Visible colorimetric fluoride and hydroxide sensing by asymmetric tris-urea receptors: combined experimental and theoretical studies†

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Supplementary Information

Contents:

Fig. S1. Visible change in color of **L1** in DMSO solution on the addition of 10 equiv. of fluoride ions: (a) 1×10^{-2} M of **L1**; (b) 1×10^{-3} M of **L1**; (c) 1×10^{-4} M of **L1**; (d) 1×10^{-5} M of **L1** (a, b, c and d, left to right).

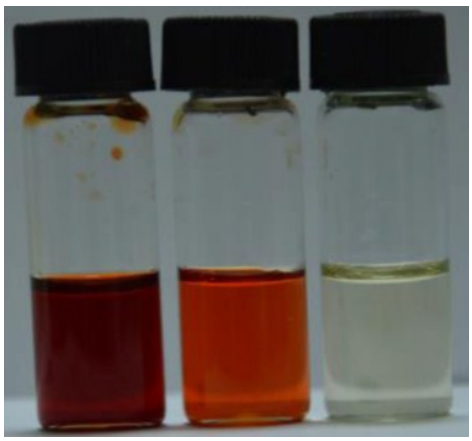

Fig. S2. Visible change in color of **L2** in DMSO solution on the addition of 10 equiv. of fluoride ions: (a) 1×10^{-2} M of **L2**; (b) 1×10^{-3} M of **L2**; (c) 1×10^{-4} M of **L2** (a, b, and c, left to right).

Fig. S3. Visible change in color of **L3** in DMSO solution on the addition of 10 equiv. of fluoride ions: (a) 1×10^{-2} M of **L3**, (b) 1×10^{-3} M of **L3**, (c) 1×10^{-4} M of **L3** (a, b, and c, left to right).

Fig. S4. Visible change in color of **L1** in DMSO solution on the addition of 10 equiv. of hydroxide ions: (a) 1×10^{-2} M of **L1**; (b) 1×10^{-3} M of **L1**; (c) 1×10^{-4} M of **L1**; (a, b, and c left to right).

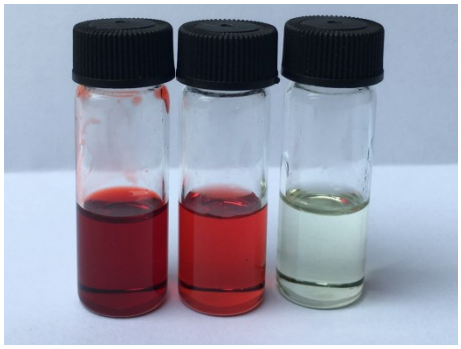

Fig. S5. Visible change in color of **L2** in DMSO solution on the addition of 10 equiv. of hydroxide ions: (a) 1×10^{-2} M of **L2**; (b) 1×10^{-3} M of **L2**; (c) 1×10^{-4} M of **L2** (a, b, and c, left to right).

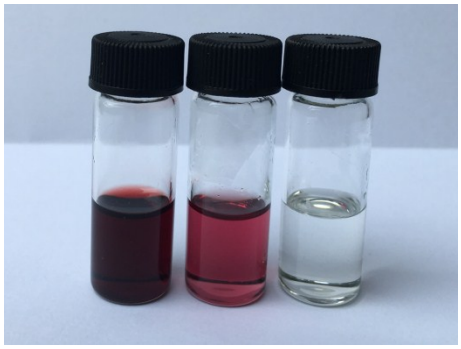

Fig. S6. Visible change in color of **L3** in DMSO solution on the addition of 10 equiv. of hydroxide ions: (a) 1×10^{-2} M of **L3**, (b) 1×10^{-3} M of **L3**, (c) 1×10^{-4} M of **L3** (a, b, and c, left to right).

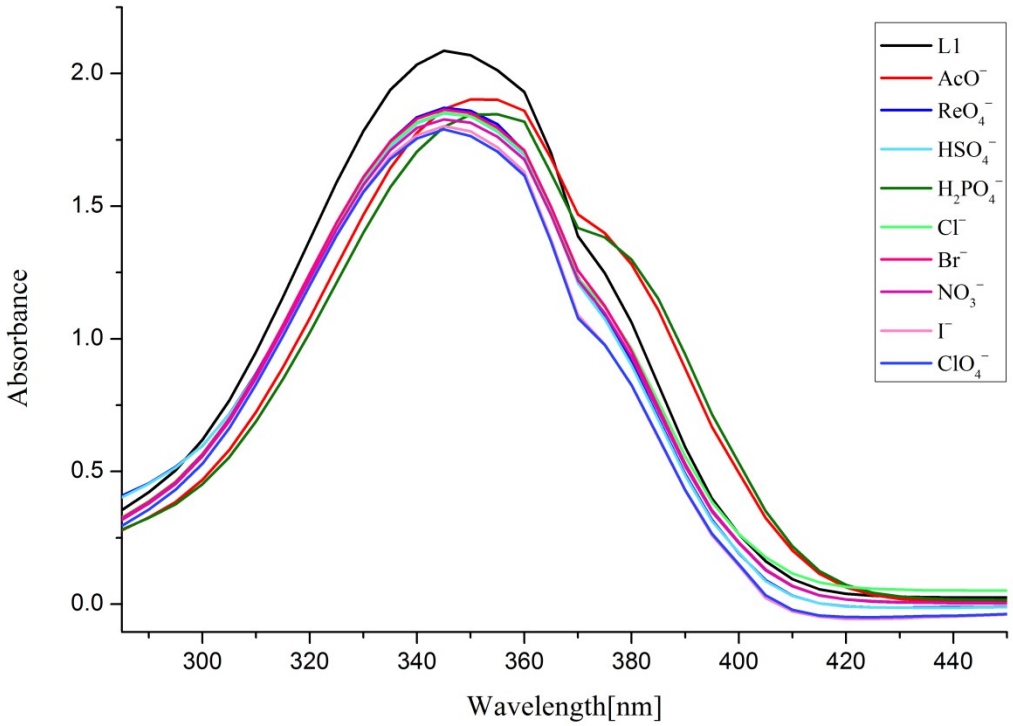

Fig. S7. UV–Vis spectral changes of **L1** (5×10^{-5} M) in DMSO solution on the addition of 10 equiv. of TBA anions or $[NH_4][ReO_4]$.

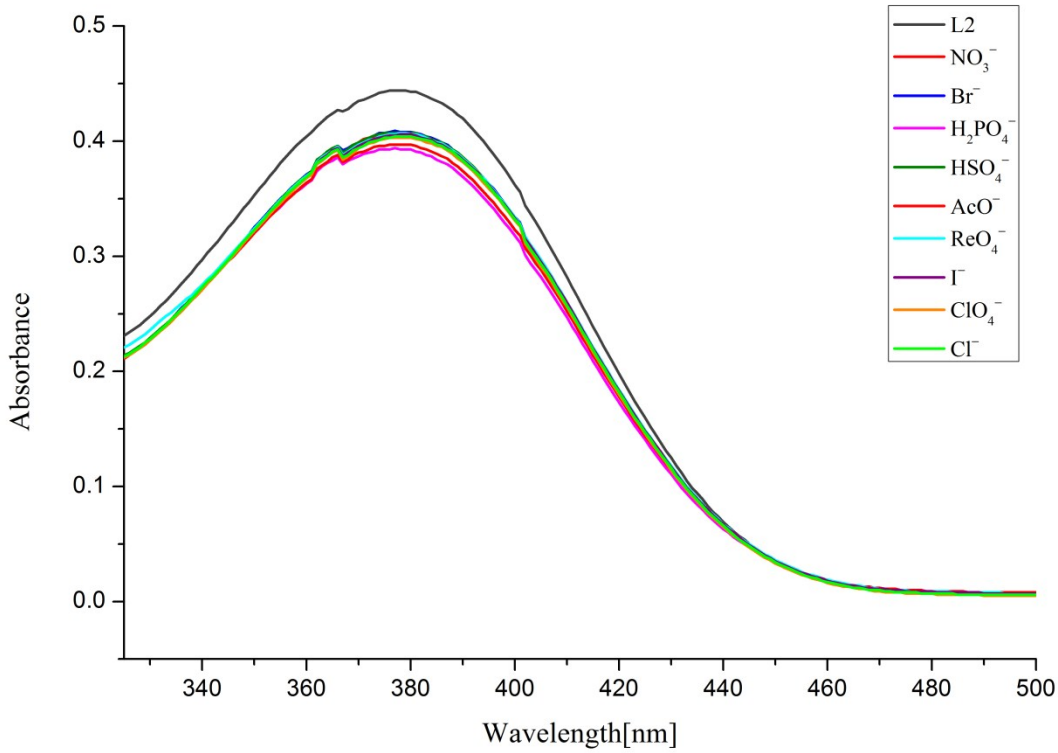

Fig. S8. UV–Vis spectral changes of **L2** (5×10^{-5} M) in DMSO solution on the addition of 10 equiv. of TBA anions or $[NH_4][ReO_4]$.

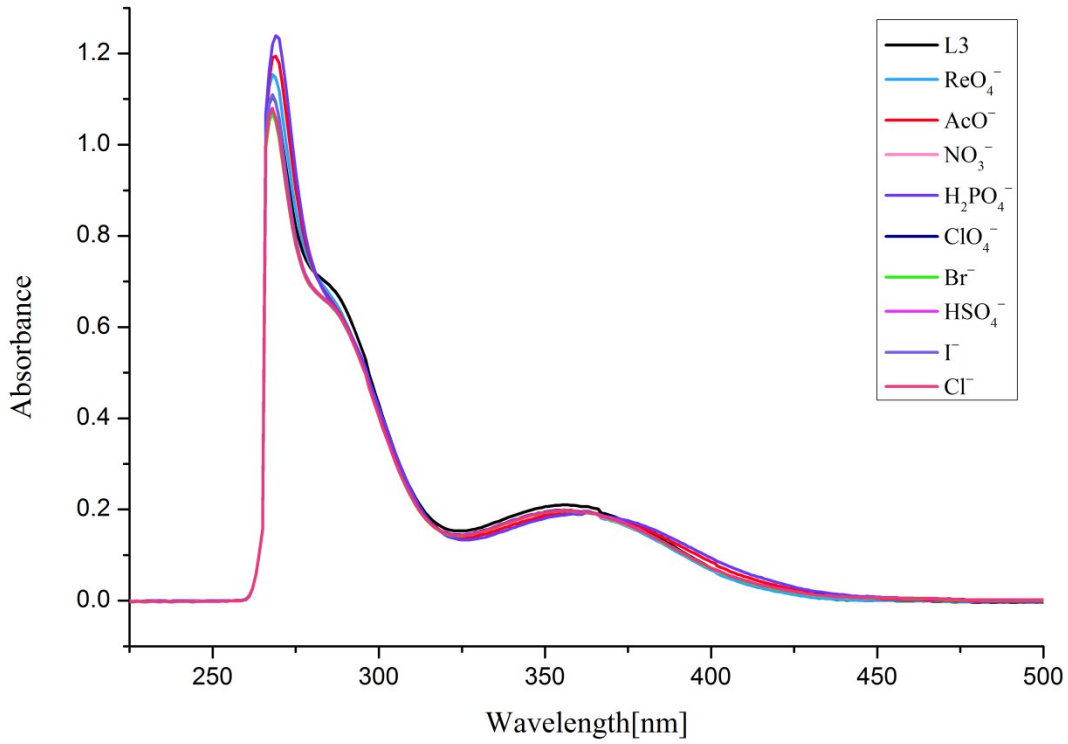

Fig. S9. UV–Vis spectral changes of **L3** (5×10^{-5} M) in DMSO solution on the addition of 10 equiv. of TBA anions or $[NH_4][ReO_4]$.

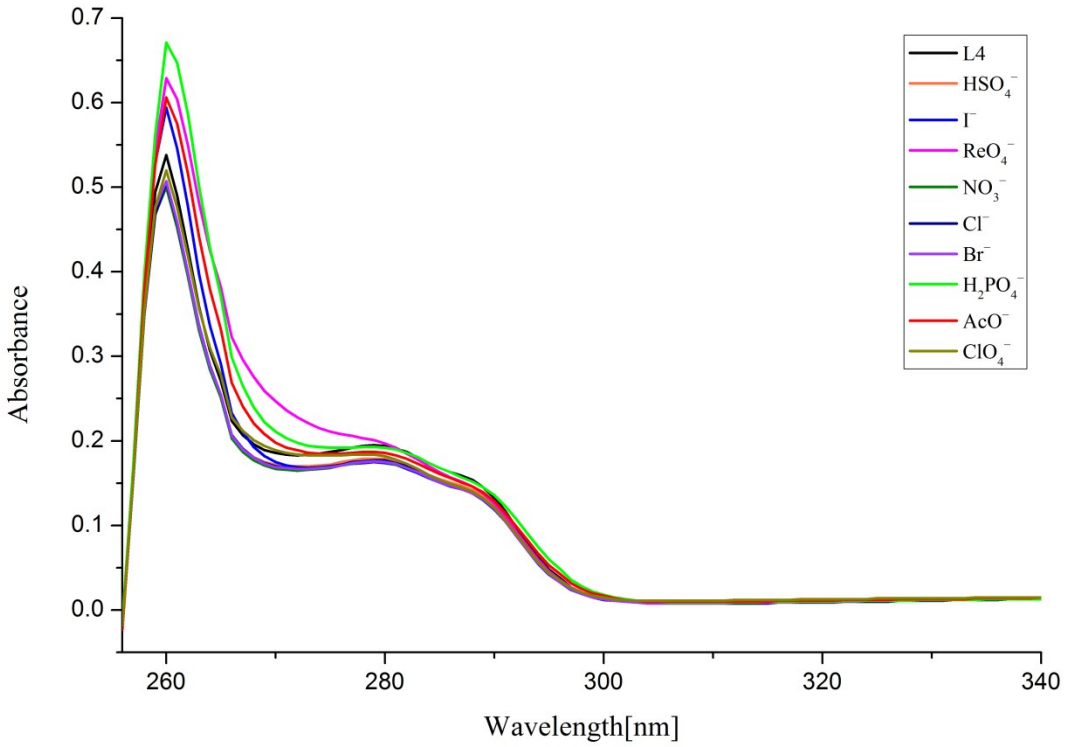

Fig. S10. UV–Vis spectral changes of **L4** (5×10^{-5} M) in DMSO solution on the addition of 10 equiv. of TBA anions or $[NH_4][ReO_4]$.

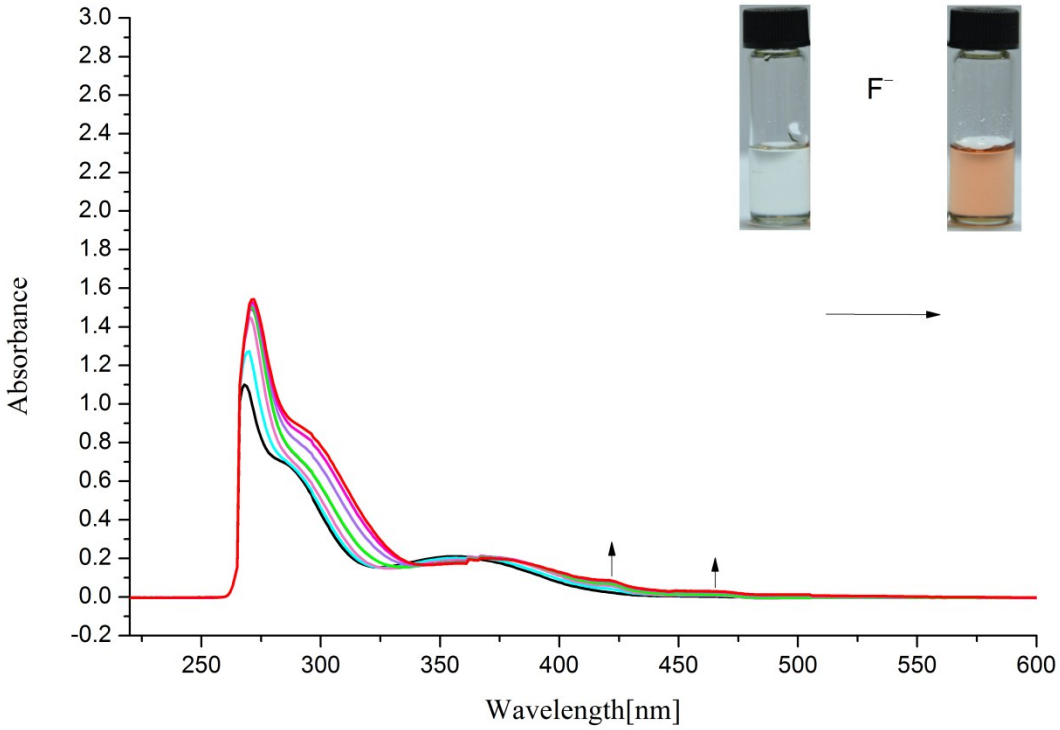

Fig. S11. UV-Vis absorption spectra of **L3** (5×10^{-5} M) to 0-100 equiv. fluoride ions in DMSO solution.

