Supporting information for

Bis(imidazolium) salts derived from amino acids as receptors and transport agents for chloride anion

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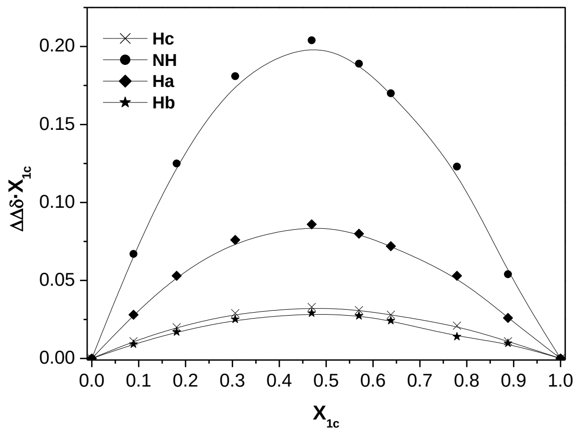
Table of contents:

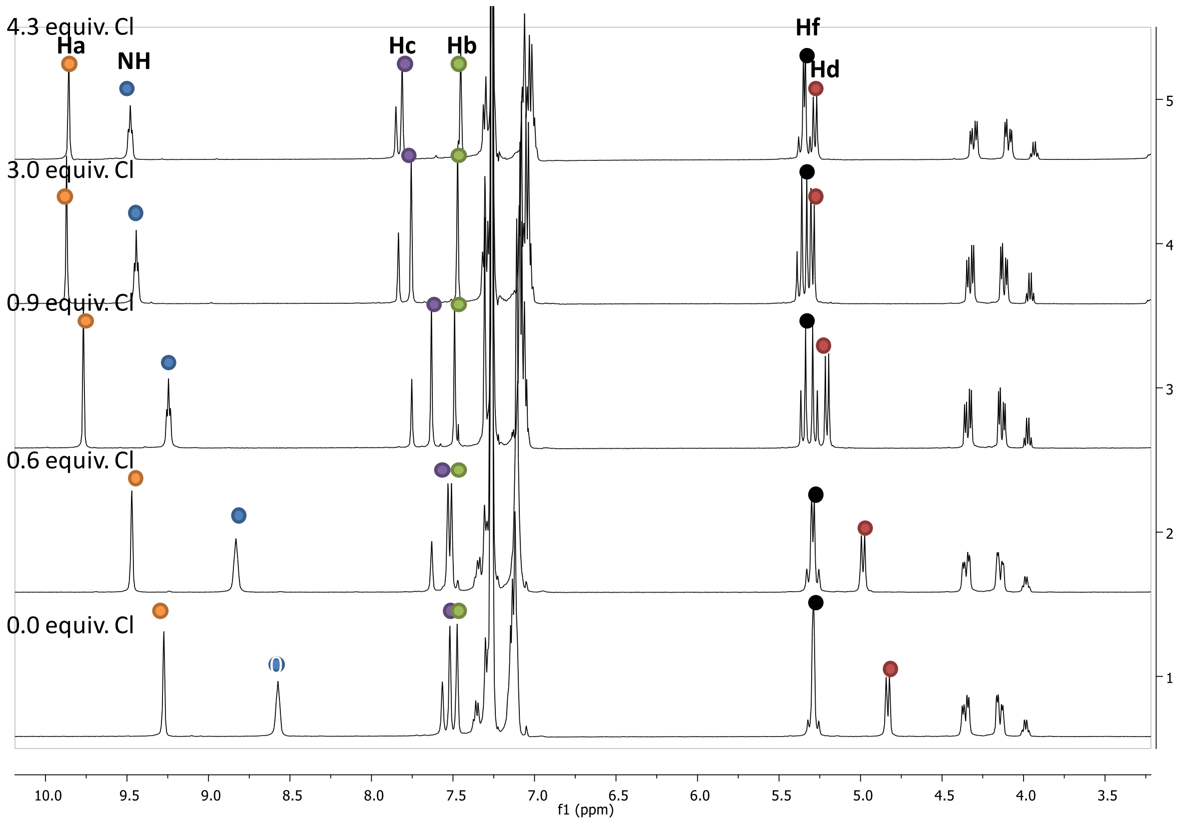
Job plot analysis for 1c and chloride

Figure S1. Job plot for the complexation of **1c** with chloride anion. The *Δδ* stands for the chemical shift change of the different protons of 1c in the presence of TBACl. Total concentration is 8 mM.



