596
C	0.0000000	0.0000000	-0.7851424
H	0.0000000	0.0000000	-1.8751419
C	-1.2116523	-0.0007831	-0.0856596
C	-1.2112455	-0.0002028	1.3211174
C	0.0000000	-0.0000000	2.0131454
H	0.0000000	0.0000000	3.1032008
C	1.2112455	0.0002028	1.3211174
H	2.1582589	-0.0000568	1.8600025
C	2.4661804	0.0029415	-0.8851480
O	3.5600383	-0.0008225	-0.0269832
O	2.5384731	0.0072064	-2.0921200
C	4.8715530	0.0027437	-0.4046945
C	5.7505812	-0.0116022	0.8193771
O	5.2555918	-0.0261507	1.9419897
C	7.2182159	-0.0072350	0.5880735
C	8.0840041	-0.0190743	1.6902364

H	7.6526146	-0.0313447	2.6913430
C	9.4634363	-0.0149705	1.4915090
H	10.1358167	-0.0239999	2.3500992
C	9.9866136	0.0009576	0.1919800
H	11.0667618	0.0041142	0.0398871
C	9.1304802	0.0127272	-0.9091191
H	9.5123566	0.0253084	-1.9304383
C	7.7446388	0.0086888	-0.7185755
O	7.2684762	0.0358878	-3.0535847
C	6.8327014	0.0216160	-1.9012731
C	5.3786059	0.0175098	-1.6620097
H	4.7451129	0.0273873	-2.5440402
H	-2.1582589	0.0000568	1.8600025
C	-2.4661804	-0.0029415	-0.8851480
O	-2.5384731	-0.0072064	-2.0921200
O	-3.5600383	0.0008225	-0.0269832
C	-4.8715530	-0.0027437	-0.4046945
C	-5.7505812	0.0116022	0.8193771
C	-5.3786059	-0.0175098	-1.6620097
C	-7.2182159	0.0072350	0.5880735
C	-6.8327014	-0.0216160	-1.9012731
H	-4.7451129	-0.0273873	-2.5440402
C	-8.0840041	0.0190743	1.6902364
C	-7.7446388	-0.0086888	-0.7185755
C	-9.4634363	0.0149705	1.4915090
C	-9.1304802	-0.0127272	-0.9091191
C	-9.9866136	-0.0009576	0.1919800
H	-9.5123566	-0.0253084	-1.9304383
H	-11.0667618	-0.0041142	0.0398871
H	-7.6526146	0.0313447	2.6913430
H	-10.1358167	0.0239999	2.3500992
O	-5.2555918	0.0261507	1.9419897
O	-7.2684762	-0.0358878	-3.0535847

Receptor 4, non-planar conformation

C	-2.2968646	2.0686762	0.9123499
C	-0.9138560	2.0563083	0.6968327
H	-0.4842049	1.3985809	-0.0543624
C	-0.0847624	2.8832223	1.4635519
C	-0.6397957	3.7150818	2.4492286
C	-2.0175617	3.7238519	2.6621532
H	-2.4464095	4.3697405	3.4283593
C	-2.8466665	2.9046391	1.8973936
H	-3.9259499	2.8916509	2.0496662
C	-3.2267687	1.2059493	0.1438762
O	-2.5641339	0.5393104	-0.8957469
O	-4.4181931	1.1053115	0.3163398
C	-3.1987520	-0.5545299	-1.4274815
C	-3.4851381	-1.6838062	-0.4801687
O	-3.1390069	-1.6112271	0.6939714
C	-4.1570710	-2.8750704	-1.0613084
C	-4.5238747	-3.9322354	-0.2184945
H	-4.3129991	-3.8454109	0.8476096
C	-5.1446512	-5.0622027	-0.7489231
H	-5.4332298	-5.8824472	-0.0906462
C	-5.3971397	-5.1454752	-2.1241656
H	-5.8818079	-6.0315188	-2.5361047
C	-5.0305118	-4.0983222	-2.9698035
H	-5.2138737	-4.1407592	-4.0438619
C	-4.4127136	-2.9577070	-2.4458293
O	-4.2231561	-1.8939291	-4.5757060
C	-4.0273131	-1.8403148	-3.3609872
C	-3.4180336	-0.6434840	-2.7546755
H	-3.1640234	0.1770709	-3.4262392
H	0.0278236	4.3436722	3.0387748
C	1.3880682	2.9055237	1.2915782
O	2.1811513	3.5031061	1.9795154
O	1.7793187	2.1862329	0.1539535

