Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Contribution of C-H Hydrogen Bonds on anion binding

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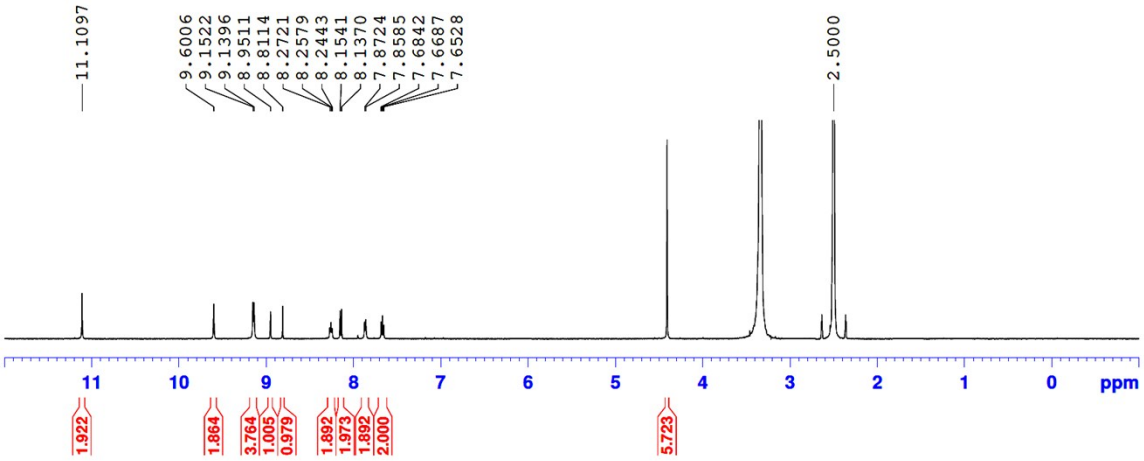