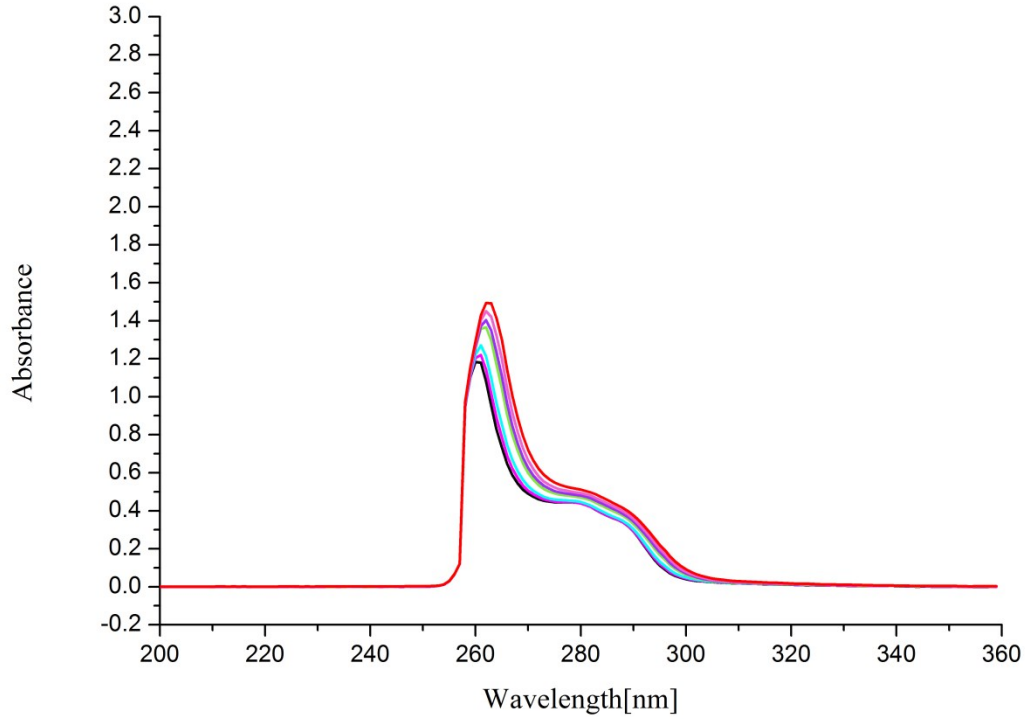

Fig. S12. UV-Vis absorption spectra of **L4** (1×10^{-4} M) to 0-230 equiv. fluoride ions in DMSO solution.

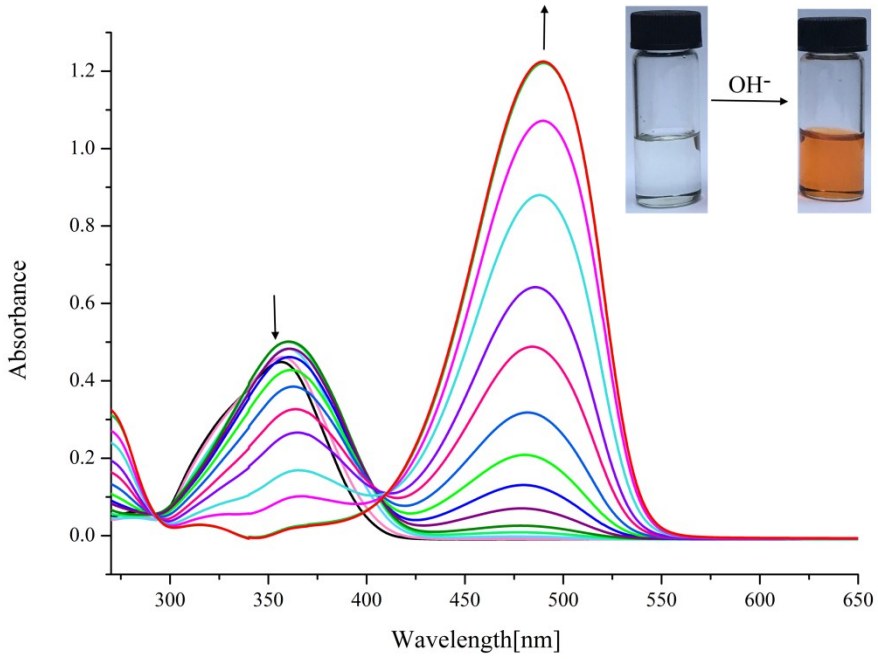

Fig. S13. UV-Vis absorption spectra of **L1** (1×10^{-5} M) to 0-120 equiv. of hydroxide ions in DMSO solution.

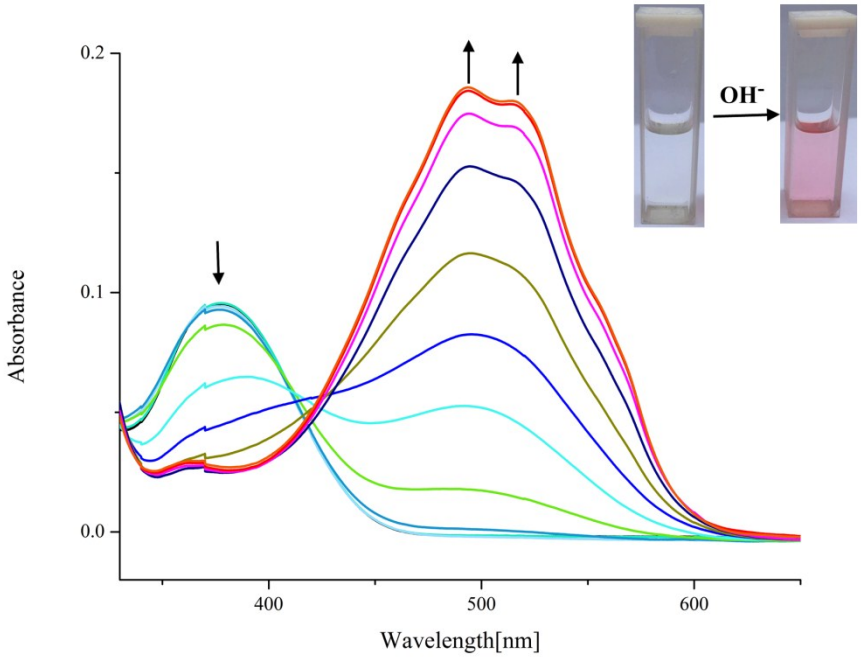

Fig. S14. UV-Vis absorption spectra of **L2** (1×10^{-5} M) to 0-150 equiv. of hydroxide ions in DMSO solution.

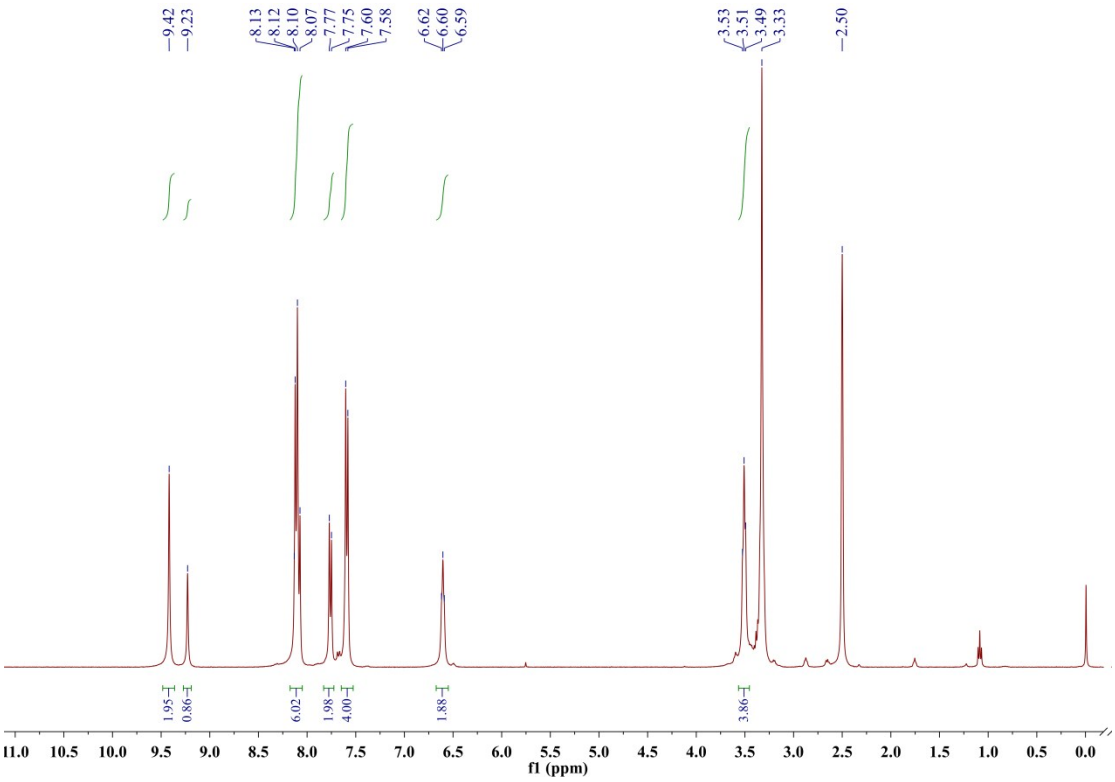

Fig. S15. ^{1}H NMR spectra of **L1** in DMSO-d_6 solution.

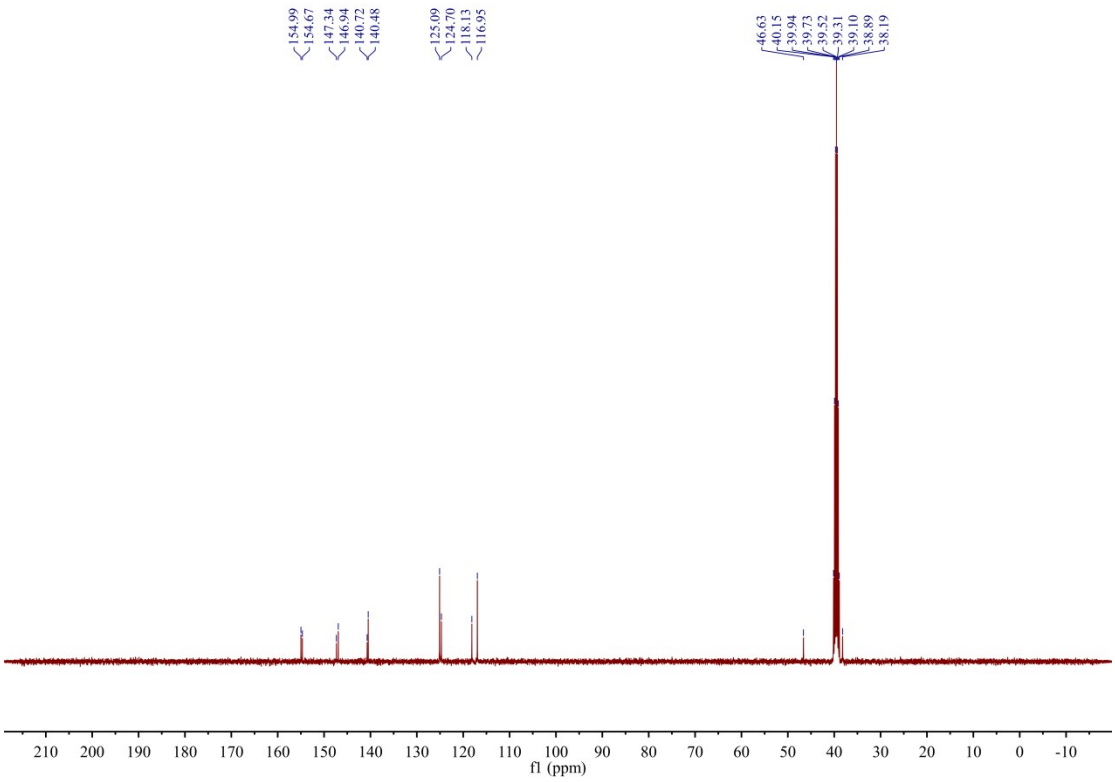

Fig. S16. ^{13}C NMR spectra of **L1** in DMSO-d_6 solution.

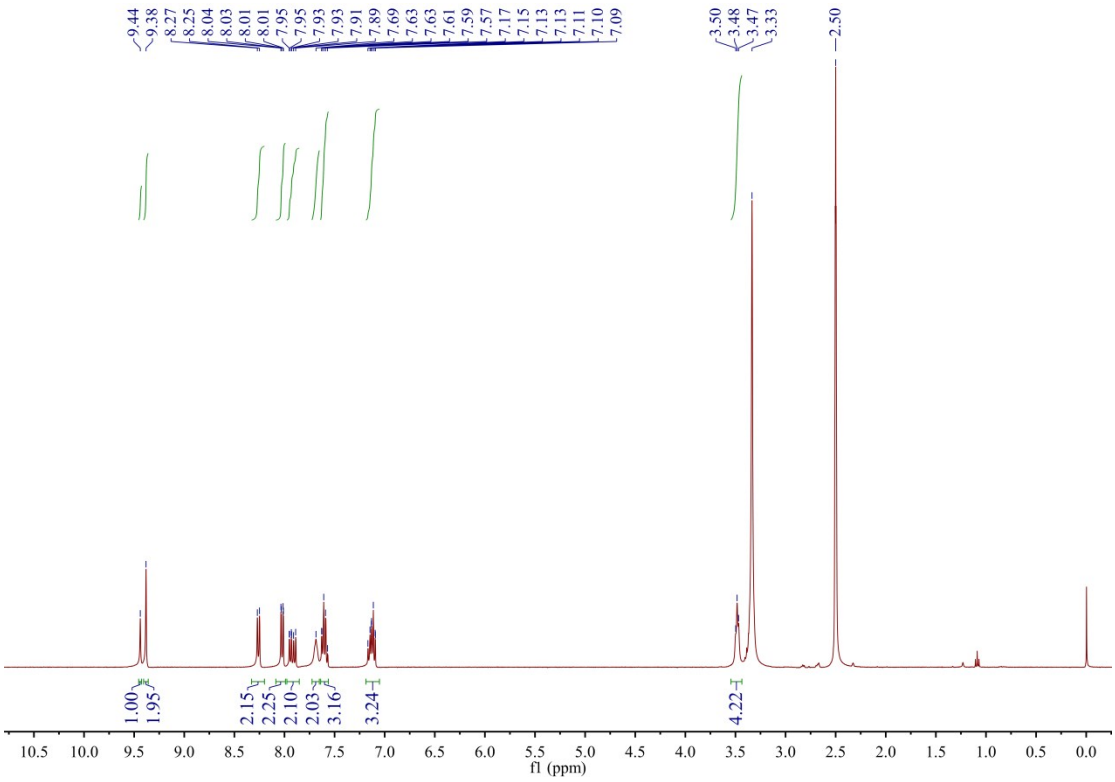

Fig. S17. ^{1}H NMR spectra of **L2** in DMSO-d_6 solution.

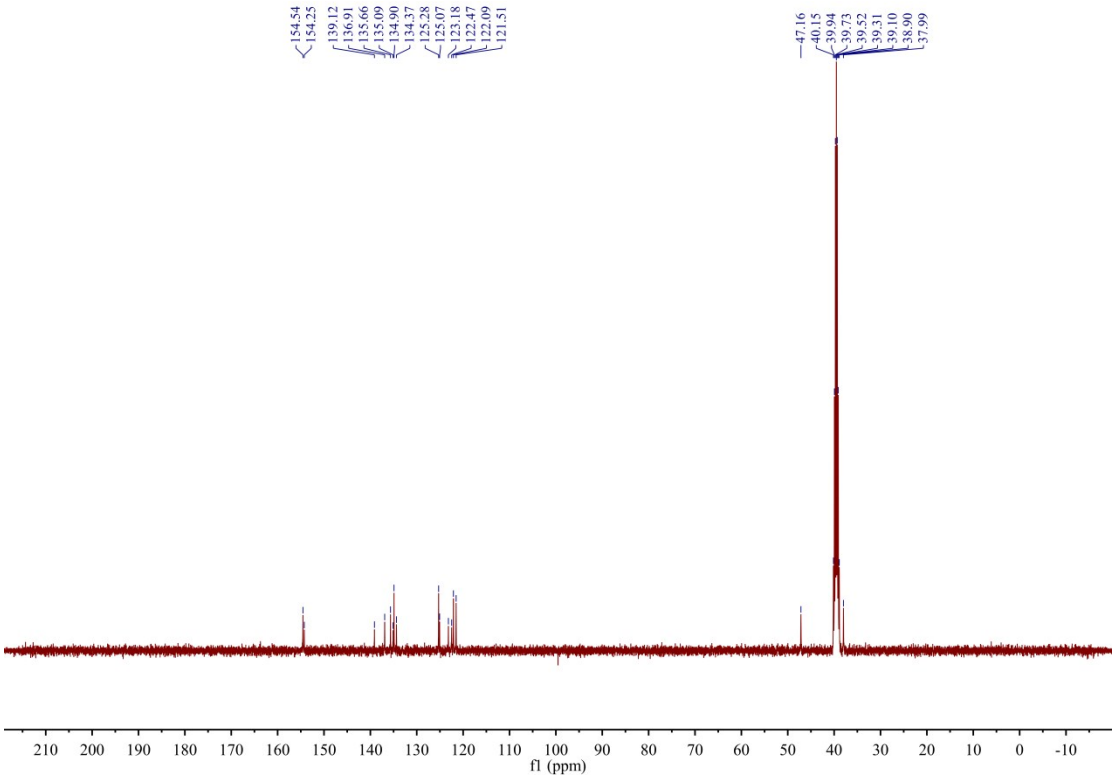

Fig. S18. ^{13}C NMR spectra of **L2** in DMSO-d_6 solution.