C	3.0970948	1.8109224	0.0865087
C	3.5875644	0.9074550	1.1807524
C	3.8504925	2.1383663	-0.9821853
C	5.0076373	0.4787894	1.0922779
C	5.2441054	1.6797355	-1.1165850
H	3.4566678	2.7679977	-1.7805310
C	5.5490260	-0.3098309	2.1156593
C	5.8047355	0.8414786	-0.0131335
C	6.8755885	-0.7318751	2.0415594
C	7.1332657	0.4086845	-0.0814088
C	7.6670434	-0.3732600	0.9430218
H	7.7285551	0.6984873	-0.9479046
H	8.7041308	-0.7064166	0.8873173
H	4.9115091	-0.5788527	2.9582286
H	7.2962996	-1.3435021	2.8405398
O	2.8240669	0.5336238	2.0644220
O	5.9143179	1.9987078	-2.0991888

Receptor 5

C	1.7021019	-1.2113544	6.6798320
C	2.0066154	-2.2678705	7.5528747
C	1.3880260	-3.5070720	7.3932453
H	1.6236699	-4.3253555	8.0737376
H	2.7290651	-2.0940222	8.3503341
C	2.3901516	0.0833638	6.8995813
O	3.2332959	0.3182953	7.7311623
O	1.9777129	1.0350089	5.9573911
C	2.3387773	2.3337222	6.1823709
C	1.7623059	2.9717766	7.4101126
C	3.0729586	3.0237282	5.2742135
C	2.1369311	4.3841549	7.6660706
C	3.4012449	4.4667115	5.4715523
C	1.6963445	5.0082424	8.8392762

C	2.9140182	5.1003580	6.7360814
C	2.0306677	6.3387617	9.0877815
C	3.2390198	6.4383906	6.9895104
C	2.8009138	7.0534072	8.1623056
H	3.8365038	6.9766858	6.2536212
H	3.0602042	8.0946965	8.3572513
H	1.0943555	4.4303467	9.5407541
H	1.6902180	6.8224018	10.0040673
O	1.0012641	2.3358053	8.1312737
O	4.0527561	5.0980042	4.6477066
C	0.7806742	-1.4010946	5.6435047
H	0.5466737	-0.5857958	4.9640544
C	0.1658034	-2.6480088	5.4835597
C	0.4694356	-3.7002162	6.3625304
H	-0.0232444	-4.6616323	6.2164377
C	-0.8078576	-2.9162822	4.3986246
O	-1.3849017	-3.9558853	4.1895917
O	-1.0417895	-1.7624852	3.6365477
C	-1.6805418	-1.9273890	2.4405111
C	-0.9554114	-2.7525378	1.4199979
C	-2.8366957	-1.2733245	2.1652158
C	-1.6300352	-2.9414388	0.1129229
C	-3.4957371	-1.3845361	0.8305374
C	-1.0431884	-3.7739329	-0.8476183
C	-2.8412294	-2.2829194	-0.1706439
C	-1.6619404	-3.9543371	-2.0837242
C	-3.4525300	-2.4636485	-1.4169308
C	-2.8659051	-3.2985598	-2.3679177
H	-4.3875798	-1.9406351	-1.6179457
H	-3.3485849	-3.4395157	-3.3357655
H	-0.1034185	-4.2691994	-0.6022182
H	-1.2064466	-4.6068616	-2.8293963
O	0.1514523	-3.2124553	1.6791623
O	-4.5324866	-0.7846272	0.5714444