Fig S1. ^{1}H NMR spectrum of compound **1**

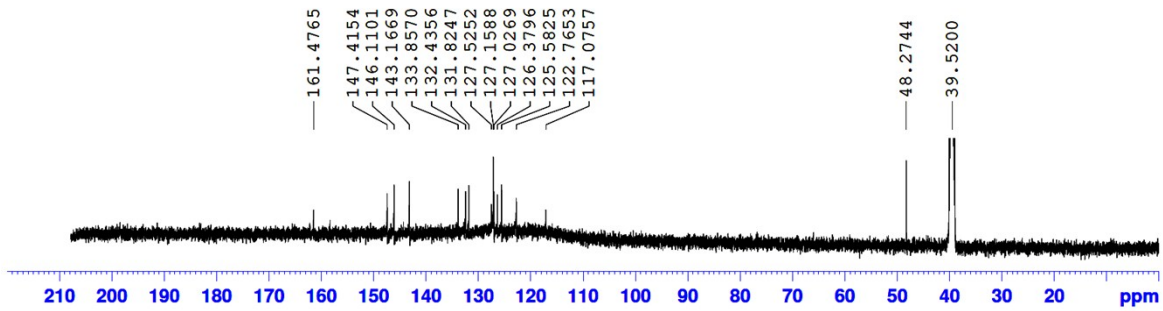


Fig S2. ^{13}C NMR spectrum of compound **1**

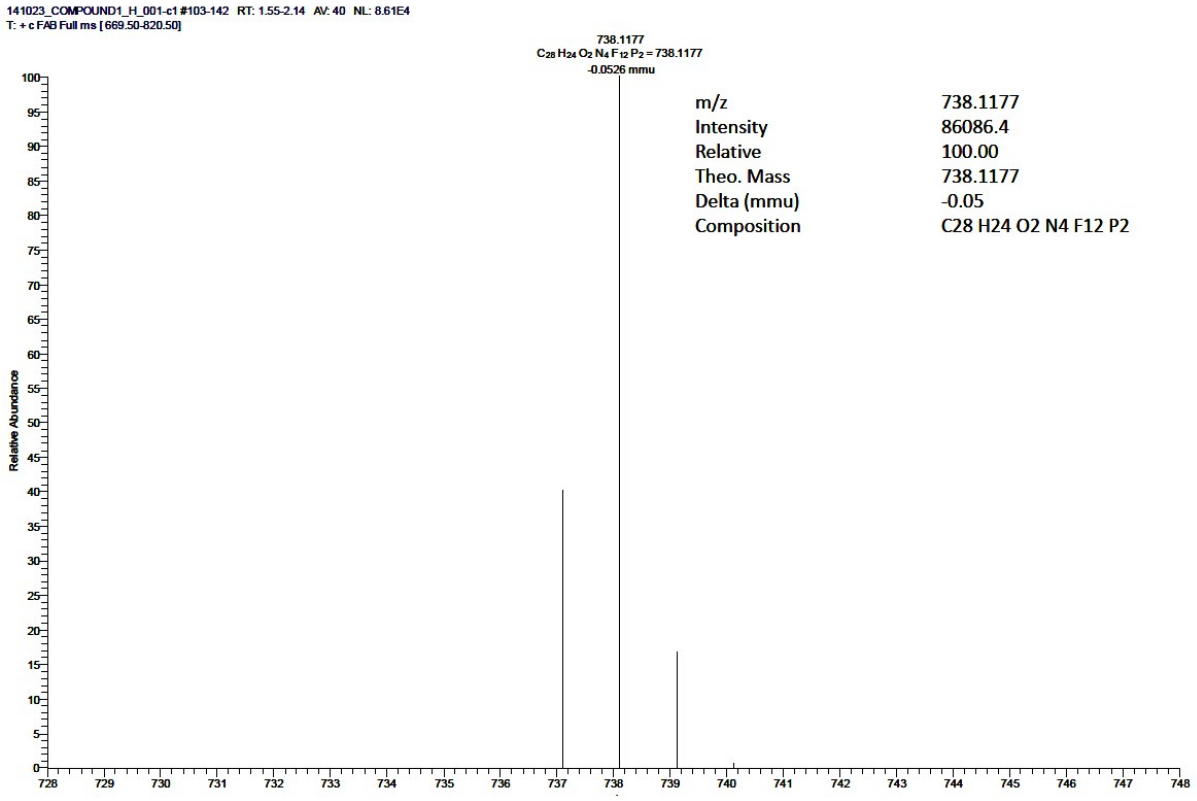


Fig S3. HRMS(FAB) spectrum of compound **1**

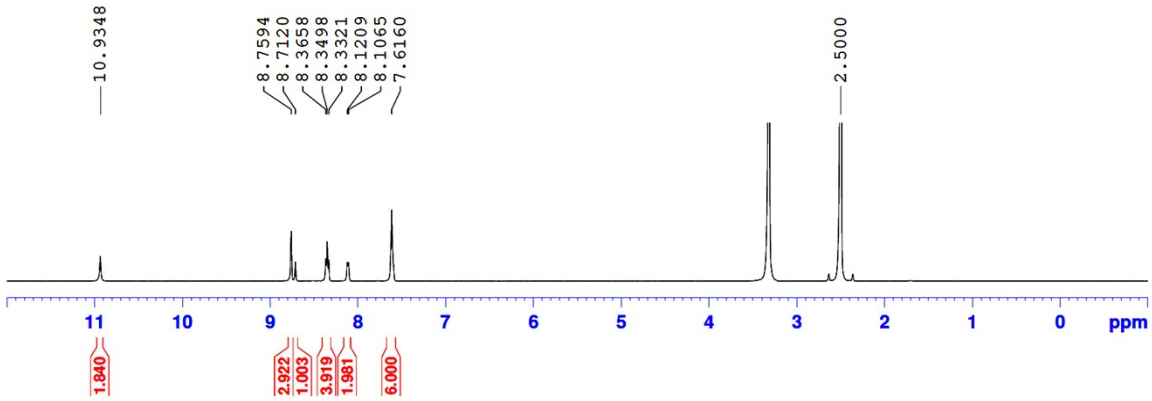