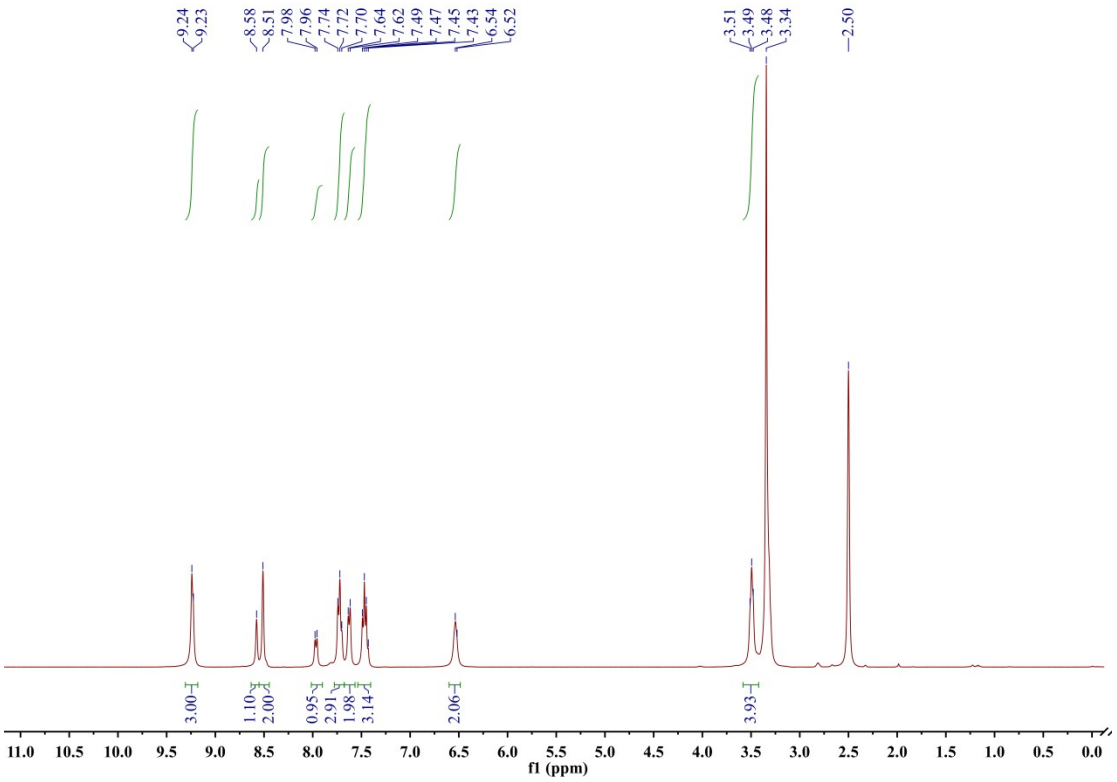

Fig. S19. ^{1}H NMR spectra of **L3** in DMSO-d_6 solution.

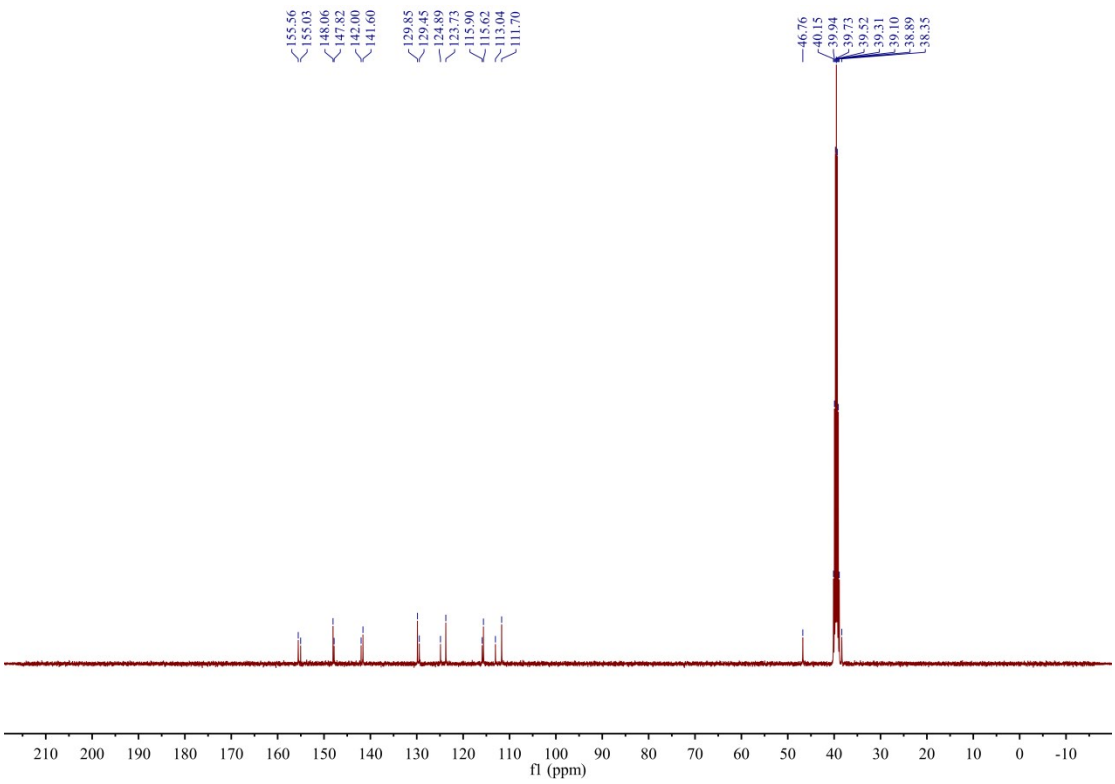

Fig. S20. ^{13}C NMR spectra of **L3** in DMSO-d_6 solution.

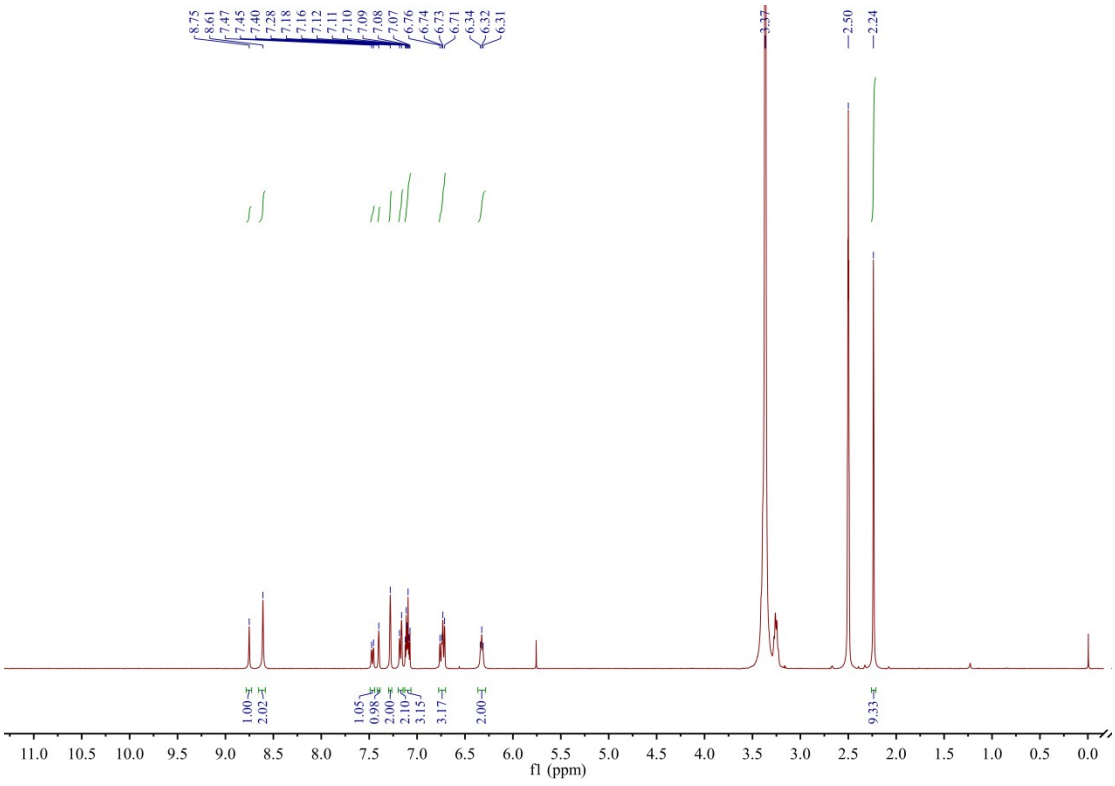

Fig. S21. ^{1}H NMR spectra of **L4** in DMSO-d_6 solution.

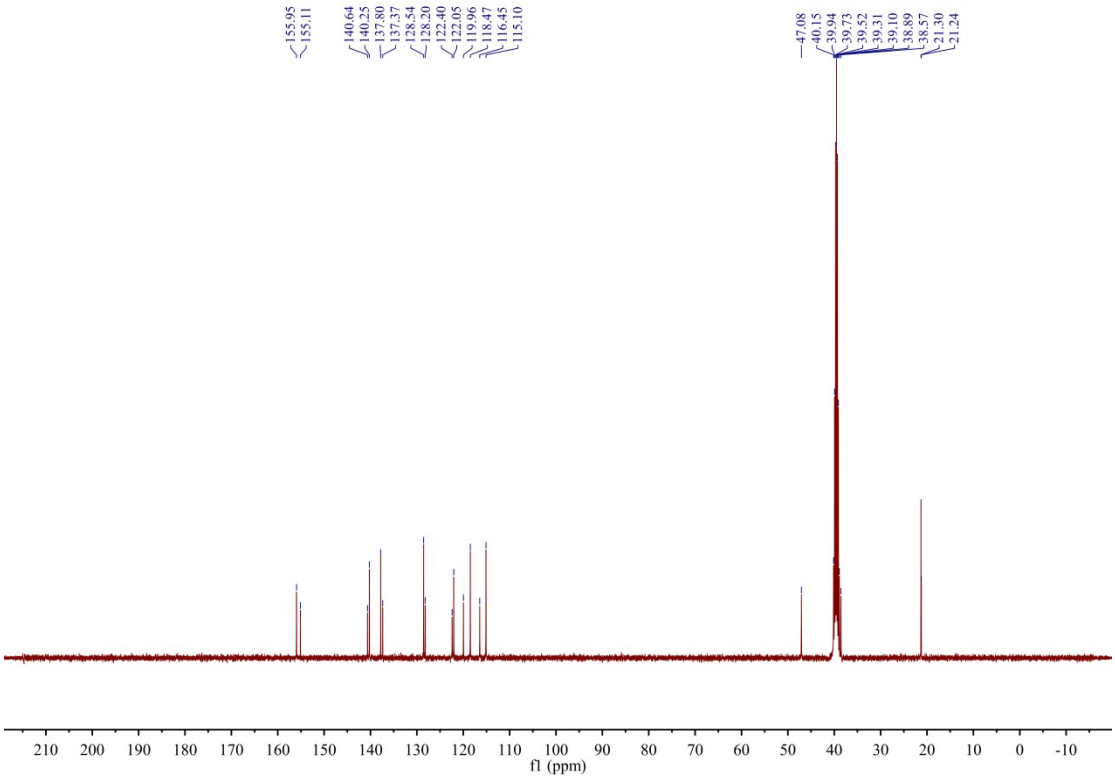

Fig. S22. ^{13}C NMR spectra of **L4** in DMSO-d_6 solution.

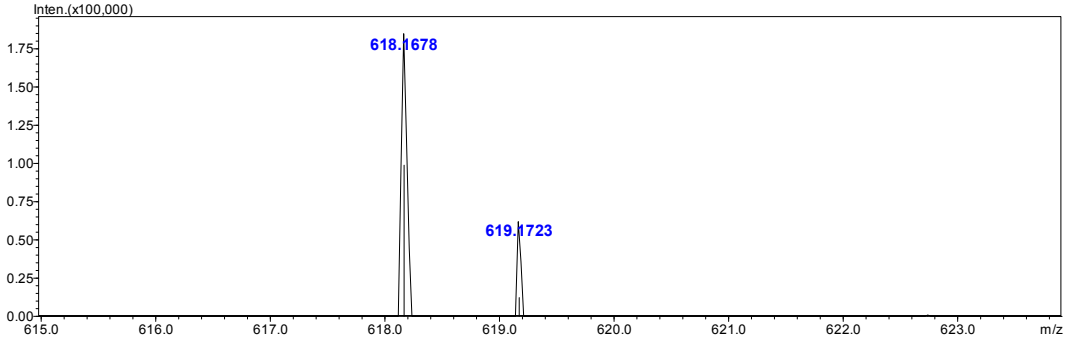

Fig. S23. HRMS-ESI spectra of **L1**.

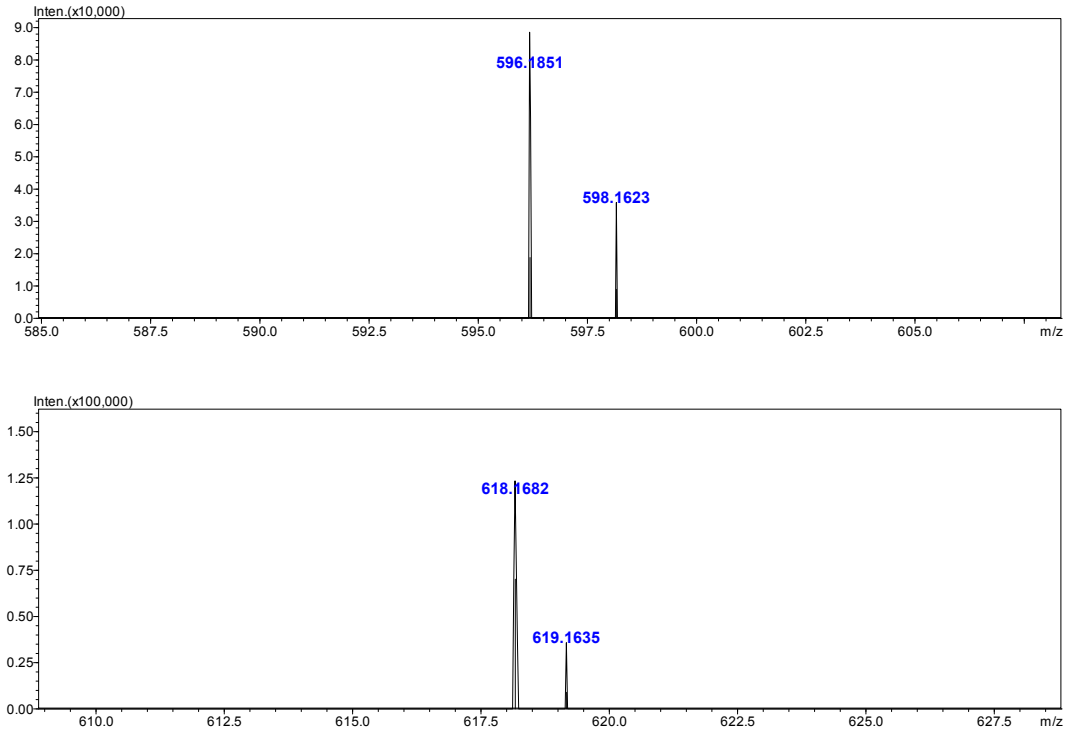

Fig. S24. HRMS-ESI spectra of **L2**.

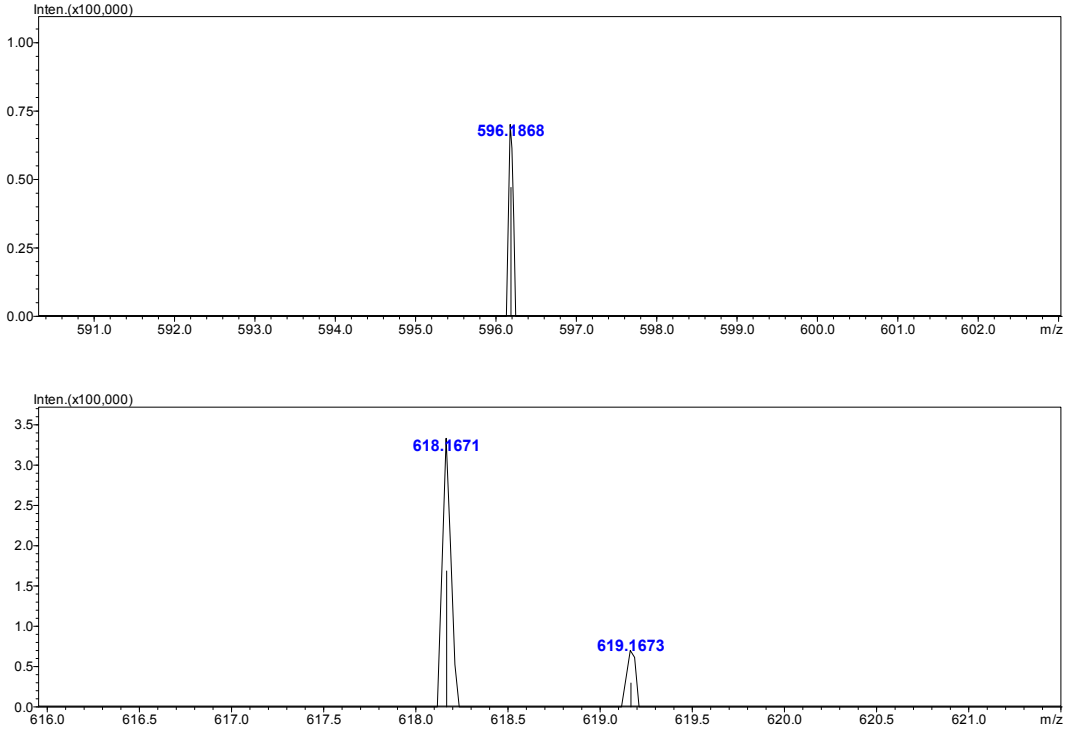

Fig. S25. HRMS-ESI spectra of **L3**.