^{1}H NMR titration in $CDCl_3$ for 1b and TBACl

Figure S2. Selected stacked ^{1}H NMR spectra for the titration of **1b** with TBACl (solvent 95 : 5 $CDCl_3$: DMSO-d_6, 0.1 M TBACl and 0.01 M receptor, **1b**)



^{1}H NMR titration procedure

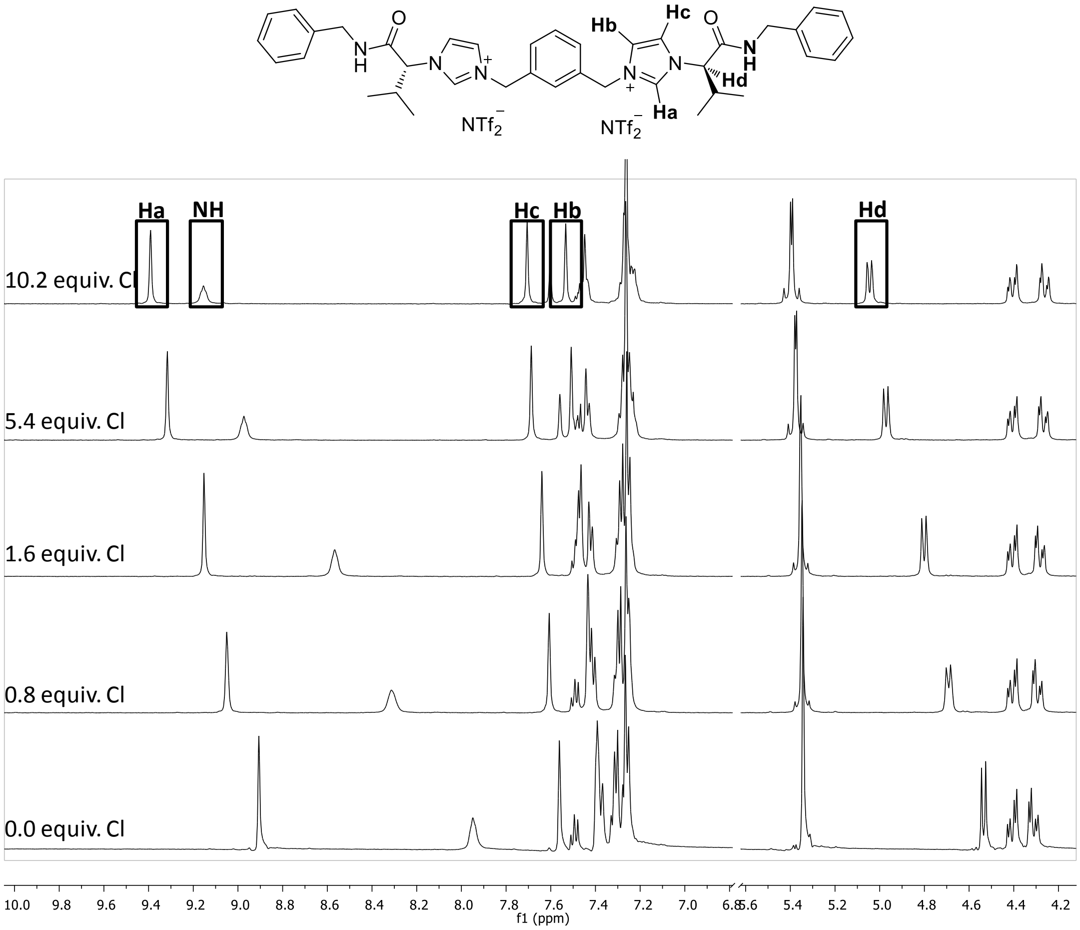
The titrations were performed with the imidazolium receptors as bis-triflamide salts.Stock solutions of the receptors were prepared by weighting the corresponding amount of the receptor and reaching a final concentration of 5 mM. The solvent used was 95 : 5 CD_3CN : D_2O, since this mixture allowed a good solubility during the titration experiment and rendered reasonably sharp and well-defined ^{1}H NMR spectra. Additionally, a stock solution of the titrant containing 0.5 M tetrabutylammonium salt (TBAX) was prepared by dissolving the salt in the stock solution of the corresponding receptor. Thus, for every experiment, the solution of the titrant will be 0.5 M in TBAX and 0.005 M in the receptor, thus maintaining the concentration of the receptor constant during the titration experiment. The stock solution of the receptor was introduced in a NMR tube and the ^{1}H NMR spectrum (500 MHz, 303 K) was acquired, then small volumes of the stock solution of the titrant were added and the ^{1}H NMR spectrum recorded after each addition.