I	3.8028712	2.1028693	3.5426816
I	-3.7776051	-0.0762435	3.6004000

Complex 4-sulfate

C	0.8844623	1.1419335	4.7925104
C	1.2776012	1.1946057	6.1404124
C	0.9905494	0.1288989	6.9935833
H	1.2773259	0.1778340	8.0441555
H	1.7938859	2.0810131	6.5102125
C	1.2072646	2.3017013	3.9223051
O	2.0711820	3.1327140	4.1386992
O	0.4263170	2.3019498	2.7927536
C	0.6267182	3.3077660	1.8709955
C	0.1810974	4.6751272	2.2624608
C	1.0717553	2.9931487	0.6372768
C	0.3619984	5.7404565	1.2427354
C	1.3436740	4.0494271	-0.3491841
H	1.2532514	1.9403581	0.3699798
C	-0.0509971	7.0467338	1.5285111
C	0.9244782	5.4427108	-0.0168193
C	0.0894108	8.0507668	0.5699391
C	1.0677544	6.4580195	-0.9683899
C	0.6494342	7.7569695	-0.6785185
H	1.4911185	6.2069508	-1.9411322
H	0.7458326	8.5395250	-1.4312159
H	-0.4890461	7.2589409	2.5038261
H	-0.2465657	9.0638335	0.7919518
O	-0.3444518	4.8779354	3.3570908
O	1.9271326	3.7858867	-1.4066258
O	-1.1792657	0.0929511	1.3832782
C	0.2459771	0.0043499	4.2777700
H	-0.0657296	-0.0340155	3.2253473
C	-0.0111412	-1.0730529	5.1408383

C	0.3370736	-1.0011837	6.4976320
H	0.1055729	-1.8429805	7.1513191
C	-0.6900208	-2.3013068	4.6362227
O	-1.3286486	-3.0909962	5.3115169
O	-0.5237451	-2.3843178	3.2938737
C	-1.1324774	-3.3647674	2.5246704
C	-0.6002270	-4.7240893	2.5776967
C	-2.0271084	-2.9353287	1.5995596
C	-1.0959862	-5.6538614	1.5172726
C	-2.5846692	-3.8481304	0.5938220
H	-2.3774395	-1.9051883	1.6144088
C	-0.6299984	-6.9729120	1.4937180
C	-2.0012977	-5.2185741	0.5250965
C	-1.0251825	-7.8420658	0.4766374
C	-2.3902878	-6.0958435	-0.4936205
C	-1.8967769	-7.4007487	-0.5259934
H	-3.0833414	-5.7368788	-1.2552820
H	-2.1923024	-8.0761103	-1.3297665
H	0.0654393	-7.2932260	2.2683563
H	-0.6403205	-8.8618425	0.4559174
O	0.2367178	-5.0780286	3.4205573
O	-3.5238918	-3.5037867	-0.1333748
S	-0.4304863	-0.3717725	0.1728190
O	1.0377745	-0.0500052	0.3119642
O	-0.9785525	0.2899009	-1.0535466
O	-0.5529057	-1.8768594	0.0332305
C	1.2564119	-1.2206951	-4.3481290
C	1.4824927	-1.3172772	-5.7310465
C	0.8738442	-0.4179273	-6.6064975
H	1.0320472	-0.5080807	-7.6812631
H	2.1220223	-2.1155060	-6.1089349
C	1.8969870	-2.2393353	-3.4721317
O	2.9035236	-2.8690179	-3.7488728
O	1.2229162	-2.3621124	-2.2907190

C	1.6190780	-3.3424245	-1.4008630
C	1.4472235	-4.7519480	-1.8201347
C	1.9525998	-2.9797625	-0.1437570
C	1.8735388	-5.7855796	-0.8350003
C	2.3582617	-3.9800513	0.8504667
H	1.9407485	-1.9265373	0.1529008
C	1.8541669	-7.1361102	-1.2019347
C	2.3030682	-5.4188254	0.4578951
C	2.2710637	-8.1146521	-0.2980398
C	2.7036205	-6.4065023	1.3630443
C	2.6941728	-7.7505392	0.9857151
H	3.0110950	-6.1015407	2.3630492
H	3.0078499	-8.5172312	1.6950713
H	1.5118127	-7.4041571	-2.2014579
H	2.2571779	-9.1650753	-0.5907282
O	0.9511145	-5.0419382	-2.9122894
O	2.7814999	-3.6251224	1.9568924
C	0.4675975	-0.1852989	-3.8242658
H	0.2663802	-0.0964290	-2.7496116
C	-0.1131165	0.7294469	-4.7149744
C	0.0600622	0.5969849	-6.1011691
H	-0.4274453	1.3053541	-6.7720098
C	-0.9641716	1.8425978	-4.2183241
O	-1.9788607	2.2541432	-4.7491532
O	-0.4603272	2.3475908	-3.0478354
C	-1.1093956	3.3973448	-2.4389807
C	-1.0800656	4.7109390	-3.1433704
C	-1.6026555	3.2301132	-1.1929037
C	-1.7802098	5.8319342	-2.4662333
C	-2.2043953	4.3561100	-0.4651136
H	-1.5298332	2.2390653	-0.7229527
C	-1.8768430	7.0722775	-3.1081976
C	-2.3071002	5.6698699	-1.1668824
C	-2.4943440	8.1467233	-2.4667228