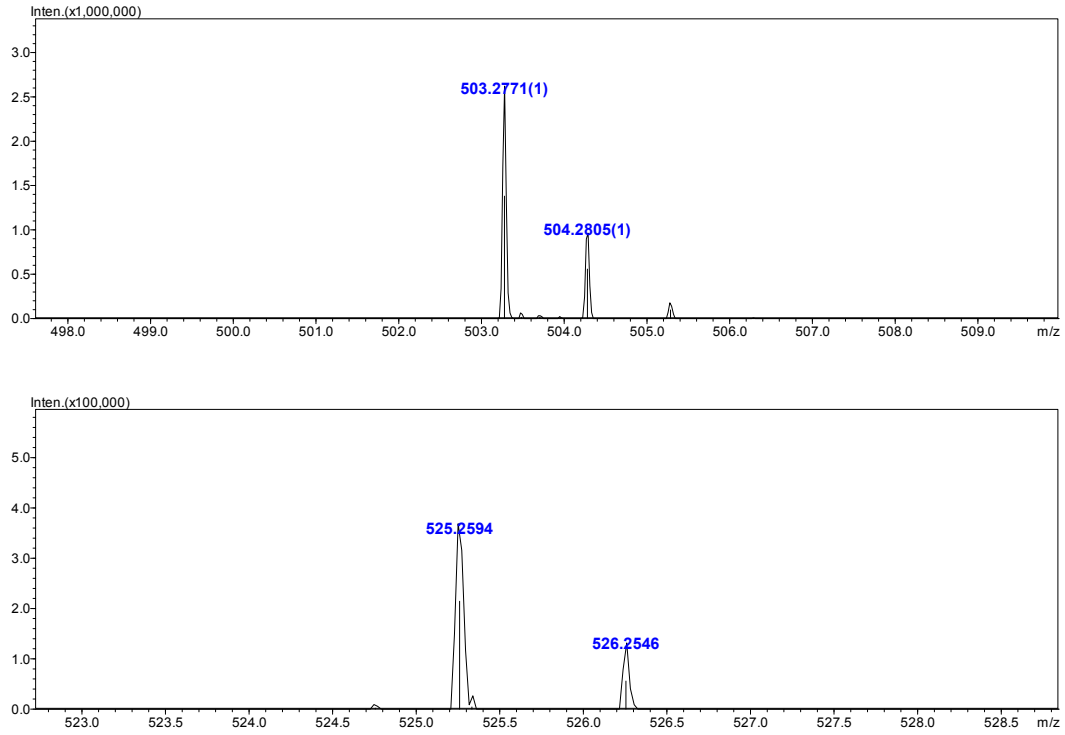

Fig. S26. HRMS-ESI spectra of **L4.**

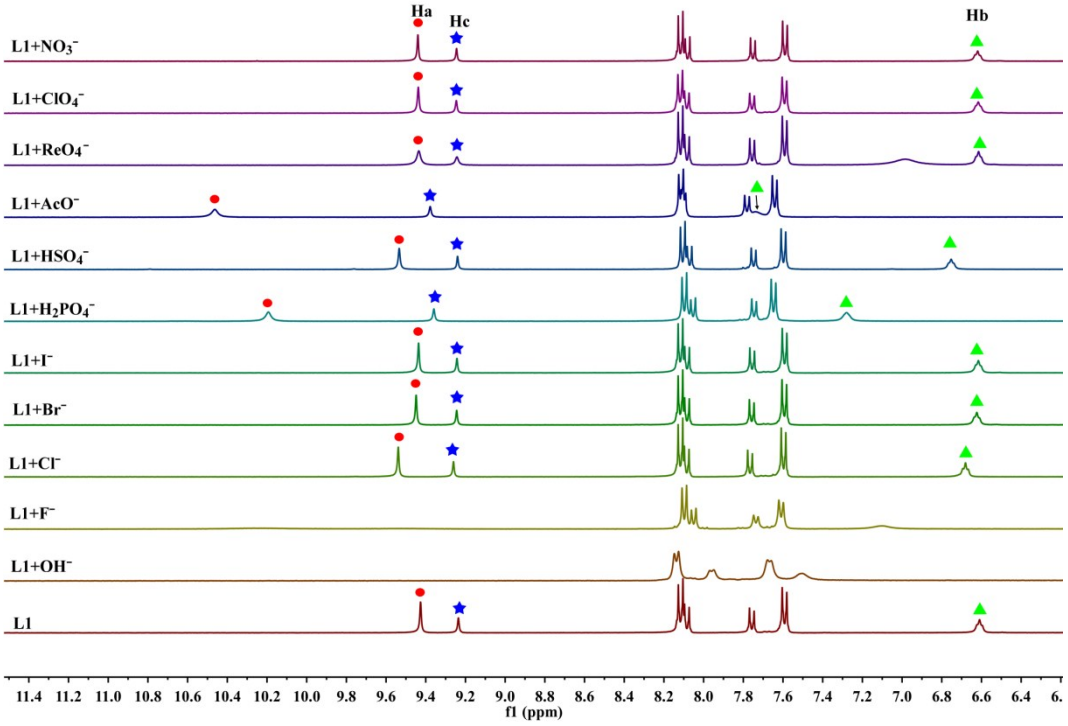

Fig. S27. Partial ^{1}H NMR spectra of receptor **L1** in DMSO-d_6 (5×10^{-3} M) in the presence of 1 equiv. different TBA anions.

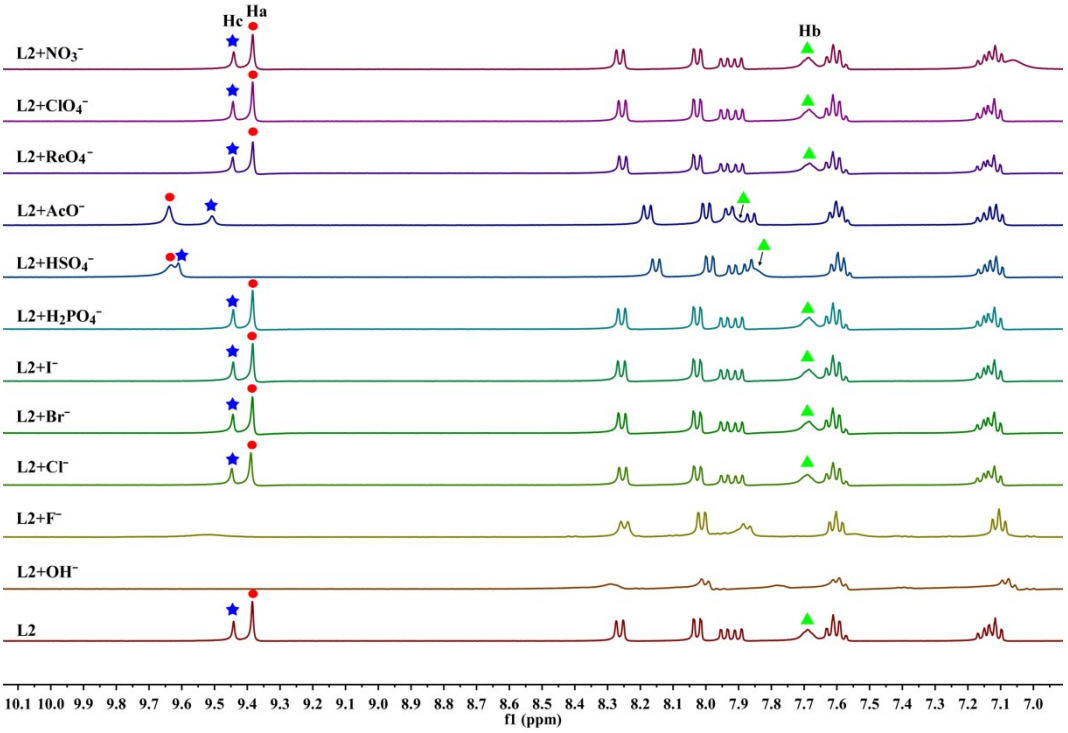

Fig. S28. Partial ^{1}H NMR spectra of receptor **L2** in DMSO-d_6 (5×10^{-3} M) in the presence of 1 equiv. of different TBA anions.

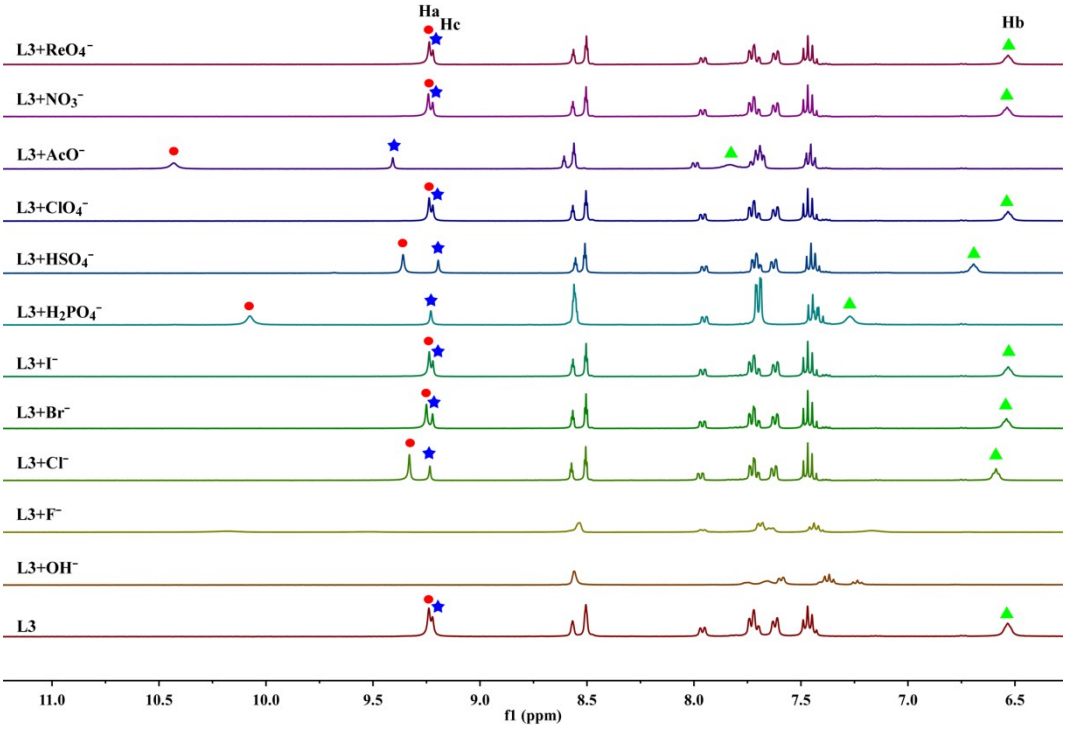

Fig. S29. Partial ^{1}H NMR spectra of receptor **L3** in DMSO-d_6 (5×10^{-3} M) in the presence of 1 equiv. of different TBA anions.

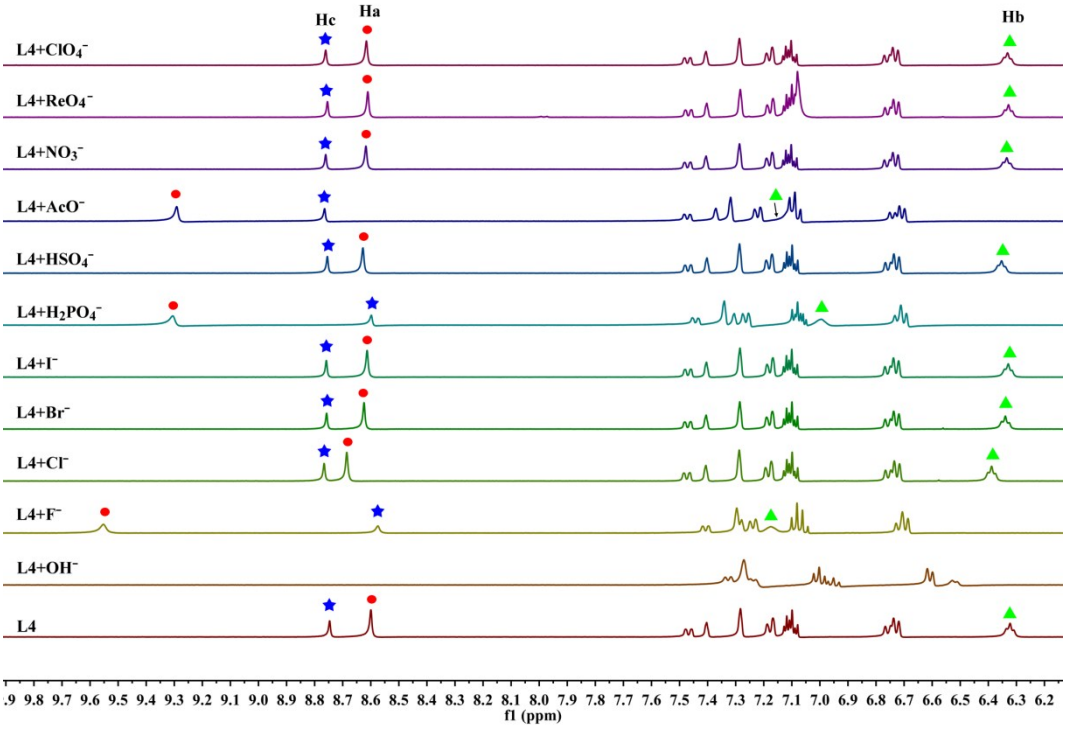

Fig. S30. Partial ^{1}H NMR spectra of receptor **L4** in DMSO-d_6 solution (5×10^{-3} M) in the presence of 1 equiv. of different TBA anions.

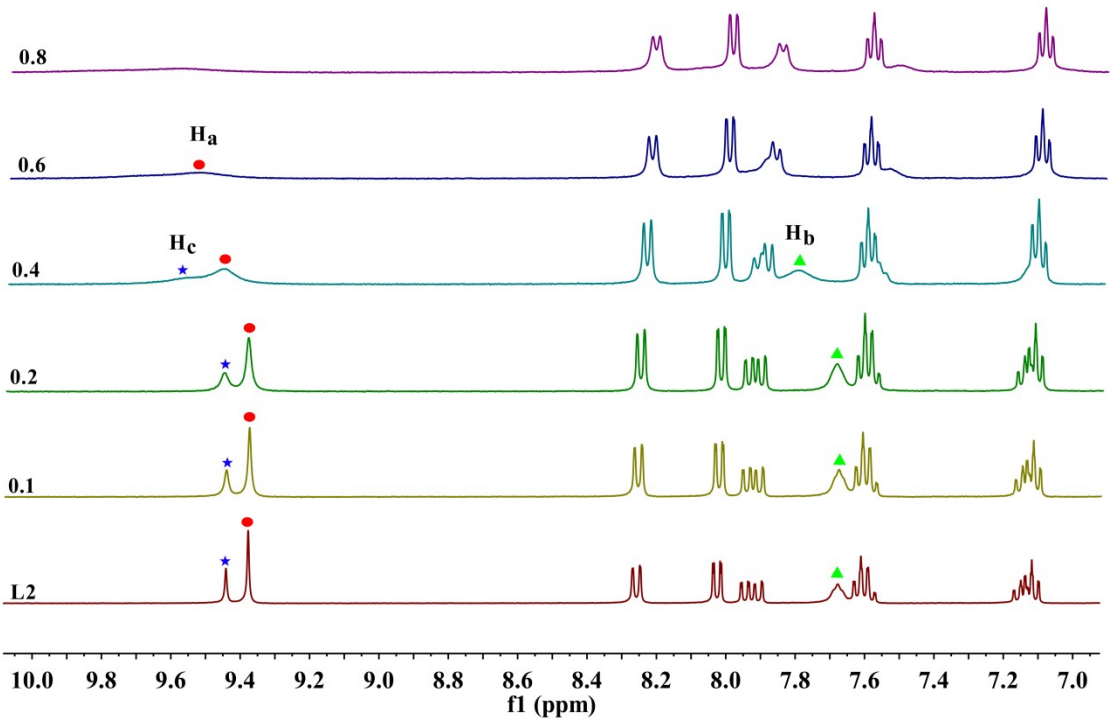

Fig. S31. Partial ^{1}H NMR titration spectra of receptor **L2** (5×10^{-3} M) upon addition of increasing amounts of TBAF recorded in DMSO-d_6 solution.

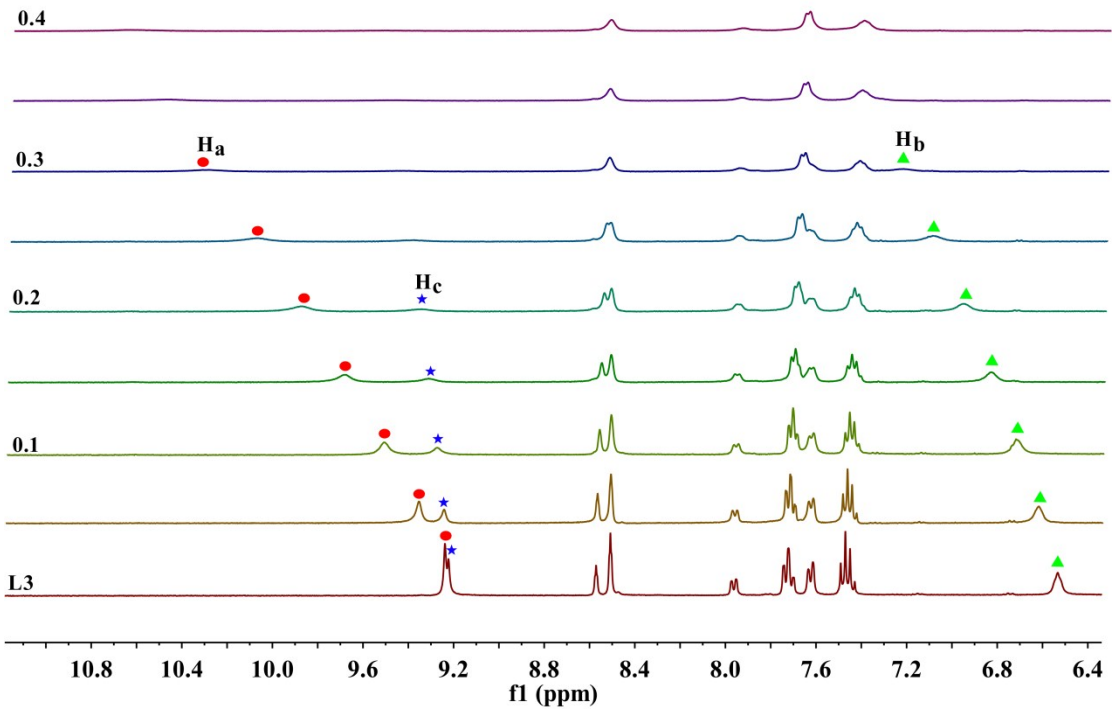

Fig. S32. Partial ^{1}H NMR titration spectra of receptor **L3** (5×10^{-3} M) upon addition of increasing amounts of TBAF recorded in DMSO-d_6 solution.