Different signals changed upon addition of diferents anions, and their variations were fitted to the simplest model using HypNmr 2008 version 4.0.71 software. For further details concerning the way the program works see: C. Frassineti, S. Ghelli, P. Gans, A. Sabatini, M.S. Moruzzi and A. Vacca, "Nuclear Magnetic Resonance as a Tool for Determining Protonation Constants of Natural Polyprotic Bases in Solution", Analytical Biochemistry 1995, 231, 374-382; C. Frassineti, L. Alderighi, P. Gans, A. Sabatini, A.Vacca, S. Ghelli, "Determination of protonation constants of some fluorinated polyamines by means of 13C NMR data processed by the new computer program HypNMR2000. Protonation sequence in polyamines", Anal. Bioanal. Chem. 2003, 376, 1041-1052.

For a suitable comparison of the systems, we calculated the BC_{50} parameter, using the BC50 calculator version 2.37.1 program. For a detailed discussion on this parameter and the use of this program, see: (a) C. Nativi, O. Francesconi, G. Gabrielli, A. Vacca, S. Roelens, “Chiral Diaminopyrrolic Receptors for Selective Recognition of Mannosides, Part 1: Design, Synthesis and Affinities of Second-Generation Tripodal Receptors” Chem. Eur. J. 2011, 17, 4814 – 4820. (b) A. Vacca, C. Venturi, S. Roelens, “Binding of Ionic Species. A General Approach to Measuring Binding Constants and Assessing Affinities” Chem. Eur. J. 2009, 15, 2635 – 2644. (c) S. Roelens, A. Vacca, O. Francesconi, C. Venturi, “Ion-pair Binding: Is Binding Both Binding Better?” Chem. Eur. J. 2009, 15, 8296 – 8302. (d) C. Nativi, M. Cacciarini, O. Francesconi, A. Vacca, G. Moneti, A. Ienco, S. Roelens, “Pyrrolic Tripodal Receptors Effectively Recognizing Monosaccharides. Affinity Assessment through a Generalized Binding Descriptor” J. Am. Chem. Soc. 2007, 129, 4377 – 4385.

Following, we show the stacked plot of the NMR spectra for the titration experiments, the corresponding data set introduced (experimental) and obtained (fit) during the fitting process, the output values (both logβ and BC^{0}_{50}) for the binding for every supramolecular complex, the plot of the experimental (symbols) and the fitted (lines) values of the chemical shifts, and the plot of the simulated species distribution obtained with HySS2009 software (for details, see: L. Alderighi , P. Gans, A. Ienco , D. Peters, A. Sabatini and A. Vacca, "Hyperquad simulation and speciation (HySS): a utility program for the investigation of equilibria involving soluble and partially soluble species", Coordination Chemistry Reviews 1999, 184, 311-318).

Figure S3. Selected stacked ^{1}H NMR spectra for the titration of **1b** with TBACl.