Fig S4. ^{1}H NMR spectrum of compound **2**

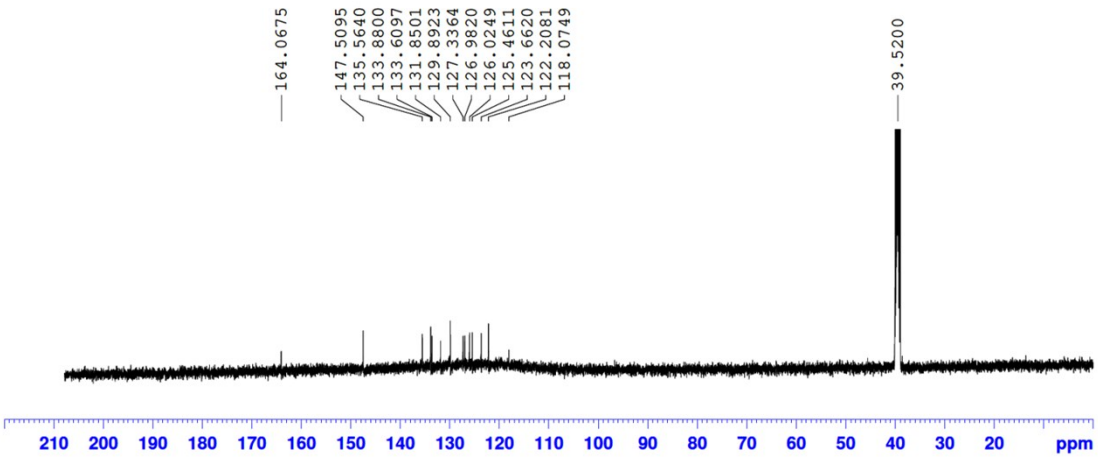


Fig S5. ^{13}C NMR spectrum of compound **2**

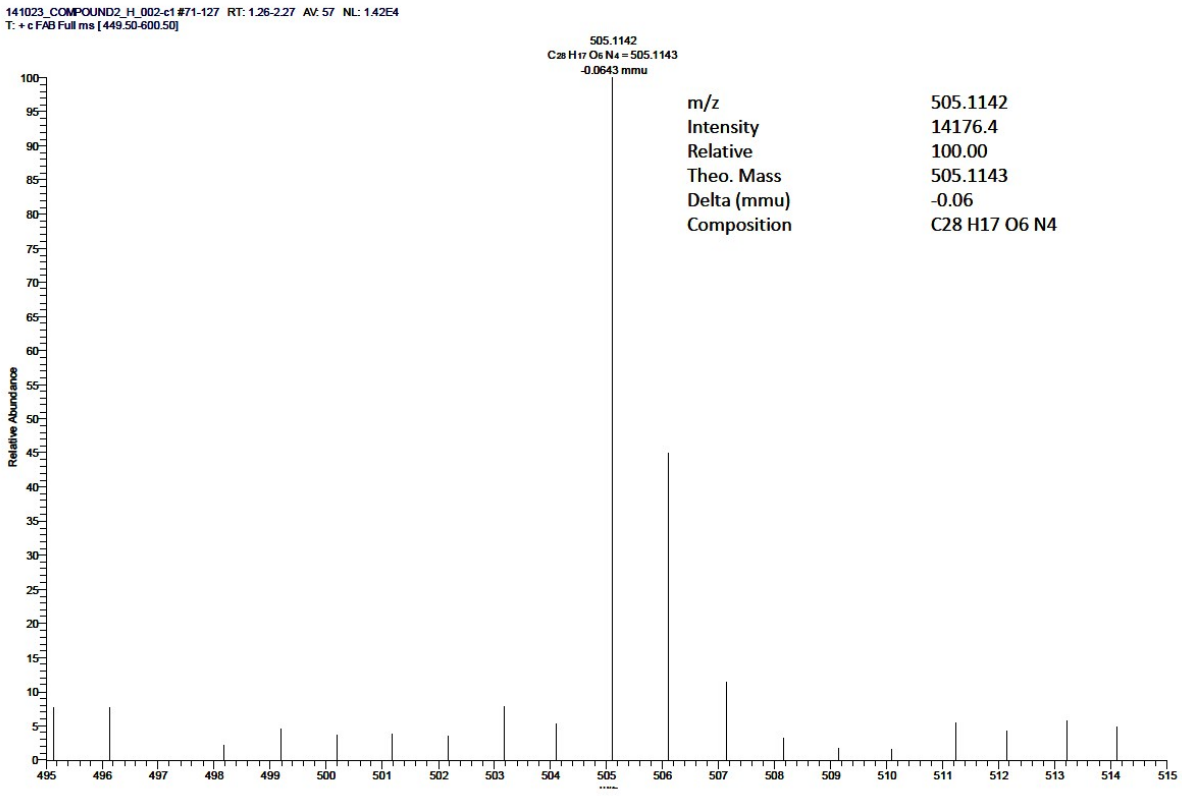


Fig S6. HRMS(FAB) spectrum of compound **2**

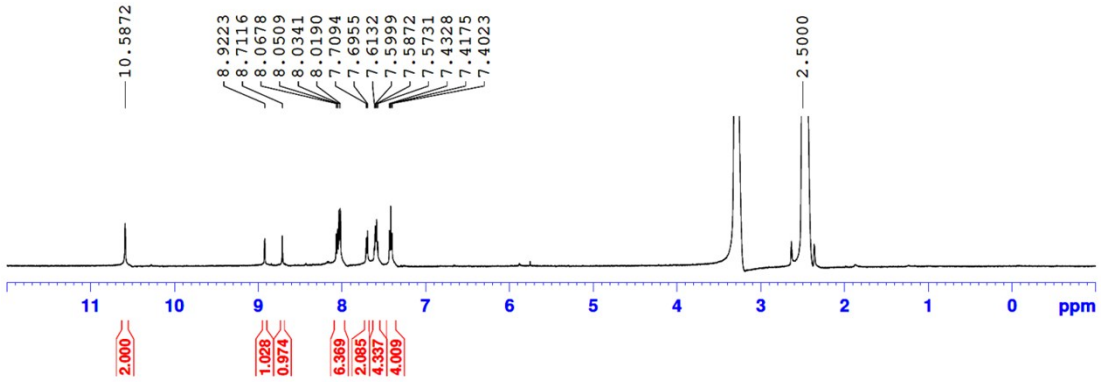


Fig S7 ^{1}H NMR spectrum of compound **3**