C	-2.9083490	6.7568825	-0.5259725
C	-3.0067032	7.9898332	-1.1741091
H	-3.2897448	6.6212443	0.4860358
H	-3.4785496	8.8326345	-0.6681423
H	-1.4571011	7.1815455	-4.1084369
H	-2.5697229	9.1103461	-2.9714728
O	-0.4708339	4.8450063	-4.2053318
O	-2.6105454	4.2071541	0.6934401

Complex 5-sulfate

C	1.5076276	-1.2592844	6.4710227
C	2.0582893	-2.3263404	7.1954527
C	1.4844398	-3.5950564	7.1127390
H	1.9133033	-4.4255348	7.6757683
H	2.9373809	-2.1388195	7.8126057
C	2.1622716	0.0707687	6.5834203
O	3.3050577	0.2661203	6.9431336
O	1.2978925	1.0692300	6.1967577
C	1.7368061	2.3797283	6.2780769
C	1.8986105	2.9108341	7.6416272
C	1.8718657	3.1077882	5.1288438
C	2.3652387	4.3245131	7.7462604
C	2.2567904	4.5460310	5.2235236
C	2.6188130	4.8753430	9.0086032
C	2.5383390	5.1064612	6.5917411
C	3.0506269	6.1963500	9.1210541
C	2.9671278	6.4340602	6.7122229
C	3.2256705	6.9769215	7.9707299
H	3.0883784	7.0182924	5.7993598
H	3.5636019	8.0112783	8.0580563
H	2.4685086	4.2426354	9.8842915
H	3.2516095	6.6219047	10.1061780
O	1.6481729	2.2359259	8.6449058

O	2.3548587	5.2693986	4.2367889
O	0.2047030	-0.8117408	1.9454196
C	0.4092052	-1.4702616	5.6295393
H	0.0311589	-0.6636463	5.0039102
C	-0.1739412	-2.7416541	5.5645754
C	0.3594629	-3.7997919	6.3132785
H	-0.1157657	-4.7782141	6.2367566
C	-1.3641987	-3.0115628	4.7131540
O	-2.0494393	-4.0091404	4.7490075
O	-1.7063251	-1.8729690	3.9845869
C	-2.0489770	-1.9838082	2.6758559
C	-1.1803587	-2.8972501	1.8621817
C	-3.0480573	-1.2410746	2.1388325
C	-1.4396500	-2.9183439	0.4080892
C	-3.3852225	-1.3098355	0.7057665
C	-0.6084360	-3.6691250	-0.4305513
C	-2.5134899	-2.1882933	-0.1349250
C	-0.8673317	-3.7298683	-1.7968497
C	-2.7817293	-2.2770632	-1.5056135
C	-1.9726260	-3.0562860	-2.3288717
H	-3.6218644	-1.7106544	-1.9062043
H	-2.1945120	-3.1175513	-3.3940436
H	0.2582520	-4.1675731	-0.0017237
H	-0.1938002	-4.2818576	-2.4543204
O	-0.3763635	-3.6402770	2.4286426
O	-4.3505798	-0.7162306	0.2232690
S	0.2308675	0.0319179	0.7124193
O	1.2261709	1.1568091	0.9024129
O	-1.1506523	0.6090914	0.4919528
O	0.6308364	-0.7598197	-0.4902143
C	1.8728061	-2.4709774	-4.0355245
C	1.8911627	-3.6798782	-4.7451630
C	0.8045402	-4.0413777	-5.5417692
H	0.8096226	-4.9935146	-6.0747608