Data set:

Conc. Cl	equiv. Cl	Hd	Hd_fit	NH	NH_fit	Ha	Ha_fit	Hc	Hc_fit	Hb	Hb_fit
0.000	0.000	4.526	4.526	7.949	7.949	8.907	8.907	7.562	7.562	7.392	7.392
0.004	0.804	4.683	4.688	8.313	8.325	9.050	9.056	7.607	7.610	7.434	7.433
0.008	1.594	4.793	4.790	8.567	8.563	9.152	9.150	7.640	7.639	7.465	7.459
0.012	2.372	4.856	4.855	8.716	8.715	9.212	9.211	7.658	7.658	7.481	7.477
0.015	3.137	4.893	4.889	8.805	8.796	9.248	9.244	7.669	7.667	7.490	7.487
0.019	3.889	4.923	4.923	8.875	8.876	9.276	9.276	7.677	7.677	7.498	7.497
0.023	4.630	4.947	4.948	8.932	8.937	9.300	9.301	7.683	7.684	7.504	7.505
0.026	5.359	4.963	4.964	8.973	8.973	9.316	9.316	7.687	7.688	7.509	7.510
0.030	6.077	4.978	4.980	9.008	9.015	9.331	9.333	7.691	7.692	7.513	7.516
0.037	7.480	5.002	5.004	9.069	9.072	9.355	9.357	7.698	7.698	7.520	7.524
0.050	10.159	5.036	5.035	9.154	9.149	9.391	9.390	7.706	7.705	7.533	7.537
0.068	13.891	5.065	5.064	9.232	9.226	9.424	9.423	7.713	7.712	7.547	7.551
0.096	19.447	5.095	5.097	9.310	9.310	9.459	9.460	7.719	7.719	7.564	7.567
0.120	24.309	5.118	5.117	9.364	9.365	9.486	9.485	7.722	7.723	7.579	7.578
0.141	28.599	5.132	5.132	9.403	9.405	9.502	9.503	7.725	7.725	7.592	7.586

Results of the HypNMR fitting:

log β_1 = 2.28 ± 0.02 (1:1)

log β_2 = 3.0 ± 0.1 (1:2)

BC_{50} = 4.99 ± 0.21 mM = 4990 ± 211 µM

Figure S4. Plot of the experimental (symbols) and fitting (lines) data.

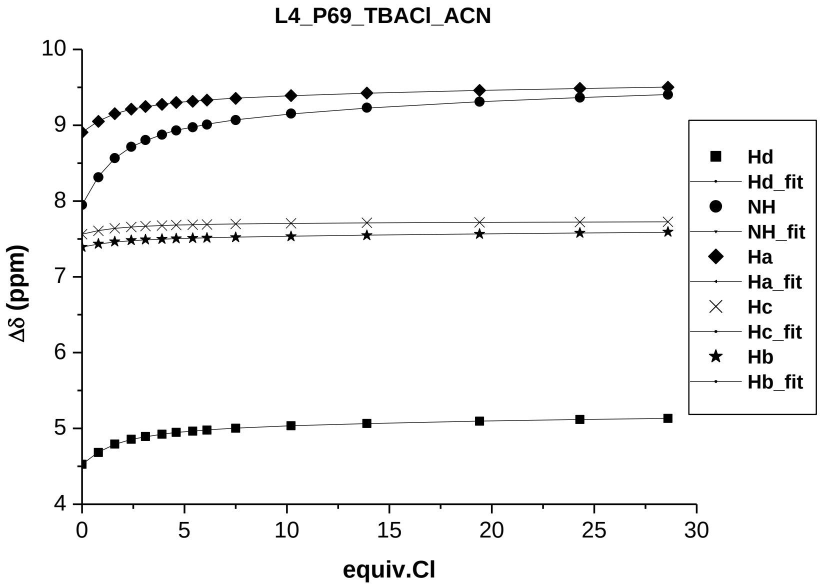


Figure S5. Species distribution as a function of the chloride (B) concentration**.**