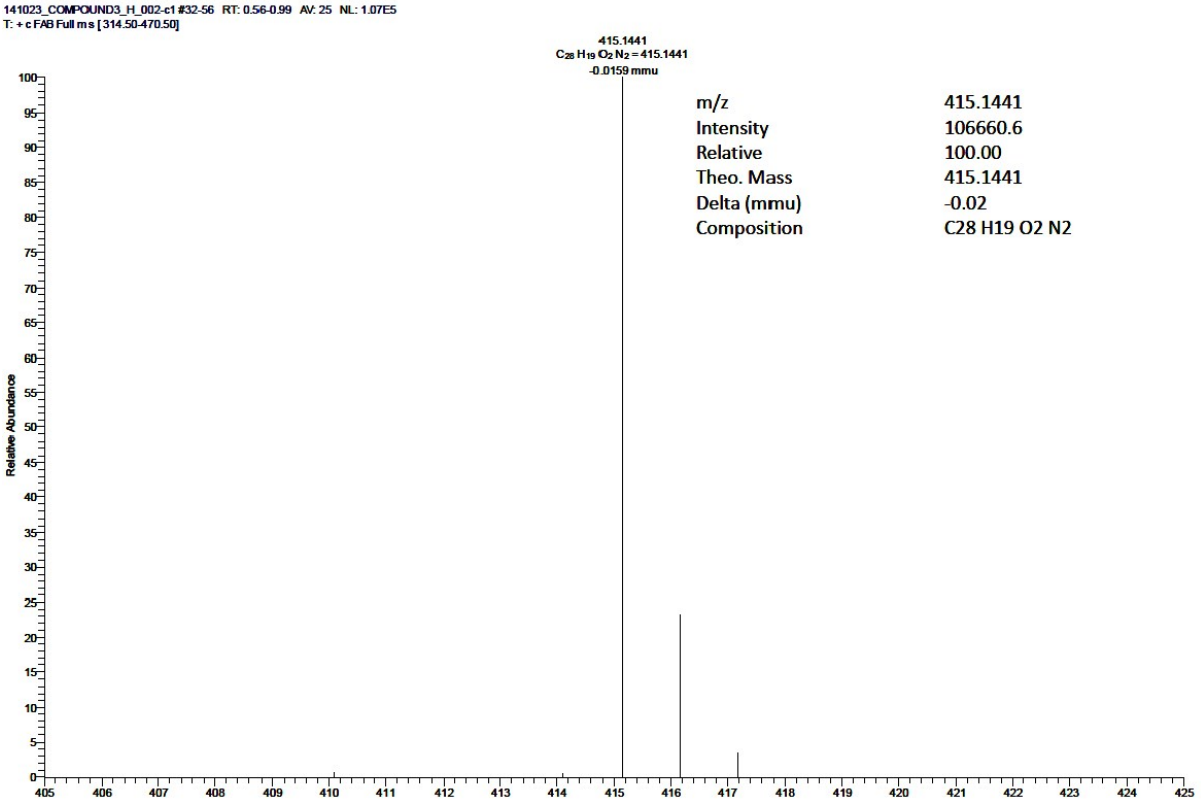


Fig S8. HRMS(FAB) spectrum of compound **3**

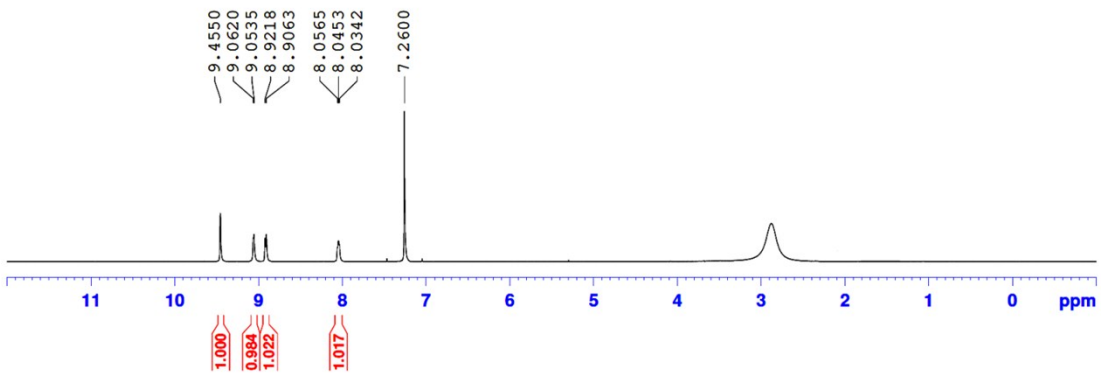


Fig S9 ^{1}H NMR spectrum of compound **4**

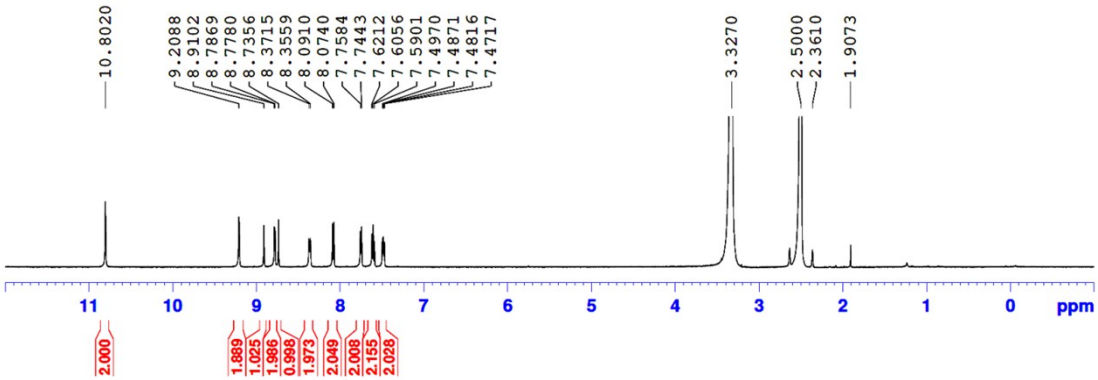
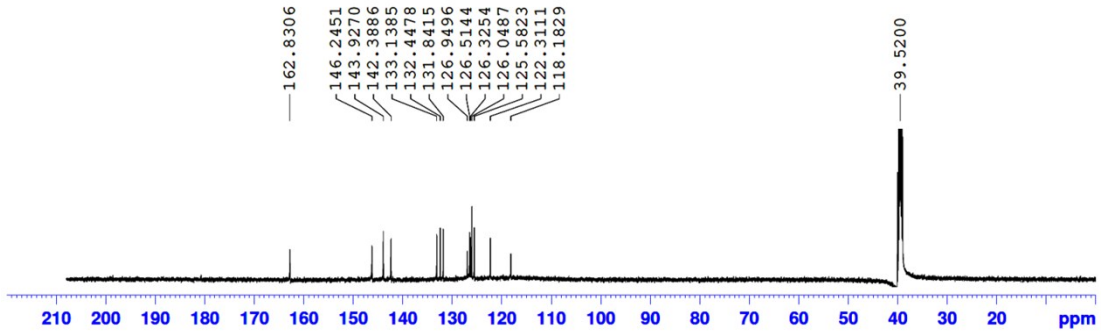