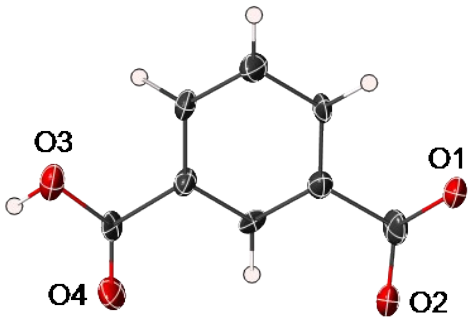
H	2.7623870	-4.3268473	-4.6402331
C	3.0470496	-2.1398868	-3.1833133
O	4.1083135	-2.7230752	-3.1830145
O	2.8303618	-0.9424363	-2.5037100
C	3.1797439	-0.8347913	-1.1958575
C	2.8055113	-2.0047140	-0.3348880
C	3.7396798	0.2968659	-0.7021526
C	3.0327972	-1.8447832	1.1161611
C	4.0607473	0.4469201	0.7289345
C	2.6118871	-2.8487568	1.9954916
C	3.6618709	-0.6891920	1.6165075
C	2.8509846	-2.7256055	3.3612335
C	3.9229896	-0.5871966	2.9876566
C	3.5320741	-1.6061438	3.8530479
H	4.4181460	0.3110829	3.3548602
H	3.7407218	-1.5131310	4.9187732
H	2.0641633	-3.7002958	1.5973367
H	2.4841575	-3.4890893	4.0489528
O	2.4228855	-3.0521508	-0.8601537
O	4.6583399	1.4276689	1.1740916
C	0.7713325	-1.6117941	-4.1375540
H	0.7313594	-0.7016681	-3.5415081
C	-0.2951676	-1.9578937	-4.9757801
C	-0.2880806	-3.1821391	-5.6598772
H	-1.1506086	-3.4407784	-6.2748543
C	-1.4890801	-1.0846070	-5.1257501
O	-2.5937180	-1.4540613	-5.4676303
O	-1.1825199	0.2162233	-4.7977350
C	-2.1766666	1.1714129	-4.9253854
C	-2.5761041	1.4919223	-6.3057399
C	-2.6239547	1.8185654	-3.8073448
C	-3.6498354	2.5169538	-6.4588406
C	-3.6264137	2.9132742	-3.9559015
C	-4.1468659	2.8098273	-7.7348743

C	-4.1543014	3.1954961	-5.3365201
C	-5.1475755	3.7678564	-7.8922824
C	-5.1547788	4.1610773	-5.5025235
C	-5.6528341	4.4442836	-6.7741093
H	-5.5235888	4.6754094	-4.6142593
H	-6.4363789	5.1943256	-6.8971969
H	-3.7293508	2.2687975	-8.5849659
H	-5.5371099	3.9904740	-8.8876041
O	-2.0469584	0.9577156	-7.2853412
O	-4.0297207	3.5727593	-3.0024207
I	1.5432655	2.2403488	3.2254550
I	-1.9253505	1.3038254	-1.8767173
I	4.1528228	1.9331827	-1.9554759
I	-4.1610539	0.0909282	3.3247104

PART VII: Fast scan X-ray data.

Fast scan crystal data for 3-carboxybenzoate of tetrabuthylammonium: $C_{24}H_{41}NO_4$, M = 407.58, triclinic, a = 12.483(9), b = 13.829(8), c = 14.388(12) Å, α = 78.81(2)º, β = 83.38(4)º, γ = 75.57(2)º, V = 2354(3) Å^3, space group Pī, Z = 4, T = 120(2) K, λ = 0.71073 Å, D_{calcd} = 1.150 gcm^{-3}, μ = 0.077 cm^{-1}, 13290 reflections measured by a FAST SCAN of 180 frames at a rate 1s/frame, 7559 unique, 2125 observed (28%), R_{int} = 0.2955, colourless crystals obtained by Et_2O/CH_3CN vapor diffusion, crystal structure solved by dual-space methods with all non hydrogen atoms refined anisotropically on F^2 using the programs SHELXT and SHELXL-2018, there is two independent molecules in the asymmetric unit, one of the independent molecules OH hydrogen atom is probably disordered over two positions, hydrogen atoms were included using a *riding* model, GOF = 0.981, R (F_o, I > 2σ(I)) = 0.1303, R_w (F_o^2, all data) = 0.3275. The 180 frames fast scan shows an electron density map that was preliminary refined for all non-hydrogen atoms, with a good convergence and a C-C bond precision of 0.01462 Å.