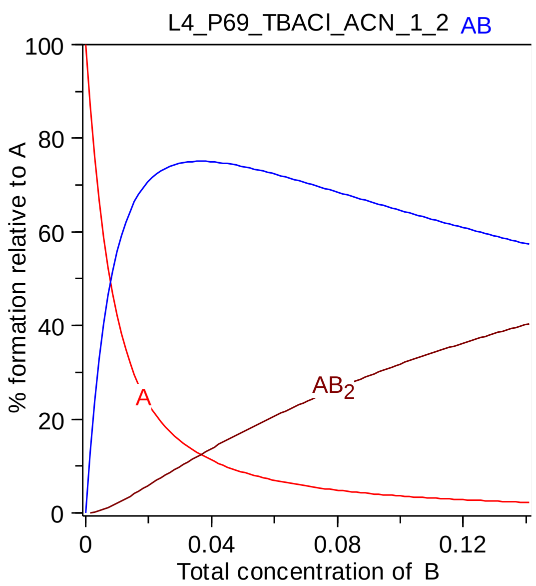
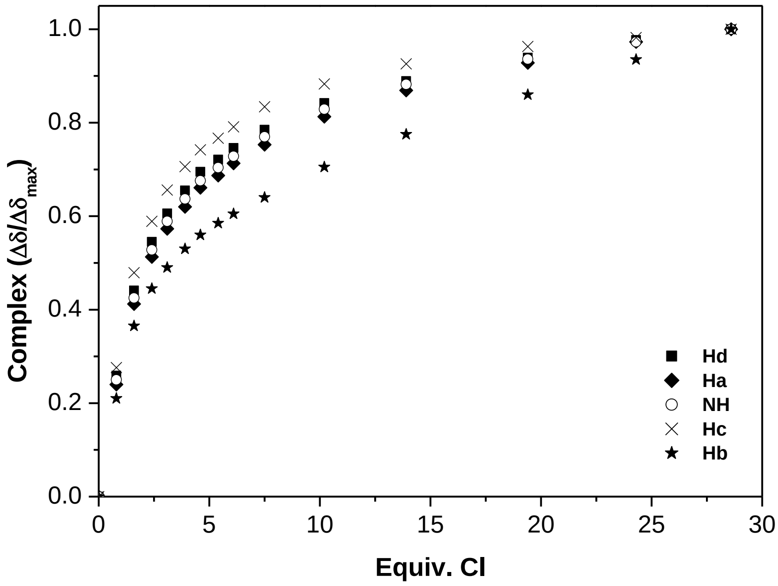


Figure S6. Plot of the chloride –induced chemical shifts observed for the different signals.