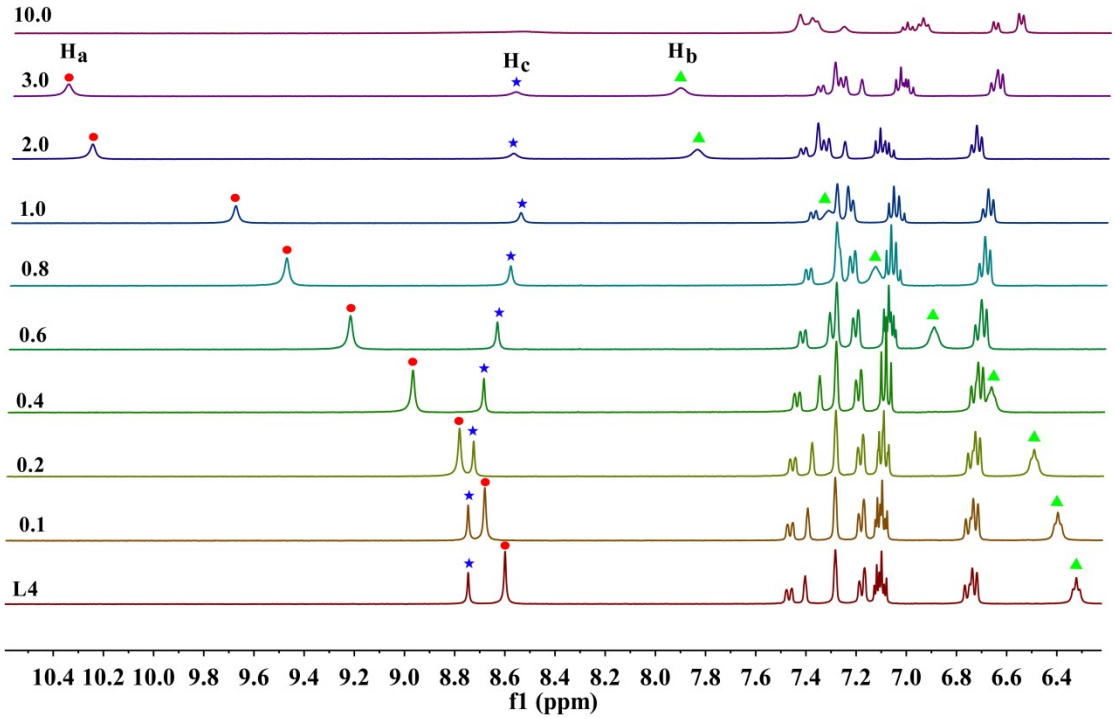

Fig. S33. Partial ^{1}H NMR titration spectra of receptor **L4** (5×10^{-3} M) upon addition of increasing amounts of TBA recorded in DMSO-d_6 solution.

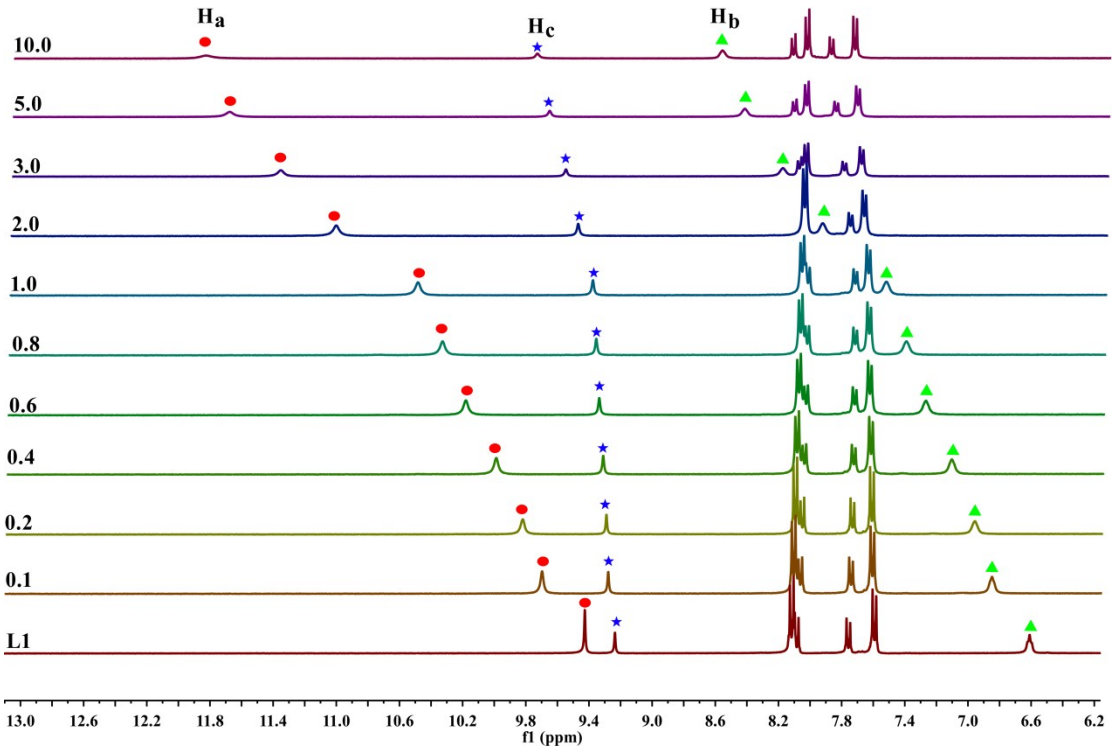

Fig. S34. Partial ^{1}H NMR titration spectra of receptor **L1** (5×10^{-3} M) upon addition of increasing amounts of $TBAH_2PO_4$ recorded in DMSO-d_6 solution.

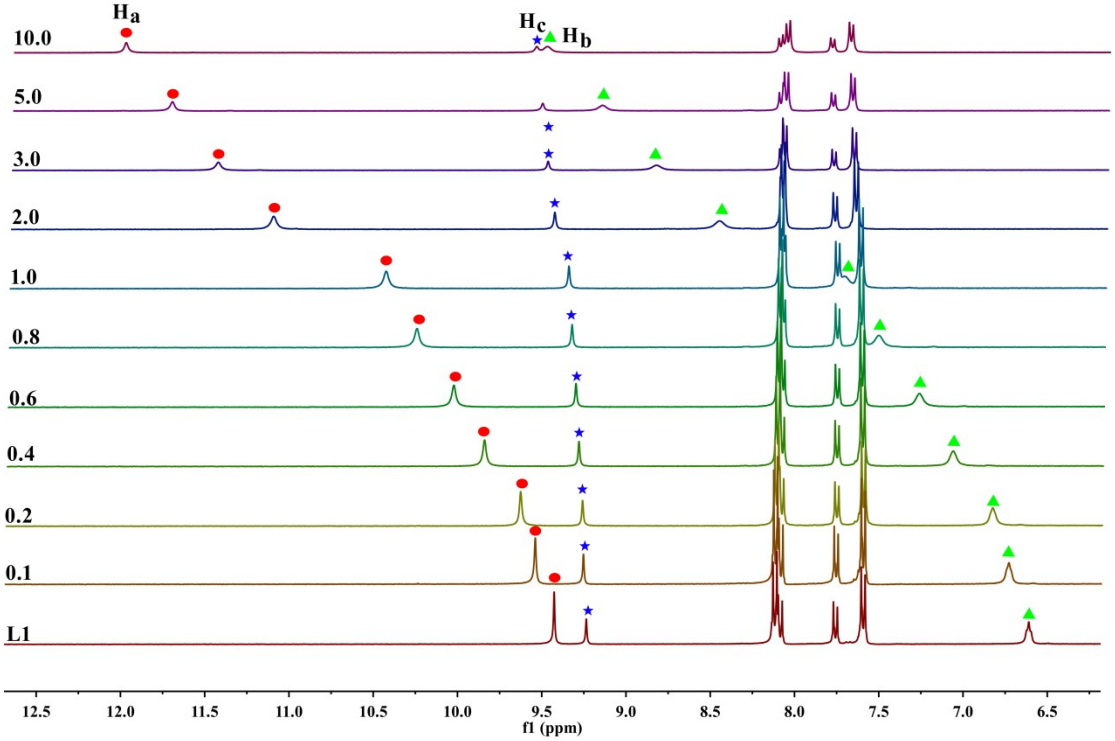

Fig. S35. Partial ^{1}H NMR titration spectra of receptor **L1** (5×10^{-3} M) upon addition of increasing amounts of TBA(CH_3COO) recorded in DMSO-d_6 solution.

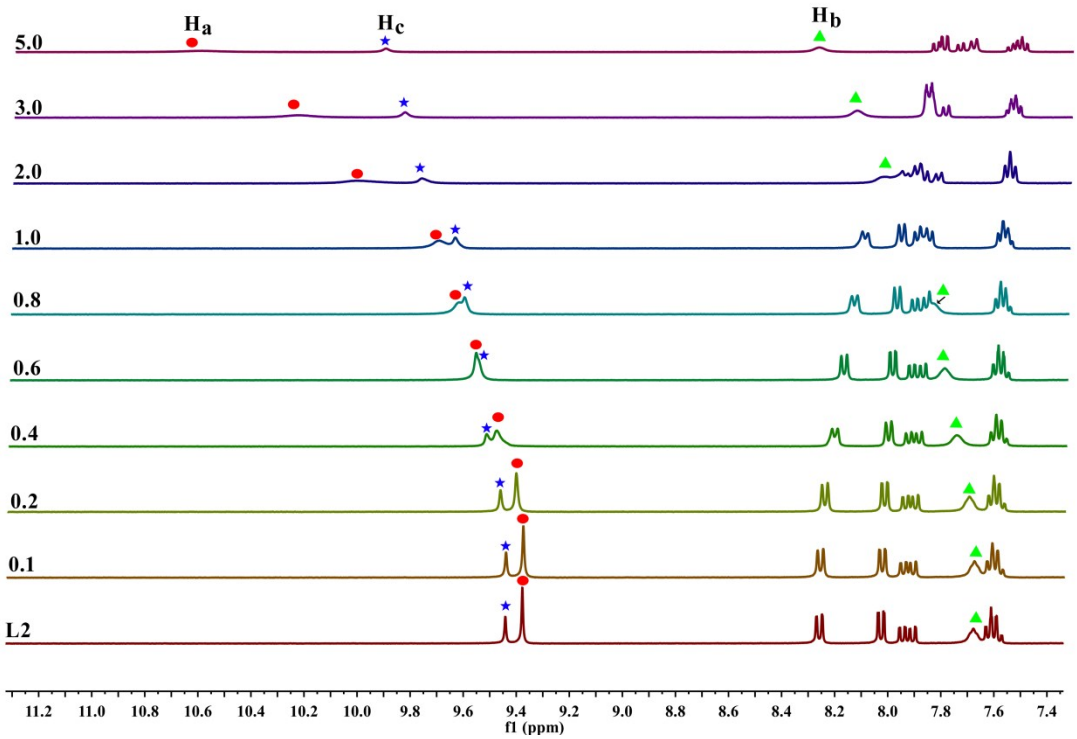

Fig. S36. Partial ^{1}H NMR titration spectra of receptor **L2** (5×10^{-3} M) upon addition of increasing amounts of $TBAH_2PO_4$ recorded in DMSO-d_6 solution.

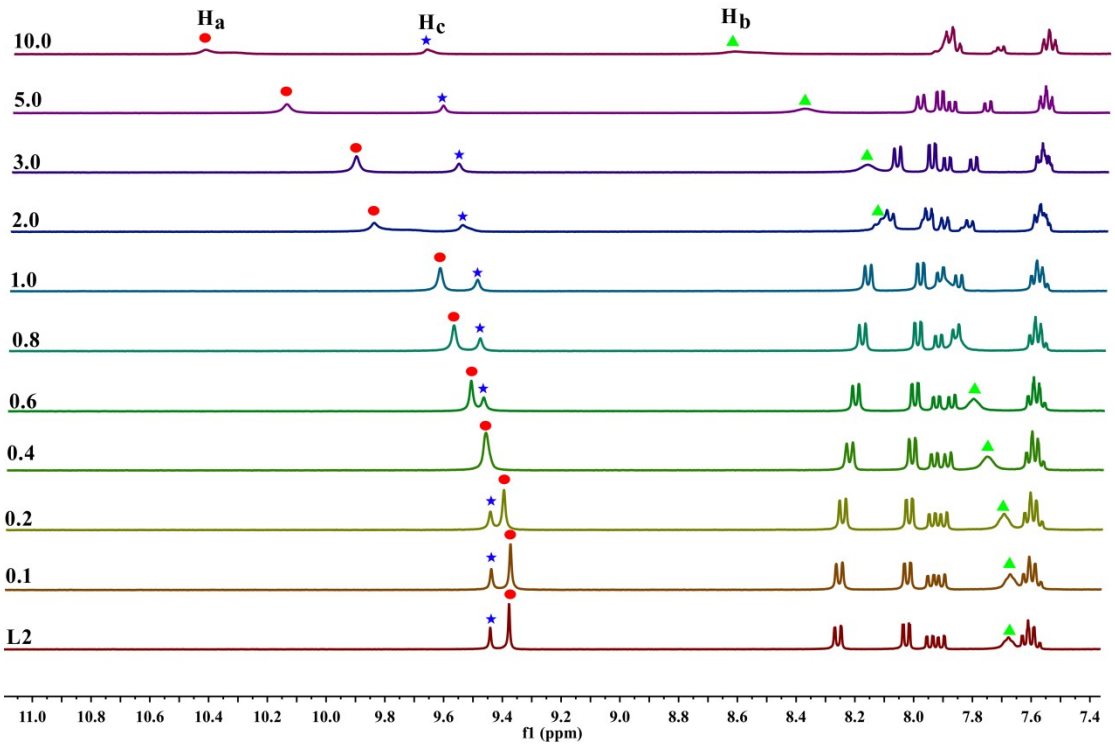

Fig. S37. Partial ^{1}H NMR titration spectra of receptor **L2** (5×10^{-3} M) upon addition of increasing amounts of TBA(CH_3COO) recorded in DMSO-d_6 solution.

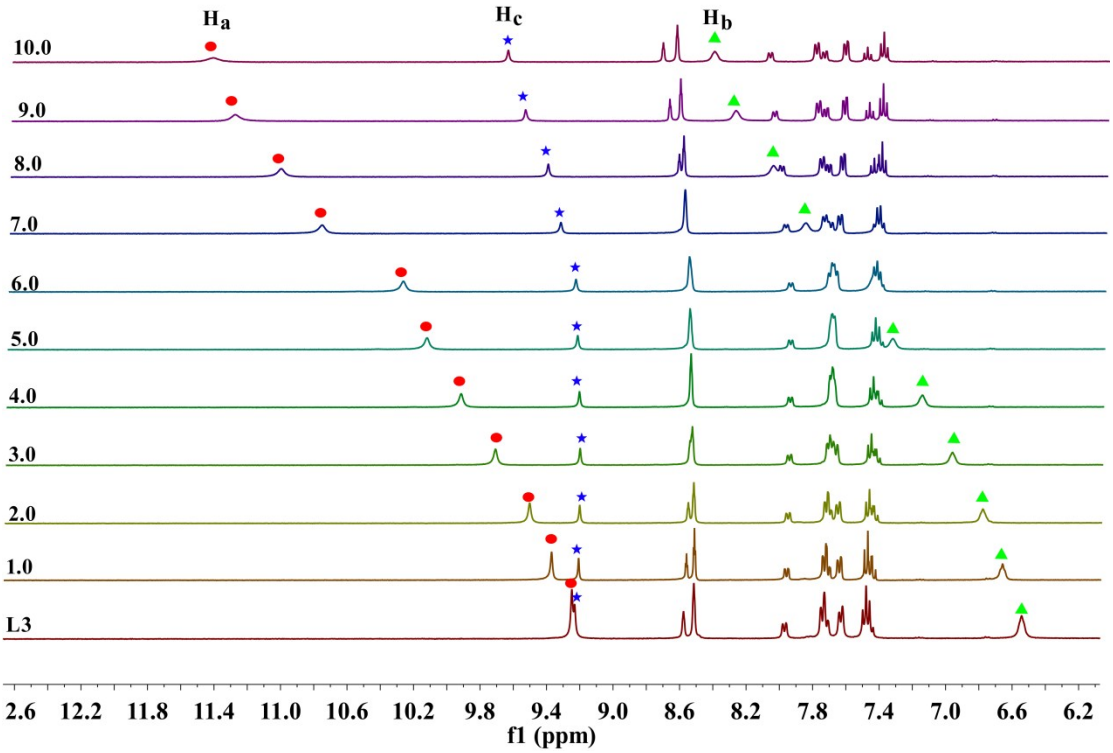

Fig. S38. Partial ^{1}H NMR titration spectra of receptor **L3** (5×10^{-3} M) upon addition of increasing amounts of $TBAH_2PO_4$ recorded in DMSO-d_6 solution.