Fig S10. ^{1}H NMR spectrum of compound **5**



11. Fig S11. ^{13}C NMR spectrum of compound **5**

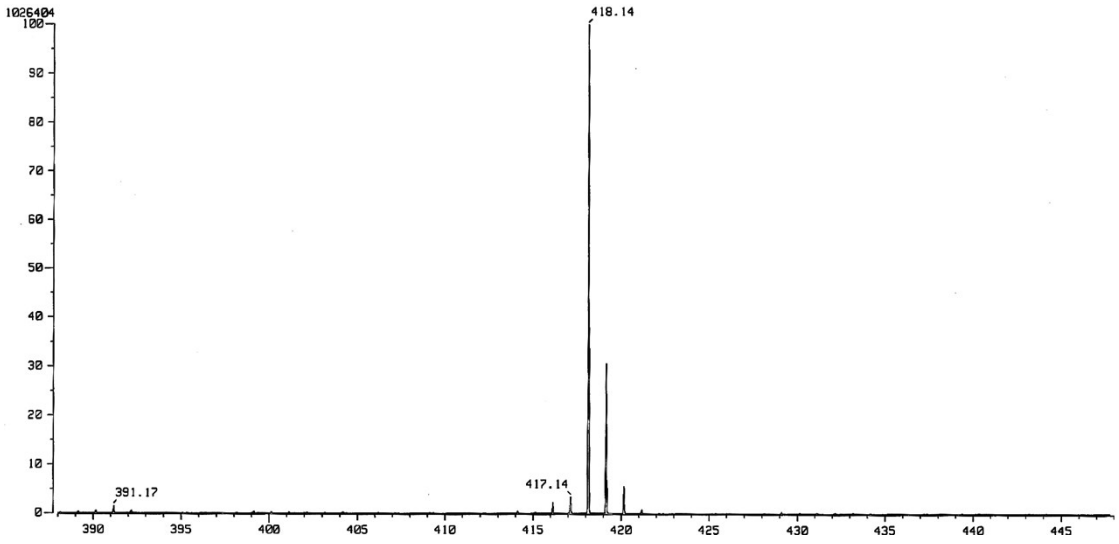


Fig S12. HRMS(EI) spectrum of compound **5**

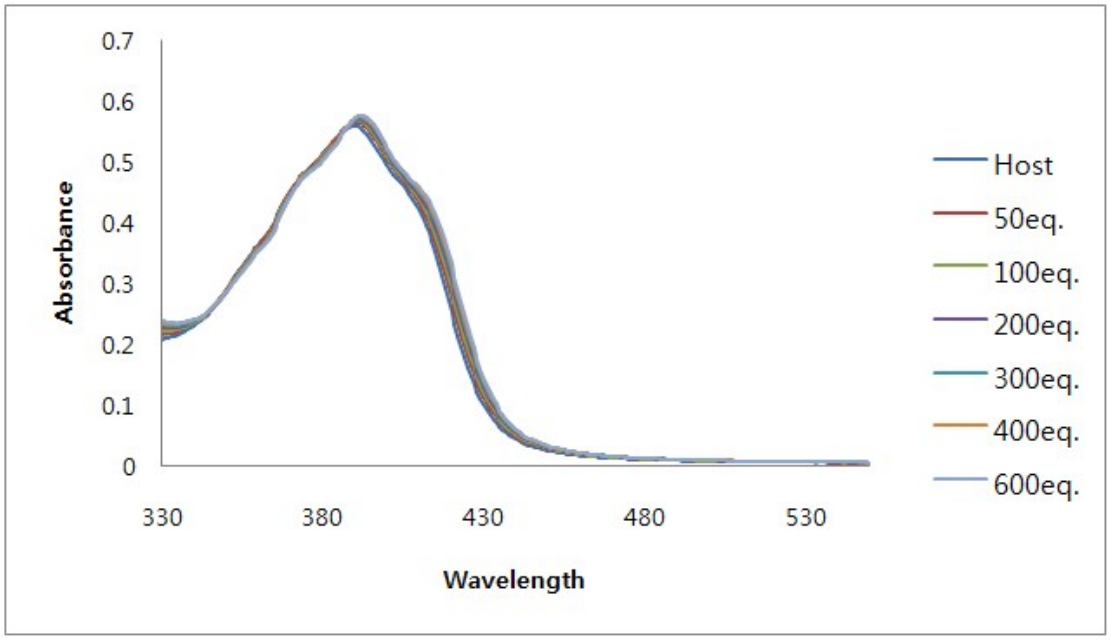


Fig S13. A family of UV-vis spectra recorded over the course of titrating a 100 μM DMSO solution of receptor **1** with increased amounts of tetrabutylammonium bromide