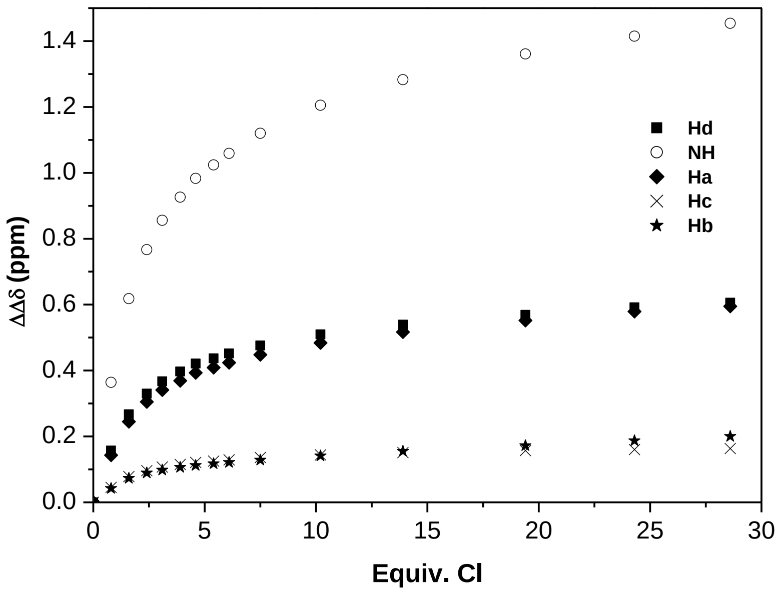
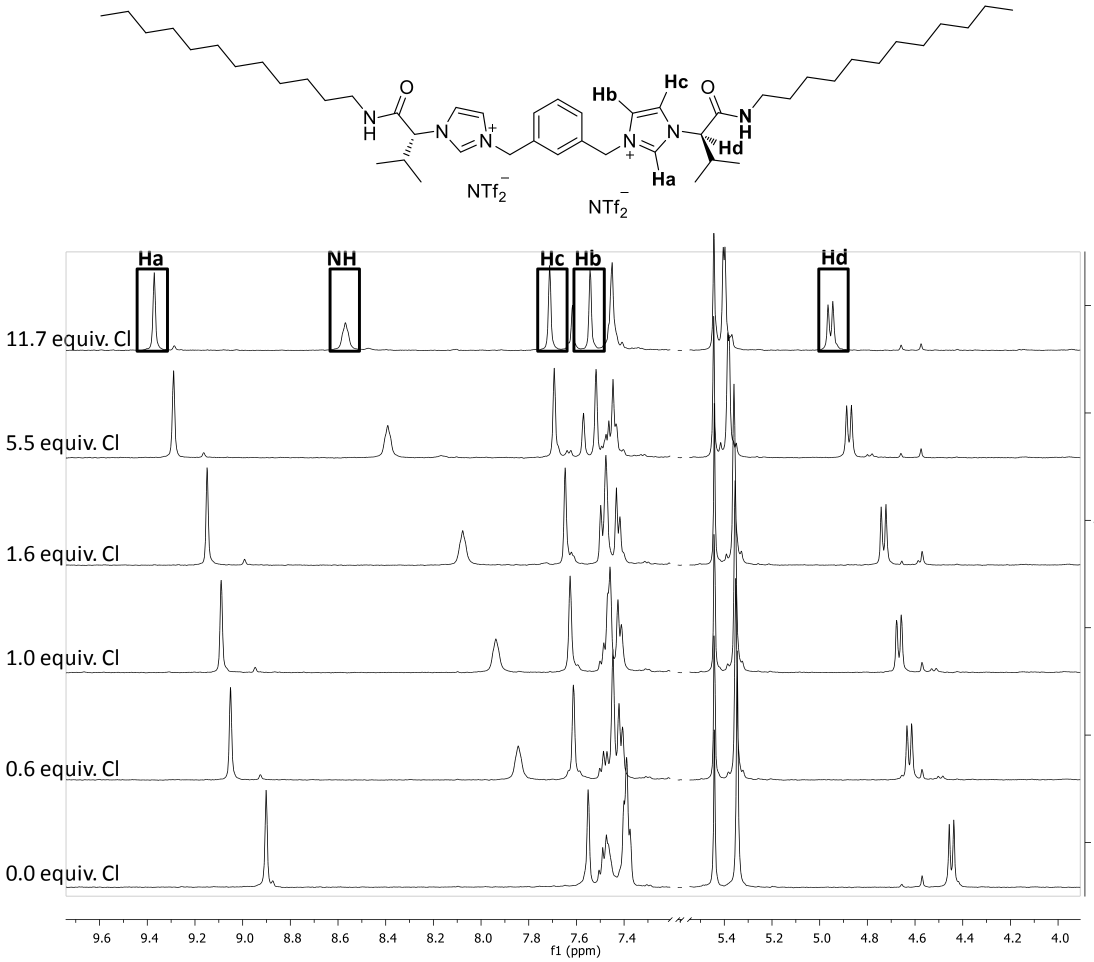


Figure S7. Selected stacked ^{1}H NMR spectra for the titration of **1c** with TBACl.



Data set:

Conc. Cl	equiv.Cl	Hd	Hd_fit	NH	NH_fit	Ha	Ha_fit	Hc	Hc_fit	Hb	Hb_fit
0.000	0.000	4.437	4.437	7.475	7.475	8.901	8.901	7.551	7.551	7.389	7.389
0.003	0.659	4.615	4.600	7.844	7.817	9.051	9.040	7.613	7.608	7.447	7.438
0.005	0.985	4.658	4.659	7.938	7.940	9.090	9.091	7.627	7.627	7.459	7.456
0.006	1.309	4.697	4.700	8.023	8.027	9.126	9.128	7.639	7.641	7.470	7.468
0.008	1.630	4.722	4.728	8.077	8.088	9.149	9.154	7.647	7.650	7.477	7.477
0.009	1.950	4.746	4.749	8.126	8.134	9.171	9.173	7.655	7.657	7.483	7.483
0.011	2.426	4.771	4.774	8.184	8.187	9.195	9.197	7.663	7.664	7.489	7.491
0.015	3.208	4.804	4.804	8.256	8.254	9.227	9.227	7.673	7.673	7.498	7.500
0.019	3.978	4.829	4.828	8.311	8.307	9.252	9.251	7.680	7.680	7.506	7.508
0.022	4.736	4.851	4.847	8.356	8.350	9.274	9.270	7.688	7.685	7.513	7.514
0.026	5.482	4.867	4.863	8.392	8.387	9.290	9.287	7.693	7.690	7.518	7.519
0.029	6.216	4.878	4.877	8.420	8.418	9.301	9.302	7.694	7.694	7.519	7.523
0.036	7.650	4.902	4.901	8.471	8.471	9.326	9.326	7.702	7.700	7.528	7.530
0.043	9.041	4.917	4.919	8.508	8.513	9.342	9.345	7.705	7.705	7.532	7.536
0.055	11.700	4.945	4.947	8.569	8.575	9.371	9.374	7.713	7.713	7.543	7.545
0.067	14.208	4.966	4.966	8.617	8.619	9.394	9.394	7.719	7.718	7.553	7.551
0.078	16.576	4.980	4.981	8.651	8.651	9.409	9.409	7.720	7.722	7.558	7.556
0.089	18.816	4.992	4.992	8.681	8.677	9.424	9.421	7.723	7.725	7.565	7.559