CCDC 1915912 contains the supplementary fast scan crystallographic data. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures.



PART VIII: Detection Limits.

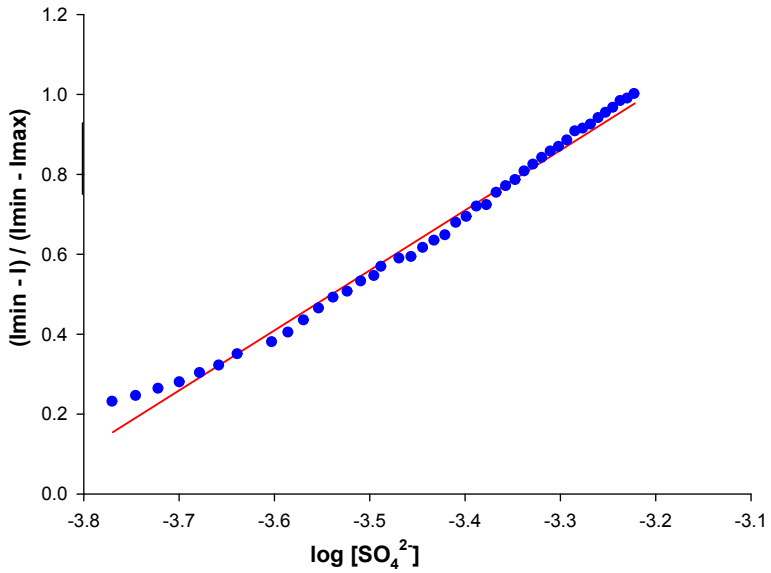


Figure S41. Fluorescence intensity of 4 (in CH_3CN) at each concentration of SO_4^{2-} added, normalized between the minimum fluorescence intensity, found at zero equiv of SO_4^{2-}; and the maximum fluorescence intensity, found at $[SO_4^{2-}]= 1.34 \times 10^{-4}$ M.

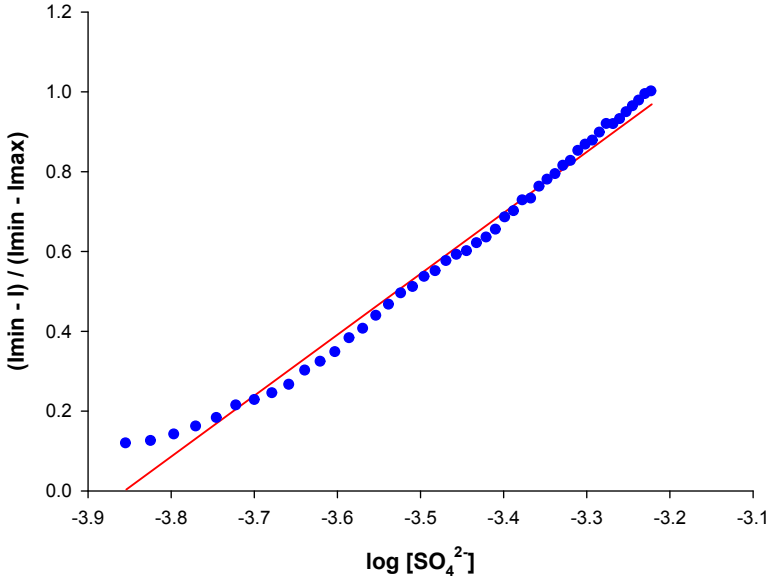


Figure S42. Fluorescence intensity of 4 (in CH_3CN) at each concentration of SO_4^{2-} added, normalized between the minimum fluorescence intensity, found at zero equiv of SO_4^{2-}; and the maximum fluorescence intensity, found at $[SO_4^{2-}]= 1.39 \times 10^{-4}$ M.