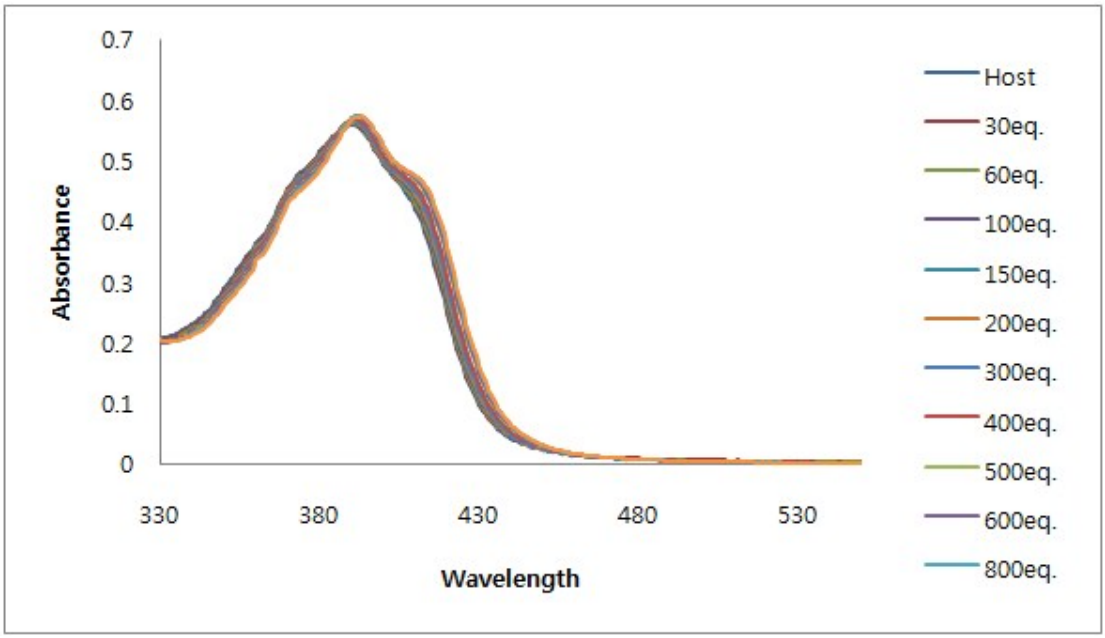


Fig S14. A family of UV-vis spectra recorded over the course of titrating a 100 μM DMSO solution of receptor **1** with increased amounts of tetrabutylammonium hydrogen sulfate

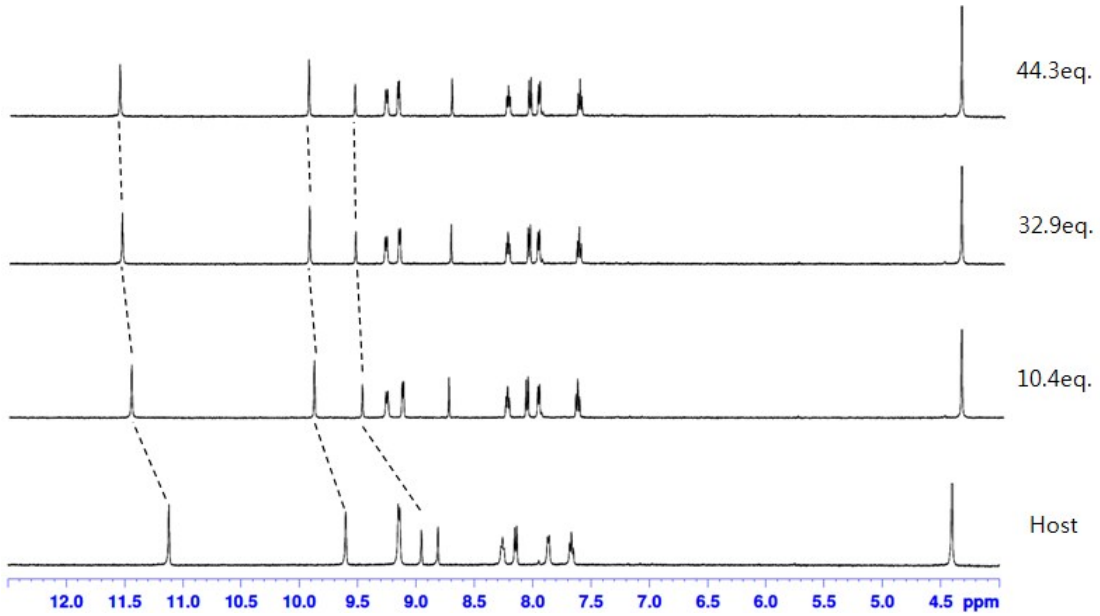


Fig S15. ^{1}H NMR spectra of 2 mM of receptor **1** containing increasing amounts of tetrabutylammonium chloride (0 –44 equiv.) in DMSO-d_6