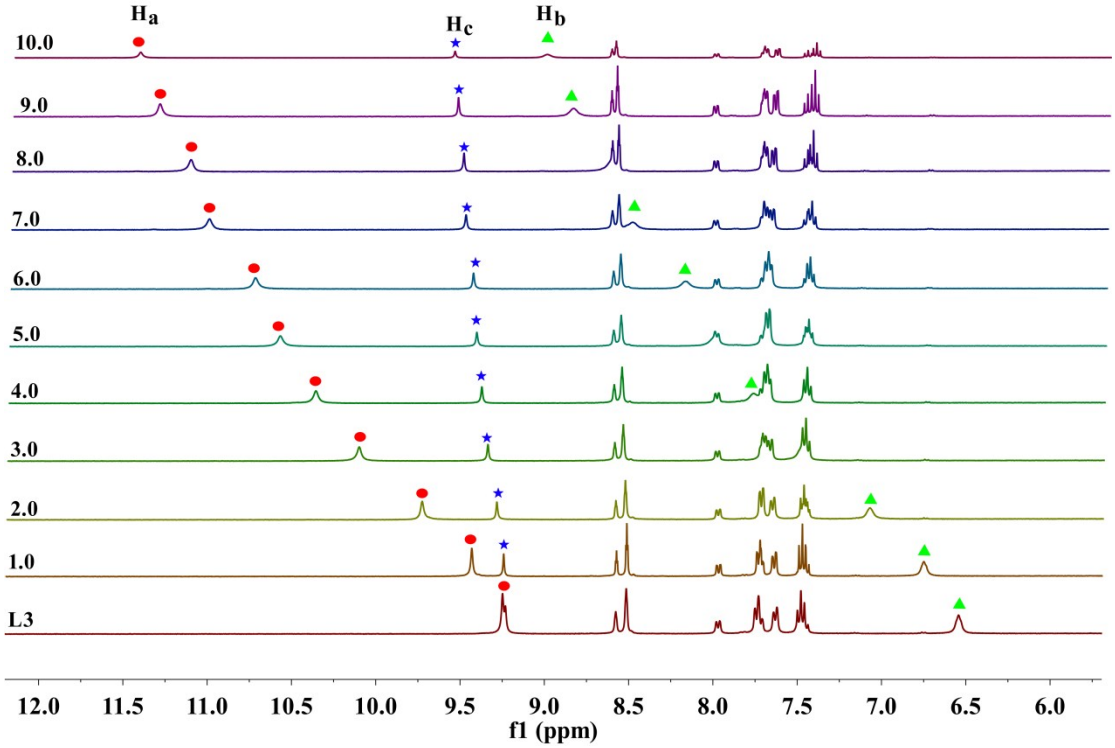

Fig. S39. Partial ^{1}H NMR titration spectra of receptor **L3** (5×10^{-3} M) upon addition of increasing amounts of TBA(CH_3COO) recorded in DMSO-d_6 solution.

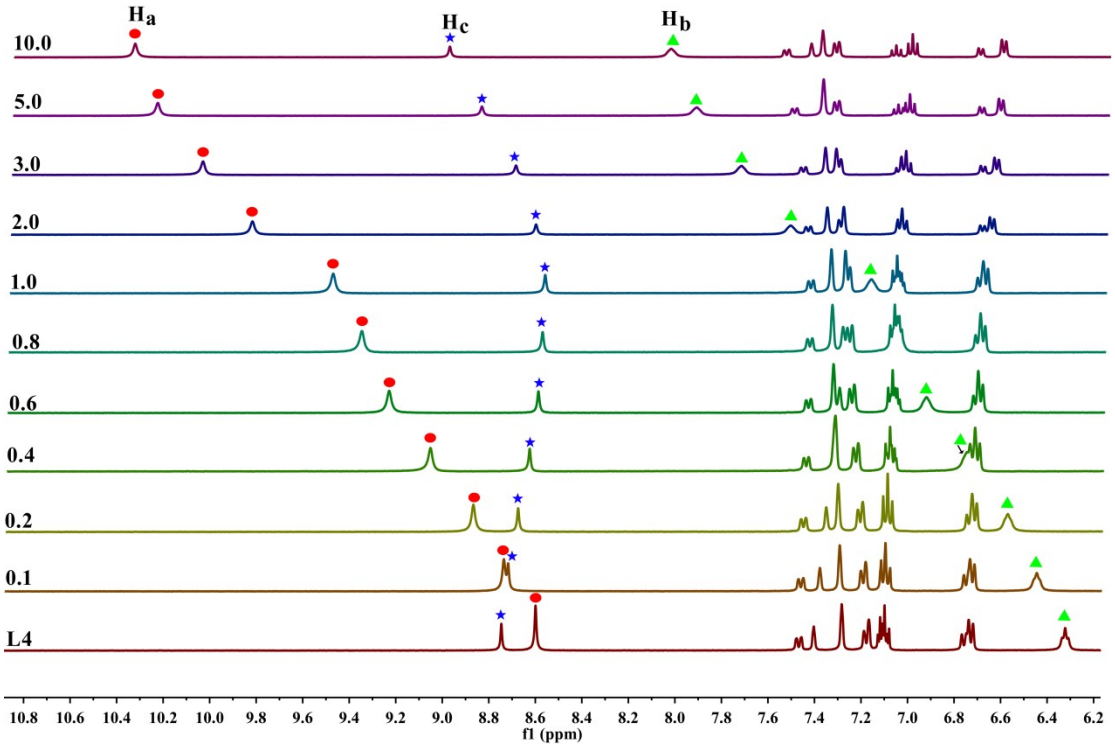

Fig. S40. Partial ^{1}H NMR titration spectra of receptor **L4** (5×10^{-3} M) upon addition of increasing amounts of $TBAH_2PO_4$ recorded in DMSO-d_6 solution.

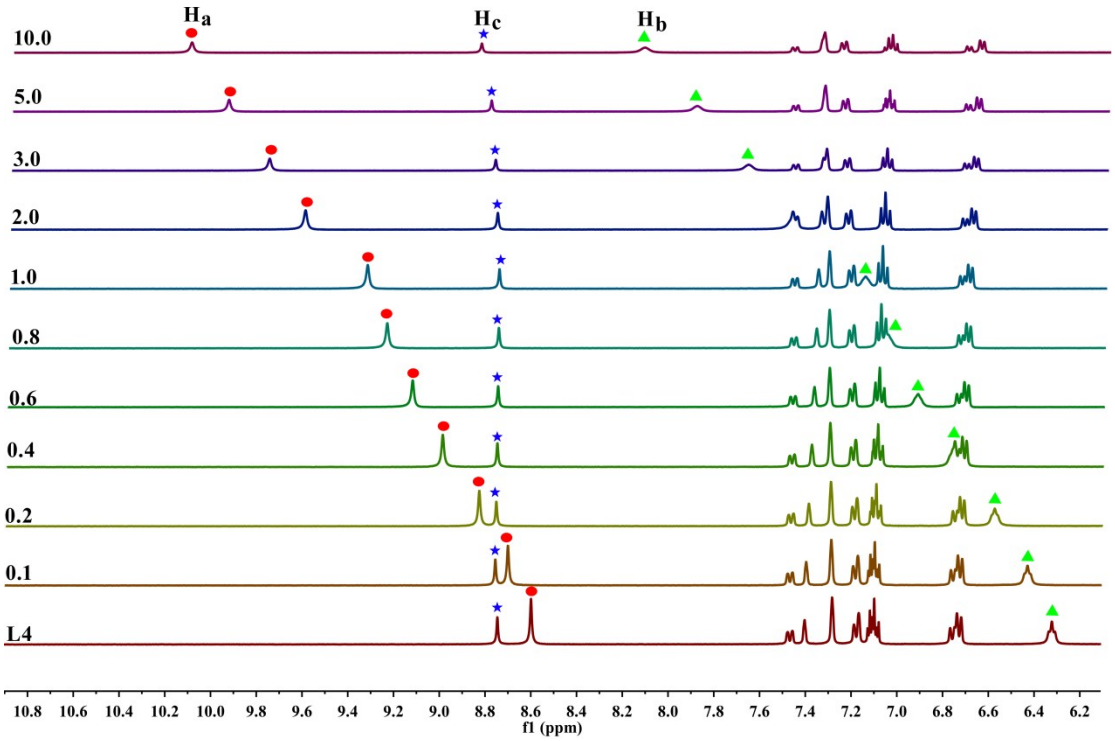

Fig. S41. Partial ^{1}H NMR titration spectra of receptor **L4** (5×10^{-3} M) upon addition of increasing amounts of TBA(CH_3COO) recorded in DMSO-d_6 solution.

Table S1. The association constants (logK_a) for the interaction of receptors L1-L4 with $TBAH_2PO_4$ and $TBA(CH_3COO)$ in DMSO solution determined by NMR titration (at 25℃).[a]

L, Anion	$H_2PO_4^-$		CH_3COO^-	
	$K_{a,\,1:1}$ [M^{-1}]	$K_{a,\,2:1}$ [M^{-1}]	$K_{a,\,1:1}$ [M^{-1}]	$K_{a,\,2:1}$ [M^{-1}]
L1	2.42[b]	-	2.20[b]	-
L2	1.90[b]	-	1.65[b]	-
L3	2.44[b]	-	3.14[c]	3.11[c]
L4	2.52[b]	-	2.29[c]	2.31[c]

[a] Estimated errors in *K*a < 21%. [b] Obtained by fitting all data points to a 1:1 binding model using a least-square fitting procedure.[c] Obtained by fitting all data points to a 2:1 (receptor:anion) binding model (Nelder–Mead method) using the Bindfit (available as freeware from app.supramolecular.org).

Table S2. The deprotonation energies (E_d, kcal/mol) of **L1-L4** for one N–H_c and two N–H_a (or N–$H_{a'}$) protons according to Eqs. (3)-(5), calculated in DMSO solution by M06-2X/6-311+G(d,p)//6-311G(d,p) with PCM model.

	$\mathbf{L1^{3-}}$	$\mathbf{L2^{3-}}$	$\mathbf{L3^{3-}}$	$\mathbf{L4^{3-}}$
$\boldsymbol{E_d}$	−66.24	−55.78	−49.22	−39.09

Table S3. The calculated absorption spectra, oscillator strengths *f* and the assignment of S_0 to S_i transitions for **L1** and its deprotonated anions, along with experimental data using TDDFT at PBE0 /def2-TZVP level in DMSO solution.

Receptor anions	**$L1^-$ (H_c)**		**$L1^{2-}$ (H_cH_a)**	
Excited state	1	3	1	6
Transition Wavelength (nm)	469	400	480	386
f	0.0069	0.8904	0.0094	0.7328
Main configuration[a]	H→ L+1	H → L+2	H → L	H−1 → L+2
Contribution (%)	99.7	98.6	99.1	60.6
Integral of hole–electron distribution overlap (S)	0.008	0.284	0.005	0.291
Distance between thecentroids of the hole and electron regions (D) (Å)	9.912	3.074	12.929	4.113
Δ*r* index (Å)	9.907	3.075	12.924	4.513

[a] H: HOMO, L: LUMO

Table S4. Analysis of electron transitions between S_0 and S_i by Multiwfn program package at PBE0 /def2-TZVP level.

	Excited State	Integral of hole–electron distribution overlap (S)	Distance between thecentroids of the hole and electron regions (D) (Å)	Variation of dipole moment with respect to ground state (a.u.)	Δ*r* index(Å)
L1	1	0.207	3.863	2.673	6.510
L1^{3-}	1	0.265	2.218	4.115	6.095
L2	1	0.135	2.329	1.110	3.382
	2	0.191	2.551	1.689	6.170
L2^{3-}	1	0.172	2.452	1.705	6.294
	4	0.241	2.096	2.275	2.896
L3	1	0.212	3.051	0.989	4.024
	4	0.181	4.323	0.868	4.442
L3^{3-}	1	0.233	3.400	1.176	3.880
	4	0.241	3.838	1.020	5.207
L4	1	0.445	0.968	0.958	2.021
	5	0.471	0.564	2.365	3.420
L4^{3-}	1	0.316	1.756	1.373	4.473
	7	0.402	1.053	3.519	3.256

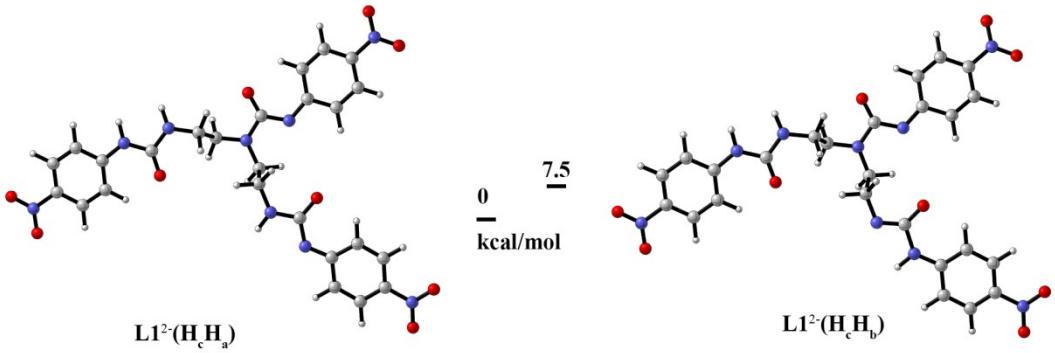

Figure S42. The energy difference of deprotonated dianion of $L1^{2-}(H_cH_a)$ and $L1^{2-}(H_cH_b)$ calculated in DMSO by M06-2X/6-311+G(d,p)//6-311G(d,p) with PCM model.

Optimized geometries

L1

68
-2137.076474 a.u.

O	-0.059661	3.455661	-0.638335
O	2.539122	-0.842340	0.202278
N	1.596289	1.880662	-0.427255
H	1.793524	0.897959	-0.247029
O	-4.392733	-0.120297	0.348625
O	8.773612	-3.573456	-0.771526
N	2.607212	-3.126796	0.422608
H	2.053051	-3.929377	0.687215
N	-4.026423	2.112246	0.426045
H	-4.409750	3.041240	0.354807
N	8.021839	-4.422802	-0.336057
N	-6.184179	1.323086	0.298256
H	-6.435574	2.301313	0.315863
N	-0.608391	1.271311	-0.877231
C	0.285463	2.282564	-0.647785
C	3.963882	-3.377197	0.229739
C	6.618245	-4.064125	-0.139257
O	-10.518852	-3.223295	-0.122093
C	2.686712	2.721033	-0.225373
O	6.133847	6.212436	0.152501
C	6.200555	-2.775370	-0.436527
H	6.912087	-2.053475	-0.813094
C	4.873139	-2.424608	-0.254843
H	4.541715	-1.426269	-0.488085
C	4.412290	-4.676571	0.519636
H	3.711476	-5.414355	0.892228
C	-7.252190	0.441447	0.196696
C	5.735056	-5.024794	0.337904
H	6.085329	-6.022582	0.561597
N	-10.678294	-2.018152	-0.132159
C	3.852657	2.125035	0.291979
H	3.843060	1.067785	0.529713
C	-4.829728	1.019346	0.353250
N	6.173856	5.027159	0.420738
C	-8.534369	1.010346	0.088976
H	-8.642148	2.088657	0.087923
C	-2.019155	1.637783	-0.930128

H	-2.564559	0.797531	-1.360096
H	-2.145365	2.506065	-1.577962
C	-7.118390	-0.956451	0.199646
H	-6.142253	-1.403359	0.287631
C	-9.497677	-1.166533	-0.016645
C	4.973156	4.228035	0.195436
C	4.993211	2.872009	0.502526
H	5.889906	2.420946	0.903980
C	1.955953	-1.912272	0.366033
C	2.694517	4.090569	-0.537004
H	1.810468	4.556674	-0.938594
C	-8.245181	-1.753624	0.091399
H	-8.156240	-2.831210	0.092226
C	-9.655517	0.214550	-0.017789
H	-10.641924	0.648455	-0.103299
C	-2.586127	1.946668	0.460180
H	-2.346470	1.131294	1.145282
H	-2.142707	2.863495	0.846362
O	-11.763769	-1.480306	-0.233529
C	3.839426	4.838483	-0.322112
H	3.858711	5.893458	-0.558551
O	7.157758	4.469009	0.867074
O	8.367039	-5.553334	-0.054164
H	-1.161633	-0.983056	0.877458
C	-0.242731	-0.136010	-0.901555
H	0.711575	-0.258507	-1.415736
H	-0.985540	-0.667731	-1.496341
C	-0.163088	-0.752370	0.507139
N	0.612675	-1.978544	0.515093
H	0.291778	-0.036827	1.197804
H	0.137868	-2.865605	0.572662

L2

68

-2137.069902 a.u.