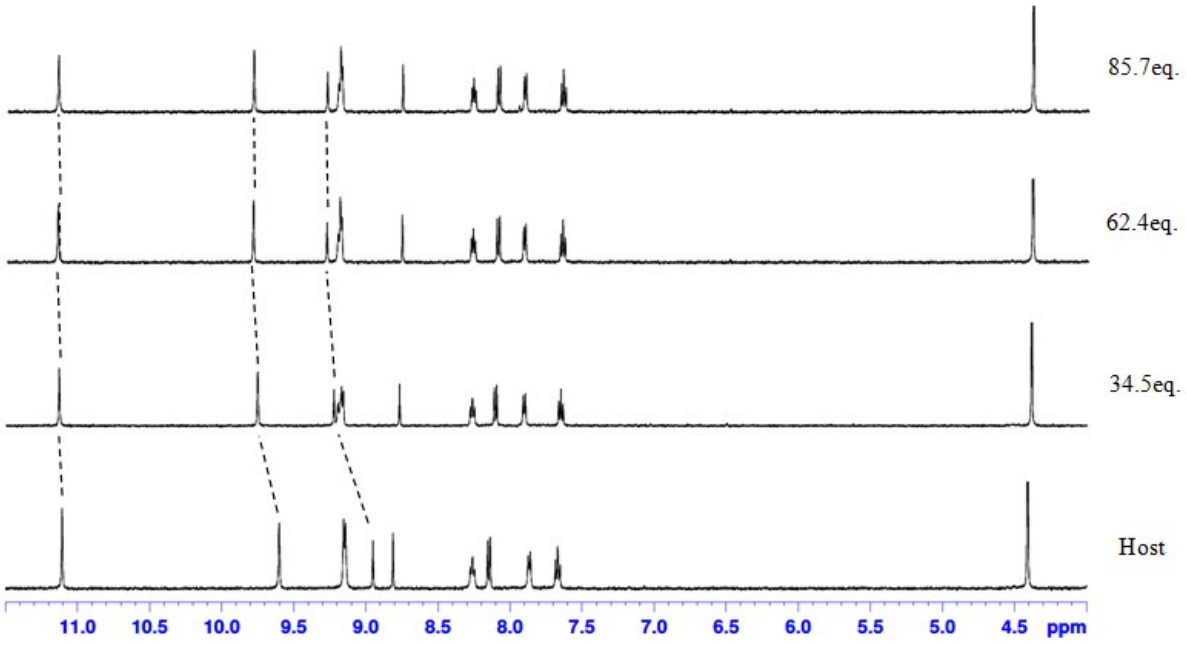


Fig S16. ^{1}H NMR spectra of 2 mM of receptor **1** containing increasing amounts of tetrabutylammonium bromide (0 –86 equiv.) in DMSO-d_6

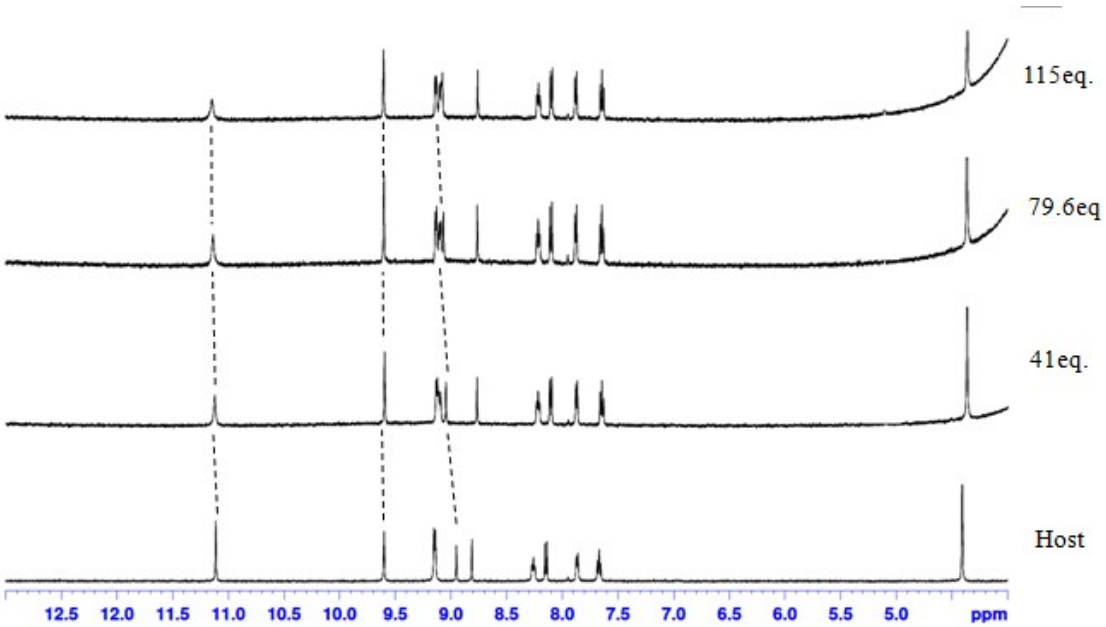


Fig S17. ^{1}H NMR spectra of 2 mM of receptor **1** containing increasing amounts of tetrabutylammonium hydrogen sulfate (0 –115 equiv.) in DMSO-d_6

Table 1. PDB file of receptor 1 in complex with $H_2PO_4^-$ anion.

TITLE	COMPLEX1 WITH H2PO4-					
HETATM	1	C	0	-3.936	4.000	-0.341
HETATM	2	C	0	-4.720	2.893	-0.182
HETATM	3	C	0	-4.134	1.592	-0.128
HETATM	4	C	0	-2.701	1.453	-0.240
HETATM	5	C	0	-1.914	2.652	-0.371
HETATM	6	C	0	-2.524	3.880	-0.428
HETATM	7	C	0	-4.918	0.443	0.004
HETATM	8	C	0	-2.141	0.169	-0.242
HETATM	9	C	0	-2.931	-0.981	-0.119
HETATM	10	C	0	-4.362	-0.839	0.010
HETATM	11	C	0	-5.178	-2.007	0.108
HETATM	12	H	0	-6.251	-1.885	0.203
HETATM	13	C	0	-4.615	-3.251	0.073
HETATM	14	C	0	-3.208	-3.404	-0.047
HETATM	15	C	0	-2.385	-2.312	-0.138
HETATM	16	H	0	-5.995	0.549	0.086
HETATM	17	H	0	-4.382	4.986	-0.387
HETATM	18	H	0	-5.798	2.982	-0.101
HETATM	19	H	0	-1.919	4.770	-0.532
HETATM	20	H	0	-1.072	0.061	-0.356
HETATM	21	H	0	-5.235	-4.137	0.146
HETATM	22	H	0	-2.779	-4.397	-0.064
HETATM	23	N	0	-0.496	2.541	-0.402
HETATM	24	C	0	0.285	3.178	-1.313
HETATM	25	H	0	-0.080	1.975	0.351
HETATM	26	O	0	-0.138	3.830	-2.260
HETATM	27	C	0	1.786	3.059	-1.135
HETATM	28	C	0	2.593	3.419	-2.217
HETATM	29	C	0	2.401	2.674	0.047
HETATM	30	H	0	2.119	3.739	-3.135
HETATM	31	H	0	1.853	2.365	0.932
HETATM	32	C	0	4.536	2.975	-0.901
HETATM	33	H	0	5.603	2.922	-0.738
HETATM	34	C	0	3.977	3.367	-2.100