O	3.692273	-2.202139	0.754805
O	-1.185276	-0.262316	-1.374951
N	2.422100	-0.528710	-0.110677
N	4.724534	-0.367798	-0.176403
H	4.583309	0.594783	-0.442111
O	5.719999	2.033081	-0.594855
O	-0.307622	2.849952	-0.751184

N	-0.756746	-2.359266	-0.649591
H	-1.110571	-3.234556	-0.298124
O	-4.803109	-3.266733	0.217769
N	-2.936309	-1.637661	-0.757283
H	-3.160984	-2.531563	-0.340447
O	7.714391	2.435971	0.055932
O	-1.846330	-0.506680	2.223131
N	1.185408	2.009009	0.740487
H	1.300254	1.488269	1.597873
N	6.825361	1.661664	-0.215020
N	-1.066174	1.772632	1.141411
H	-0.809051	1.025089	1.770494
O	-3.891290	-1.113099	2.088373
N	-5.593470	-2.334400	0.197000
N	-3.018484	-0.279654	1.951689
C	3.614187	-1.121946	0.193253
C	-1.593531	-1.336922	-0.960201
C	1.201587	-1.212139	0.298771
H	0.438140	-0.456898	0.478105
H	1.388929	-1.749202	1.226824
C	6.054854	-0.732971	-0.059784
C	-4.034335	-0.878270	-1.133328
C	0.674897	-2.162746	-0.784356
H	0.881232	-1.737668	-1.769826
H	1.165119	-3.133063	-0.721604
C	7.090989	0.229026	-0.091281
C	2.274431	0.636288	-0.985738
H	1.308269	0.537823	-1.489029
H	3.042921	0.631853	-1.761813
C	-2.428494	1.959681	0.975354
C	-0.079608	2.259507	0.286163
O	-6.592856	-2.301917	0.879972
C	-5.336591	-1.209509	-0.698719
C	-3.389519	1.025762	1.420451
C	2.282242	1.959488	-0.212392
H	3.215650	2.100808	0.335666
H	2.170779	2.789734	-0.909402
C	6.452705	-2.075538	0.068979
H	5.689904	-2.836056	0.101035
C	8.436851	-0.129516	-0.005201
H	9.180480	0.653860	-0.041260
C	-2.922291	3.141742	0.396609
H	-2.213714	3.873923	0.042010

C	8.794773	-1.454875	0.116793
H	9.837880	-1.734814	0.174343
C	7.788390	-2.421082	0.153971
H	8.049215	-3.468933	0.241556
C	-3.921210	0.266968	-1.942530
H	-2.940419	0.574497	-2.266031
C	-4.761552	1.280379	1.332591
H	-5.450456	0.533419	1.702278
C	-4.279116	3.376479	0.292916
H	-4.617234	4.305032	-0.151446
C	-6.458635	-0.473678	-1.079195
H	-7.426527	-0.788190	-0.714288
C	-5.212519	2.453694	0.771574
H	-6.274045	2.648762	0.699177
C	-6.319540	0.625162	-1.899615
H	-7.188438	1.192987	-2.204386
C	-5.039064	0.991532	-2.314433
H	-4.905027	1.861315	-2.946734

L3

68

-2137.091020 a.u.

O	1.922618	-1.322477	-1.031575
O	-3.084354	-2.180466	-1.050450
O	-0.949841	-2.741466	2.494184
N	-1.305804	-3.511831	-0.557069
N	-2.427027	-1.080092	1.939833
H	-3.364652	-0.909104	1.603594
N	-0.983886	-1.275163	-1.115736
H	0.018785	-1.443760	-1.050588
O	-1.291257	4.614638	0.924914
N	2.378471	-3.527047	-1.186455
H	3.032667	-4.281791	-1.052031
N	-3.020458	-3.301366	1.710315
H	-3.758569	-2.918718	1.132066
N	-2.001505	3.644395	1.077613
N	4.066855	-2.037977	-0.671776
H	4.684391	-2.834264	-0.740842
O	-3.204024	3.649241	0.898695
O	2.758024	2.734327	0.232974
C	-1.580035	0.035120	1.919420
N	3.960110	2.749339	0.411396

C	-2.170936	1.264857	1.617988
H	-3.237549	1.347941	1.449140
C	-1.870479	-2.314273	-0.920527
C	2.739517	-2.241741	-0.965127
C	-1.363899	2.379480	1.478705
C	-2.044245	-2.404245	2.074196
C	0.106536	-3.655287	-0.227995
H	0.210802	-4.526061	0.419968
H	0.442711	-2.800842	0.362934
C	-1.312025	0.059075	-1.380537
C	4.686660	-0.813874	-0.393926
C	3.983635	0.362920	-0.128187
H	2.907243	0.393930	-0.136816
C	-2.578574	-4.619467	1.271532
H	-3.372402	-5.347343	1.442688
H	-1.722667	-4.896928	1.885419
C	-0.192909	-0.023079	2.113567
H	0.271945	-0.964302	2.359451
C	-2.205416	-4.611039	-0.223019
H	-1.719198	-5.552071	-0.487517
H	-3.103266	-4.508482	-0.829627
C	0.986022	-3.824217	-1.477520
H	0.927063	-4.844216	-1.854425
H	0.641252	-3.158981	-2.272538
C	4.714806	1.508067	0.146843
O	4.578608	3.719072	0.790750
C	-2.616271	0.561700	-1.409781
H	-3.468091	-0.075406	-1.242634
C	0.011769	2.348804	1.644917
H	0.610719	3.234953	1.496445
C	-0.239743	0.944702	-1.578813
H	0.771687	0.557079	-1.541300
C	0.578921	1.126255	1.973133
H	1.651320	1.060639	2.110425
C	6.087922	-0.792838	-0.359610
H	6.636827	-1.705006	-0.564636
N	-4.158882	2.450033	-1.587325
C	6.097195	1.556972	0.187935
H	6.610507	2.481080	0.409034
C	-2.785667	1.918805	-1.636491
O	-5.022482	1.752151	-1.096264
C	-0.457716	2.293242	-1.814568
H	0.390124	2.952858	-1.951174

C	6.778963	0.373569	-0.070660
H	7.860895	0.361157	-0.053102
C	-1.748162	2.808760	-1.855420
H	-1.947830	3.858352	-2.018939
O	-4.352923	3.561684	-2.030340

L4

71

-1641.528082 a.u.

O	3.285721	-0.630171	-0.364474
O	-1.348605	-0.870356	-2.415905
O	-3.963610	-2.811168	1.325684
N	-0.124097	-2.381799	-1.241389
N	-4.363765	-0.836194	0.213156
H	-4.148520	-0.335811	-0.636934
N	0.615134	-0.190315	-1.458584
H	1.515090	-0.487714	-1.085240
N	3.450950	-2.880177	-0.288924
H	3.923810	-3.700780	0.054029
N	-3.027547	-2.447636	-0.710747
H	-2.782941	-1.763350	-1.419458
N	5.022615	-1.580632	0.789417
H	5.501922	-2.452934	0.959723
C	-5.235899	-0.172229	1.086352
C	-5.690293	1.090878	0.678770
H	-5.354870	1.489346	-0.274790
C	-0.344433	-1.127295	-1.747785
C	3.886911	-1.632485	0.024536
C	-6.558263	1.840783	1.461988
C	-3.792933	-2.088976	0.353539
C	0.979638	-2.698538	-0.349540
H	0.686071	-3.550974	0.265427
H	1.153757	-1.866438	0.334135
C	0.542017	1.188248	-1.740338
C	5.701081	-0.427745	1.231299
C	5.115787	0.838424	1.283065
H	4.095303	0.972757	0.955921
C	-2.192216	-3.635407	-0.664073
H	-2.760608	-4.527765	-0.945107
H	-1.827172	-3.782852	0.356501
C	-5.666515	-0.689364	2.311652
H	-5.325435	-1.658562	2.637817
C	-1.022302	-3.467320	-1.628258

H	-0.445120	-4.392875	-1.658340
H	-1.392629	-3.271991	-2.635243
C	2.272503	-3.022869	-1.121496
H	2.245635	-4.043106	-1.502529
H	2.359032	-2.351830	-1.979794
C	5.843792	1.935193	1.750059
C	-0.652674	1.873363	-1.967300
H	-1.588308	1.333241	-1.972036
C	-6.986810	1.313848	2.683828
H	-7.667985	1.883536	3.306378
C	1.751465	1.897854	-1.727088
H	2.675967	1.365126	-1.534233
C	-6.539229	0.065229	3.092231
H	-6.874504	-0.341019	4.040019
C	7.021270	-0.595681	1.665609
H	7.479201	-1.578013	1.625670
C	7.158765	1.758210	2.174437
H	7.728652	2.607664	2.533724
C	-0.648740	3.252145	-2.193983
C	1.750490	3.266545	-1.945367
H	2.689567	3.807854	-1.932076
C	7.738247	0.492983	2.135551
H	8.760319	0.353501	2.467369
C	0.558378	3.946980	-2.183187
H	0.566270	5.017264	-2.356121
C	5.183222	3.289251	1.811708
H	4.621054	3.493269	0.898275
H	4.479395	3.335531	2.646982
H	5.920802	4.080398	1.949422
C	-1.954501	3.962586	-2.448952
H	-2.393400	3.636429	-3.395292
H	-2.678378	3.743154	-1.660748
H	-1.813076	5.042709	-2.494267
C	-7.012753	3.206516	1.014487
H	-8.078282	3.344517	1.206633
H	-6.477222	3.987486	1.560880
H	-6.830487	3.356312	-0.050114

$L1^{3-}(H_cH_{a2})$

65

-2135.616021 a.u.

O	-0.246869	4.026707	0.333056
O	-2.368139	-1.335183	-0.585327

N	-1.983464	2.452964	0.409703
O	3.873341	0.232144	-0.436054
O	-7.526781	-5.847218	-0.592903
N	-1.749701	-3.450178	0.254312
N	3.616959	2.469287	-0.633467
H	4.070596	3.358987	-0.505540
N	-6.517831	-6.364974	-0.124878
N	5.726078	1.688652	-0.342633
N	0.206768	1.877289	0.844128
C	-0.692075	2.880365	0.515901
C	-2.943197	-4.050012	0.124659
C	-5.320032	-5.591719	-0.037545
O	9.883002	-3.045048	0.033775
C	-2.997893	3.317649	0.253130
O	-6.424357	6.899413	-0.159566
C	-5.309450	-4.264367	-0.480468
H	-6.219862	-3.840353	-0.884349
C	-4.163395	-3.507378	-0.405643
H	-4.169905	-2.486871	-0.751126
C	-3.010618	-5.414771	0.566097
H	-2.100885	-5.843452	0.969165
C	6.687666	0.756567	-0.247707
C	-4.152956	-6.165524	0.490212
H	-4.171014	-7.192842	0.829092
N	10.061964	-1.832380	0.077819
C	-4.287414	2.735487	0.011814
H	-4.331994	1.654338	-0.049864
C	4.407000	1.353042	-0.459516
N	-6.518032	5.677544	-0.219679
C	8.023892	1.250898	-0.075481
H	8.145493	2.326456	-0.030104
C	1.625502	2.187735	0.817086
H	2.158024	1.353418	1.279680
H	1.822926	3.092064	1.398701
C	6.555743	-0.671899	-0.311226
H	5.574179	-1.096822	-0.442098
C	8.933974	-0.962144	-0.033626
C	-5.340618	4.884189	-0.060648
C	-5.423019	3.485447	-0.142281
H	-6.381822	3.018644	-0.325375
C	-1.555568	-2.149972	-0.123925
C	-2.964906	4.751280	0.328664
H	-2.020180	5.239053	0.503632

C	7.652080	-1.496423	-0.205841
H	7.534800	-2.571373	-0.256537
C	9.113413	0.428104	0.029350
H	10.108620	0.832054	0.159590
C	2.175474	2.382256	-0.604330
H	1.866800	1.538972	-1.225116
H	1.753480	3.293132	-1.028079
O	11.177437	-1.340440	0.215168
C	-4.107613	5.501668	0.177138
H	-4.066681	6.581385	0.241924
O	-7.590118	5.112976	-0.412085
O	-6.502995	-7.526315	0.271247
H	1.273761	-0.398376	-0.301835
C	-0.168132	0.490446	1.055249
H	-1.240722	0.443401	1.218397
H	0.343357	0.115151	1.949825
C	0.192254	-0.404589	-0.138243
N	-0.240664	-1.770928	0.042794
H	-0.293166	0.002279	-1.028766
H	0.352825	-2.424497	0.526688

L2^{3-}

65

-2135.589713 a.u.

O	-3.460881	-2.175905	-0.655933
O	1.348440	-0.370441	2.090108
N	-2.384877	-0.354469	0.148015
N	-4.666260	-0.298336	0.085403
O	-6.021824	1.566933	1.616683
O	0.147029	2.943046	0.565134
N	0.742902	-2.257339	0.987019
H	1.040004	-2.839211	0.217497
O	4.782089	-3.410408	-0.131856
N	2.926577	-1.636925	0.877409
O	-7.515048	2.308201	0.274103
O	1.851503	-0.562969	-2.366967
N	-1.291330	2.143951	-1.005656
H	-1.319261	1.413096	-1.703280
N	-6.823664	1.400774	0.720305
N	0.933460	1.724060	-1.278615
O	3.911080	-1.064721	-2.116607
N	5.462992	-2.413704	-0.271333
N	2.980433	-0.271108	-2.015107

C	-3.552536	-1.029764	-0.175113
C	1.701652	-1.316773	1.366580
C	-1.102584	-0.992765	-0.087641
H	-0.344651	-0.218278	-0.212624
H	-1.153384	-1.563789	-1.016793
C	-5.904787	-0.784411	-0.102457
C	4.032328	-0.941114	1.206232
C	-0.664237	-1.915159	1.057451
H	-0.833392	-1.405598	2.007016
H	-1.264502	-2.827467	1.047853
C	-7.023629	0.066269	0.167451
C	-2.383798	0.912727	0.867363
H	-1.470423	0.953859	1.469172
H	-3.250368	0.954035	1.526449
C	2.245151	1.976261	-1.103288
C	0.000173	2.327620	-0.502343
O	6.337188	-2.334480	-1.127859
C	5.300695	-1.286881	0.635244
C	3.270857	1.051298	-1.486940
C	-2.406648	2.124186	-0.069980
H	-3.337224	2.110327	-0.641104
H	-2.376701	3.041531	0.520970
C	-6.288464	-2.072065	-0.603270
H	-5.497169	-2.769033	-0.826528
C	-8.349915	-0.276255	-0.083344
H	-9.120780	0.455076	0.125387
C	2.751078	3.213486	-0.582296
H	2.023621	3.947230	-0.268808
C	-8.662531	-1.532715	-0.564438
H	-9.691476	-1.818193	-0.738614
C	-7.607199	-2.420971	-0.812428
H	-7.826635	-3.415277	-1.188537
C	4.106609	0.182294	2.097914
H	3.186271	0.505196	2.555838
C	4.637998	1.343626	-1.360298
H	5.345789	0.579178	-1.648431
C	4.092366	3.493762	-0.484486
H	4.401864	4.460844	-0.100981
C	6.482782	-0.590257	0.898930
H	7.388437	-0.921667	0.408399
C	5.063226	2.556057	-0.872802
H	6.119738	2.770860	-0.779230
C	6.496420	0.473454	1.774588

H	7.417003	0.998303	1.994458
C	5.282554	0.846720	2.367407
H	5.259634	1.684806	3.057154

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-2135.603023 a.u.

O	-2.758422	0.714011	-1.662919
O	2.765372	2.994237	-0.782462
O	0.097059	2.105882	2.676247
N	0.579094	3.508584	-0.422495
N	2.131701	1.111654	2.067309
N	1.084972	1.440849	-1.276069
O	3.011804	-4.452035	0.441501
N	-3.006710	2.970272	-1.462990
H	-3.533005	3.642485	-0.923763
N	1.922709	3.378570	2.132090
H	2.714908	3.263303	1.510249
N	3.345457	-3.352851	0.842864
N	-4.697091	1.639256	-0.722374
O	4.504240	-2.983033	0.879670
O	-3.632613	-3.319086	-0.276069
C	1.676753	-0.165173	1.939214
N	-4.808063	-3.249823	0.023696
C	2.650334	-1.125658	1.557287
H	3.671164	-0.798042	1.418408
C	1.574478	2.613463	-0.831270
C	-3.465050	1.662608	-1.277640
C	2.294583	-2.430652	1.293839
C	1.284048	2.133436	2.305018
C	-0.813091	3.106484	-0.303964
H	-1.282722	3.739505	0.455726
H	-0.881450	2.075032	0.037438
C	1.901132	0.376268	-1.501490
C	-5.289436	0.458989	-0.388752
C	-4.708786	-0.837372	-0.387317
H	-3.691503	-0.972392	-0.711536
C	1.103506	4.527753	1.788466
H	1.522158	5.441869	2.223652
H	0.121450	4.364412	2.233797
C	0.352647	-0.664779	2.090786
H	-0.420701	0.019480	2.403068

C	0.976455	4.721497	0.264594
H	0.242688	5.509233	0.061502
H	1.934701	5.040776	-0.143262
C	-1.589866	3.245218	-1.616937
H	-1.470312	4.259197	-2.010707
H	-1.172381	2.545212	-2.339761
C	-5.460144	-1.924646	0.029501
O	-5.478194	-4.220174	0.321739
C	3.297026	0.278557	-1.260915
H	3.841250	1.132698	-0.897466
C	0.992151	-2.914256	1.410990
H	0.757577	-3.943998	1.186745
C	1.280717	-0.807359	-1.988696
H	0.211722	-0.760394	-2.165042
C	0.036955	-1.996277	1.826197
H	-0.991706	-2.322280	1.938880
C	-6.640076	0.524182	0.052781
H	-7.101518	1.505072	0.066427
N	5.373616	-1.002306	-1.138741
C	-6.779940	-1.856104	0.453394
H	-7.314949	-2.741614	0.761080
C	3.944746	-0.925571	-1.478177
O	5.835152	-0.169955	-0.380582
C	1.967542	-1.990364	-2.198812
H	1.430920	-2.865604	-2.548011
C	-7.357546	-0.587697	0.456595
H	-8.384937	-0.471552	0.782028
C	3.335646	-2.079757	-1.950362
H	3.895582	-2.995159	-2.074750
O	6.034672	-1.899026	-1.626340

L4^{3-}

68

-1640.023995 a.u.