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HETATM   35  N                0       -0.972   -2.476   -0.236
HETATM   36  C                0       -0.389   -3.250   -1.187
HETATM   37  H                0       -0.417   -1.999    0.488
HETATM   38  O                0       -0.998   -3.832   -2.076
HETATM   39  C                0        1.122   -3.383   -1.145
HETATM   40  C                0        1.739   -4.004   -2.233
HETATM   41  C                0        1.918   -2.953   -0.092
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HETATM   43  H                0        1.526   -2.458    0.793
HETATM   44  C                0        3.863   -3.719   -1.181
HETATM   45  H                0        4.938   -3.817   -1.125
HETATM   46  C                0        3.119   -4.168   -2.251
HETATM   47  H                0        3.620   -4.640   -3.085
HETATM   48  H                0        4.624    3.630   -2.925
HETATM   49  C                0        4.368    2.267    1.440
HETATM   50  H                0        3.706    1.582    1.965
HETATM   51  H                0        5.322    1.786    1.243
HETATM   52  H                0        4.520    3.173    2.027
HETATM   53  C                0        4.074   -2.687    1.028
HETATM   54  H                0        5.023   -2.302    0.662
HETATM   55  H                0        3.537   -1.906    1.557
HETATM   56  H                0        4.243   -3.540    1.684
HETATM   57  N                0        3.256   -3.125   -0.130
HETATM   58  N                0        3.747    2.640    0.143
HETATM   59  P                0        0.725   -0.037    2.603
HETATM   60  O                0        0.504    1.251    1.856
HETATM   61  O                0        0.389   -1.358    1.949
HETATM   62  O                0        2.302    0.005    3.044
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Table 2. PDB file of receptor 1 in complex with Cl^- anion.

TITLE	COMPLEX1 WITH CL-					
HETATM	1	C	0	-0.183	4.204	3.648
HETATM	2	C	0	-0.256	4.889	2.468
HETATM	3	C	0	-0.205	4.191	1.224
HETATM	4	C	0	-0.062	2.755	1.224
HETATM	5	C	0	-0.026	2.074	2.493
HETATM	6	C	0	-0.078	2.788	3.664
HETATM	7	C	0	-0.266	4.864	0.000
HETATM	8	C	0	0.035	2.084	0.000
HETATM	9	C	0	-0.062	2.755	-1.224
HETATM	10	C	0	-0.205	4.191	-1.224
HETATM	11	C	0	-0.256	4.889	-2.468
HETATM	12	H	0	-0.352	5.969	-2.457
HETATM	13	C	0	-0.183	4.204	-3.648
HETATM	14	C	0	-0.078	2.788	-3.664
HETATM	15	C	0	-0.026	2.074	-2.493
HETATM	16	H	0	-0.359	5.945	0.000
HETATM	17	H	0	-0.221	4.734	4.592
HETATM	18	H	0	-0.352	5.969	2.457
HETATM	19	H	0	-0.048	2.268	4.610
HETATM	20	H	0	0.195	1.017	0.000
HETATM	21	H	0	-0.221	4.734	-4.592
HETATM	22	H	0	-0.048	2.268	-4.610
HETATM	23	N	0	0.031	0.655	2.502
HETATM	24	C	0	0.793	-0.083	3.359
HETATM	25	H	0	-0.480	0.166	1.765
HETATM	26	O	0	1.574	0.375	4.179
HETATM	27	C	0	0.639	-1.581	3.248
HETATM	28	C	0	1.730	-2.390	3.575
HETATM	29	C	0	-0.558	-2.190	2.908
HETATM	30	H	0	2.659	-1.924	3.875
HETATM	31	H	0	-1.455	-1.642	2.666
HETATM	32	C	0	0.395	-4.326	3.148
HETATM	33	H	0	0.233	-5.392	3.082
HETATM	34	C	0	1.607	-3.772	3.511

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HETATM   35  N             0        0.031    0.655   -2.502
HETATM   36  C             0        0.793   -0.083   -3.359
HETATM   37  H             0       -0.480    0.166   -1.765
HETATM   38  O             0        1.574    0.375   -4.179
HETATM   39  C             0        0.639   -1.581   -3.248
HETATM   40  C             0        1.730   -2.390   -3.575
HETATM   41  C             0       -0.558   -2.190   -2.908
HETATM   42  H             0        2.659   -1.924   -3.875
HETATM   43  H             0       -1.455   -1.642   -2.666
HETATM   44  C             0        0.395   -4.326   -3.148
HETATM   45  H             0        0.233   -5.392   -3.082
HETATM   46  C             0        1.607   -3.772   -3.511
HETATM   47 Cl             0       -1.684   -1.021    0.000
HETATM   48  H             0        2.438   -4.424   -3.741
HETATM   49  H             0        2.438   -4.424    3.741
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HETATM   51  H             0       -2.343   -3.616    1.615
HETATM   52  H             0       -1.829   -5.187    2.288
HETATM   53  H             0       -2.659   -4.005    3.332
HETATM   54  C             0       -1.969   -4.131   -2.499
HETATM   55  H             0       -1.829   -5.187   -2.288
HETATM   56  H             0       -2.343   -3.616   -1.615
HETATM   57  H             0       -2.659   -4.005   -3.332
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