O	4.017183	0.130488	-0.876741
O	-1.675093	-0.318833	-2.726595
O	-3.341649	-3.304716	0.863379
N	-0.039954	-1.619747	-1.838106
N	-4.176520	-1.248199	0.080112
N	0.164613	0.667906	-1.683795
N	3.672905	-2.070111	-1.349849

H	3.765230	-2.978071	-0.917973
N	-2.816151	-2.526870	-1.207147
H	-2.725125	-1.657067	-1.723069
N	5.183423	-1.556603	0.272033
C	-4.937458	-0.924058	1.172846
C	-5.552023	0.358514	1.141081
H	-5.357621	0.970770	0.264448
C	-0.582769	-0.360060	-2.105643
C	4.308022	-1.053656	-0.614900
C	-6.362954	0.845854	2.153761
C	-3.468111	-2.394780	0.017249
C	1.202250	-1.792420	-1.109950
H	1.153489	-2.737690	-0.555779
H	1.314776	-0.981805	-0.392063
C	-0.387040	1.923691	-1.580677
C	5.998556	-0.739208	1.018835
C	6.173514	0.663480	0.905624
H	5.593636	1.197179	0.167038
C	-1.684870	-3.421888	-1.355923
H	-1.997787	-4.408488	-1.723336
H	-1.199732	-3.581690	-0.386132
C	-5.205129	-1.706136	2.326934
H	-4.760407	-2.685760	2.404948
C	-0.681722	-2.821410	-2.342927
H	0.090144	-3.564980	-2.563813
H	-1.193295	-2.582837	-3.277158
C	2.425160	-1.809048	-2.035803
H	2.282950	-2.565471	-2.814598
H	2.500024	-0.835034	-2.517784
C	7.066252	1.368446	1.715177
C	-1.757924	2.219768	-1.391571
H	-2.468926	1.403820	-1.395611
C	-6.607024	0.043711	3.277397
H	-7.242216	0.405192	4.079453
C	0.498342	3.029659	-1.564025
H	1.557016	2.826490	-1.689960
C	-6.023271	-1.216588	3.341940
H	-6.210316	-1.844373	4.208824
C	6.788114	-1.380980	2.009292
H	6.675393	-2.454849	2.114237
C	7.825377	0.698363	2.673993
H	8.522039	1.244753	3.300777
C	-2.218144	3.519821	-1.190298

C	0.042329	4.324499	-1.378077
H	0.752969	5.145110	-1.374757
C	7.673463	-0.683513	2.810945
H	8.258069	-1.219657	3.552122
C	-1.316486	4.585658	-1.191839
H	-1.669910	5.600396	-1.043549
C	7.180795	2.867162	1.560367
H	7.131652	3.159424	0.509272
H	6.361777	3.375743	2.077668
H	8.118022	3.239552	1.978037
C	-3.691447	3.755373	-0.949826
H	-4.299310	3.254234	-1.707163
H	-3.995794	3.356332	0.022349
H	-3.931938	4.819789	-0.966314
C	-6.967616	2.226419	2.060861
H	-8.041885	2.198952	2.259792
H	-6.519972	2.900363	2.796854
H	-6.813808	2.659489	1.071106

$L1^{-}(H_c)$

67

-2136.586451 a.u.

O	-0.464706	-3.623786	0.367055
O	3.348085	0.960428	-0.501814
N	1.546359	-2.411992	0.397099
O	-4.349081	0.480996	-0.483058
O	9.012902	4.792089	0.219466
N	2.944561	3.219316	-0.371043
H	2.210792	3.913165	-0.373620
N	-3.990726	-1.741934	-0.747964
H	-4.373945	-2.669238	-0.649892
N	8.033874	5.512228	0.248986
N	-6.137279	-0.966872	-0.467664
H	-6.396585	-1.928212	-0.637671
N	-0.491633	-1.374542	0.589136
C	0.198874	-2.576063	0.442639
C	4.228707	3.721441	-0.218545
C	6.720332	4.896534	0.088874
O	-10.423357	3.500624	0.672039
C	2.384763	-3.462239	0.299785
O	5.074486	-7.632791	0.009554
C	6.629793	3.523110	-0.086780

H	7.530088	2.924345	-0.103197
C	5.389135	2.929048	-0.241121
H	5.309637	1.864029	-0.380197
C	4.350079	5.112154	-0.039050
H	3.458619	5.728208	-0.021230
C	-7.196799	-0.099130	-0.246005
C	5.587073	5.701912	0.113524
H	5.683358	6.769820	0.251275
N	-10.599882	2.323113	0.426013
C	3.777632	-3.137857	0.211274
H	4.036841	-2.085698	0.221034
C	-4.782713	-0.657056	-0.553321
N	5.409403	-6.454026	0.008604
C	-8.490671	-0.649205	-0.302732
H	-8.613596	-1.703338	-0.522178
C	-1.940901	-1.426770	0.611497
H	-2.322098	-0.504793	1.054128
H	-2.261073	-2.268651	1.228480
C	-7.043943	1.267551	0.041508
H	-6.058633	1.700568	0.087816
C	-9.427581	1.484565	0.195904
C	4.395516	-5.446463	0.104105
C	4.757068	-4.091743	0.116119
H	5.801710	-3.818239	0.049808
C	2.556751	1.887811	-0.509886
C	2.064909	-4.859077	0.281416
H	1.031302	-5.156360	0.343534
C	-8.162969	2.052234	0.260395
H	-8.058545	3.105178	0.482864
C	-9.604067	0.134272	-0.084271
H	-10.599392	-0.285033	-0.129690
C	-2.544486	-1.598476	-0.787722
H	-2.302899	-0.735996	-1.410828
H	-2.126608	-2.493798	-1.246640
O	-11.697143	1.803434	0.360209
C	3.050729	-5.816329	0.187571
H	2.794393	-6.867965	0.177377
O	6.581267	-6.104894	-0.071221
O	8.085803	6.717157	0.404635
H	-0.260274	0.478267	-1.404759
C	0.185115	-0.091370	0.642241
H	1.077050	-0.171618	1.263943
H	-0.492016	0.632936	1.102383

C	0.604604	0.417726	-0.741707
N	1.218102	1.733637	-0.675469
H	1.325505	-0.279316	-1.166687
H	0.609186	2.533716	-0.599121

$L1^{2-}(H_cH_a)$

66

-2136.101247 a.u.

O	-0.367845	3.667583	-0.364576
O	3.209053	-1.079981	0.398501
N	1.638026	2.449148	-0.379786
O	-4.243965	-0.393788	0.491099
O	8.813512	-5.019745	0.212279
N	2.726584	-3.364272	0.081062
N	-3.892884	1.837036	0.694342
H	-4.282423	2.759508	0.578064
N	7.819053	-5.689046	-0.049478
N	-6.038195	1.046861	0.455299
H	-6.299690	2.010622	0.607047
N	-0.402199	1.428003	-0.656198
C	0.291010	2.617084	-0.457855
C	3.990237	-3.813695	0.056566
C	6.535836	-5.063243	-0.017706
O	-10.318119	-3.458235	-0.549636
C	2.476808	3.495061	-0.270873
O	5.185664	7.655273	0.000053
C	6.425925	-3.707648	0.312720
H	7.324954	-3.150192	0.542448
C	5.197017	-3.091648	0.349174
H	5.127386	-2.046733	0.602659
C	4.159577	-5.200024	-0.275500
H	3.260518	-5.762169	-0.498237
C	-7.096256	0.170779	0.263608
C	5.384913	-5.810119	-0.314131
H	5.481350	-6.857474	-0.567907
N	-10.496662	-2.277142	-0.322815
C	3.865286	3.164761	-0.132524
H	4.115099	2.110556	-0.109592
C	-4.681169	0.744195	0.536005
N	5.512243	6.474022	0.035213
C	-8.391822	0.716466	0.325936
H	-8.516559	1.773913	0.527701

C	-1.851226	1.488334	-0.668442
H	-2.236316	0.553061	-1.079081
H	-2.179138	2.311346	-1.308183
C	-6.940924	-1.200271	-0.000987
H	-5.954246	-1.629764	-0.051605
C	-9.325391	-1.429906	-0.122218
C	4.495715	5.471703	-0.062351
C	4.847864	4.114020	-0.031928
H	5.888221	3.835571	0.070626
C	2.438592	-2.046748	0.312908
C	2.166091	4.895079	-0.289709
H	1.136511	5.197257	-0.384986
C	-8.059065	-1.993431	-0.191892
H	-7.952669	-3.049788	-0.396631
C	-9.504320	-0.075394	0.135294
H	-10.500792	0.340661	0.185081
C	-2.445545	1.702929	0.729167
H	-2.192707	0.864637	1.379756
H	-2.031068	2.616156	1.153057
O	-11.595417	-1.760970	-0.253103
C	3.155404	5.847357	-0.190727
H	2.906344	6.900585	-0.211676
O	6.680452	6.120636	0.150601
O	7.889784	-6.879867	-0.336745
H	-0.474574	-0.656067	1.106073
C	0.256634	0.137109	-0.771612
H	1.224397	0.271644	-1.250120
H	-0.359015	-0.508986	-1.404565
C	0.479374	-0.546871	0.583304
N	1.081816	-1.853615	0.460730
H	1.131899	0.089582	1.183505
H	0.499687	-2.653418	0.272821

$L1^{2-}(H_cH_b)$

66

-2136.087900 a.u.

O	-0.103662	3.784087	-0.371440
O	2.740513	-1.235608	0.600215
N	1.817162	2.439384	-0.432179
O	-4.099827	-0.168883	0.457108
O	8.371318	-5.174869	0.318651
N	2.343274	-3.437283	-0.001993

H	1.585227	-4.053173	-0.259107
N	-3.746244	2.062993	0.650134
H	-4.141330	2.985115	0.552413
N	7.391944	-5.846722	0.035369
N	-5.895424	1.270266	0.458946
H	-6.154921	2.234172	0.613073
N	-0.290668	1.568722	-0.759148
C	0.480239	2.693754	-0.510898
C	3.589350	-3.970492	0.024877
C	6.096605	-5.210446	0.031280
O	-10.190047	-3.237393	-0.469389
C	2.717818	3.424871	-0.293626
O	5.688845	7.393847	0.109305
C	5.989504	-3.857335	0.350956
H	6.882313	-3.299311	0.599634
C	4.758530	-3.237711	0.351376
H	4.659124	-2.193696	0.599849
C	3.732426	-5.346536	-0.295100
H	2.847981	-5.920445	-0.547338
C	-6.955954	0.393549	0.286740
C	4.963189	-5.958211	-0.292752
H	5.063735	-7.006645	-0.538094
N	-10.364993	-2.056238	-0.239913
C	4.078032	3.002810	-0.113566
H	4.256559	1.934361	-0.087601
C	-4.535991	0.969434	0.510734
N	5.934888	6.192159	0.133336
C	-8.250704	0.938772	0.369836
H	-8.372447	1.996501	0.571937
C	-1.731770	1.723586	-0.755479
H	-2.173130	0.821482	-1.185464
H	-2.018220	2.580309	-1.370944
C	-6.804743	-0.978041	0.022050
H	-5.818919	-1.407376	-0.044282
C	-9.190877	-1.208627	-0.059660
C	4.859506	5.262437	-0.009467
C	5.117514	3.883128	0.025260
H	6.132407	3.533991	0.161236
C	1.891445	-2.086355	0.255822
C	2.504781	4.844728	-0.322979
H	1.501960	5.216024	-0.453795
C	-7.925582	-1.771819	-0.149230
H	-7.822237	-2.828490	-0.353960

C	-9.365872	0.146254	0.198815
H	-10.361476	0.562206	0.264586
C	-2.298015	1.930355	0.654790
H	-2.028438	1.086737	1.291520
H	-1.875101	2.840068	1.077544
O	-11.462652	-1.540441	-0.151550
C	3.551670	5.727079	-0.186112
H	3.375375	6.794659	-0.214820
O	7.074675	5.761062	0.275657
O	7.458757	-7.033573	-0.244400
H	-1.002617	-0.749747	0.532289
C	0.248129	0.225508	-0.925530
H	1.308580	0.307738	-1.142508
H	-0.250385	-0.249720	-1.778583
C	0.068196	-0.669011	0.309133
N	0.596852	-1.999562	0.084072
H	0.550504	-0.156714	1.155159

$L1^{4-}(H_cH_{a2}H_b)$

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-2135.083515 a.u.

O	-0.625749	3.941145	-0.106451
O	-3.055691	-1.343096	0.676020
N	-2.407457	2.520916	0.448940
O	3.688869	0.204409	-0.403872
O	-4.498378	-7.569325	-2.355488
N	-2.412447	-3.293224	1.735419
N	3.098927	2.299821	-1.026777
H	3.427620	3.251217	-1.067245
N	-4.364200	-7.632209	-1.118683
N	5.301928	1.903223	-0.666505
N	-0.211370	1.886396	0.732796
C	-1.091261	2.872609	0.330893
C	-2.880747	-4.269034	1.025018
C	-3.880203	-6.536591	-0.420017
O	10.122771	-2.030681	0.388408
C	-3.397243	3.393210	0.223654
O	-6.728381	7.002644	-0.568803
C	-3.534599	-5.338989	-1.102958
H	-3.659320	-5.310195	-2.178240
C	-3.063934	-4.257268	-0.428078
H	-2.820500	-3.347583	-0.962296

C	-3.255897	-5.521024	1.678853
H	-3.134513	-5.559595	2.755843
C	6.391476	1.154761	-0.437163
C	-3.726058	-6.593695	0.993950
H	-3.991983	-7.509688	1.505513
N	10.117960	-0.816993	0.208991
C	-4.728170	2.850952	0.264664
H	-4.814141	1.786147	0.448950
C	4.044929	1.362873	-0.665266
N	-6.868811	5.801904	-0.352656
C	7.641867	1.859446	-0.410570
H	7.601727	2.930762	-0.565854
C	1.209219	2.137687	0.571589
H	1.754813	1.393474	1.156137
H	1.456186	3.132261	0.954232
C	6.472575	-0.264603	-0.230178
H	5.562517	-0.841195	-0.238447
C	8.871490	-0.153921	-0.005880
C	-5.710341	4.993083	-0.161733
C	-5.847661	3.615758	0.079007
H	-6.836681	3.178411	0.114344
C	-2.090332	-2.065177	1.051161
C	-3.308647	4.806075	-0.028129
H	-2.334054	5.263072	-0.074943
C	7.680494	-0.889058	-0.022838
H	7.724106	-1.960004	0.128645
C	8.842639	1.235496	-0.202895
H	9.768684	1.794662	-0.188427
C	1.681247	2.050826	-0.886597
H	1.459820	1.056827	-1.278464
H	1.134556	2.787505	-1.475743
O	11.149766	-0.152610	0.207364
C	-4.435951	5.571474	-0.210750
H	-4.351569	6.634983	-0.394160
O	-7.976482	5.275130	-0.294713
O	-4.661977	-8.673736	-0.503491
H	0.563847	-0.615504	-0.044538
C	-0.617194	0.598028	1.283932
H	-1.658044	0.662507	1.583318
H	-0.003613	0.391006	2.169132
C	-0.474911	-0.577391	0.307972
N	-0.798898	-1.842808	0.940728
H	-1.113583	-0.352429	-0.561160

$L1^{5-}(H_cH_{a2}H_{b2})$

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-2134.549380 a.u.

O	-0.785993	-3.948296	-0.124176
O	-2.974709	1.476676	-0.489958
N	-2.538983	-2.403226	-0.247981
O	3.525999	-0.476354	-1.364074
O	-2.877275	7.969714	2.340933
N	-2.595740	3.305152	-1.846112
N	3.193374	-2.533619	-0.331060
N	-3.175659	7.950920	1.131140
N	5.245540	-2.021423	-1.261145
N	-0.461013	-1.956459	-1.145138
C	-1.261649	-2.856216	-0.483166
C	-2.728933	4.357853	-1.104945
C	-3.031107	6.780806	0.402769
O	9.305823	1.132657	2.334371
C	-3.522310	-3.227631	0.108908
O	-6.911058	-6.708118	1.194460
C	-2.546682	5.597461	1.024305
H	-2.297605	5.637969	2.077366
C	-2.403822	4.443676	0.321266
H	-2.049210	3.547656	0.815024
C	-3.228037	5.599275	-1.693468
H	-3.481628	5.568409	-2.747422
C	6.202716	-1.426684	-0.623798
C	-3.368724	6.744612	-0.980073
H	-3.738677	7.650131	-1.443635
N	9.503972	0.278725	1.449359
C	-4.770693	-2.605642	0.468698
H	-4.795025	-1.521961	0.450315
C	3.892449	-1.617994	-0.963818
N	-6.978886	-5.479997	1.180206
C	7.588980	-1.791042	-0.908107
H	7.743821	-2.538714	-1.678069
C	0.945673	-2.288494	-1.336200
H	1.345721	-1.620735	-2.101770
H	1.031035	-3.320299	-1.688715
C	6.037523	-0.403084	0.410976
H	5.033090	-0.065824	0.633142
C	8.428845	-0.274045	0.770648
C	-5.827979	-4.726810	0.825208

C	-5.882655	-3.321038	0.815212
H	-6.806248	-2.824247	1.081309
C	-2.136367	2.097569	-1.201644
C	-3.514751	-4.668366	0.136794
H	-2.602421	-5.184570	-0.115530
C	7.099385	0.129951	1.070865
H	6.954469	0.880431	1.838110
C	8.640876	-1.249426	-0.244294
H	9.657219	-1.545516	-0.470537
C	1.817856	-2.136815	-0.080859
H	1.735519	-1.093525	0.257153
H	1.390995	-2.780087	0.695390
O	10.662992	-0.082988	1.169506
C	-4.636062	-5.381828	0.480042
H	-4.616280	-6.464124	0.487405
O	-8.016650	-4.884241	1.464593
O	-3.604107	8.978232	0.571002
H	0.651087	0.523596	-0.851378
C	-0.929877	-0.678015	-1.668158
H	-2.014823	-0.674821	-1.664048
H	-0.579274	-0.578158	-2.703110
C	-0.445369	0.542032	-0.874399
N	-0.889084	1.787173	-1.477920
H	-0.802307	0.414786	0.159735