Results of the HypNMR fitting:
log β_1 = 3.20 ± 0.08 (1:1)
log β_2 = 4.6 ± 0.1 (1:2)
BC_{50} = 0.60 ± 0.11 mM = 608 ± 112 μM

Figure S8. Plot of the experimental (symbols) and fitting (lines) data.

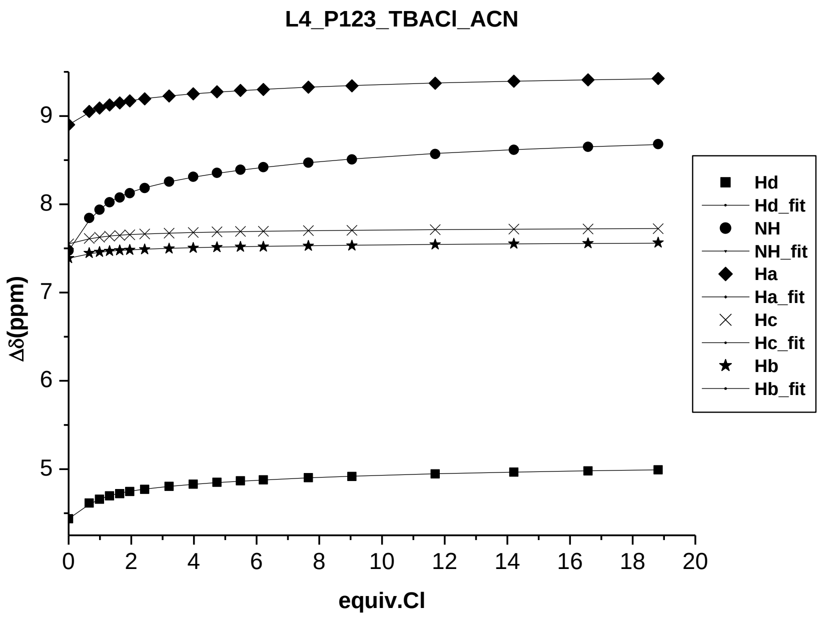


Figure S9. Species distribution as a function of the chloride (B) concentration.

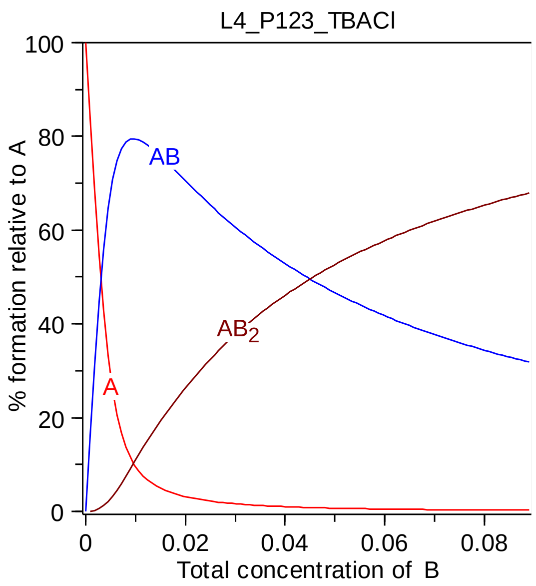
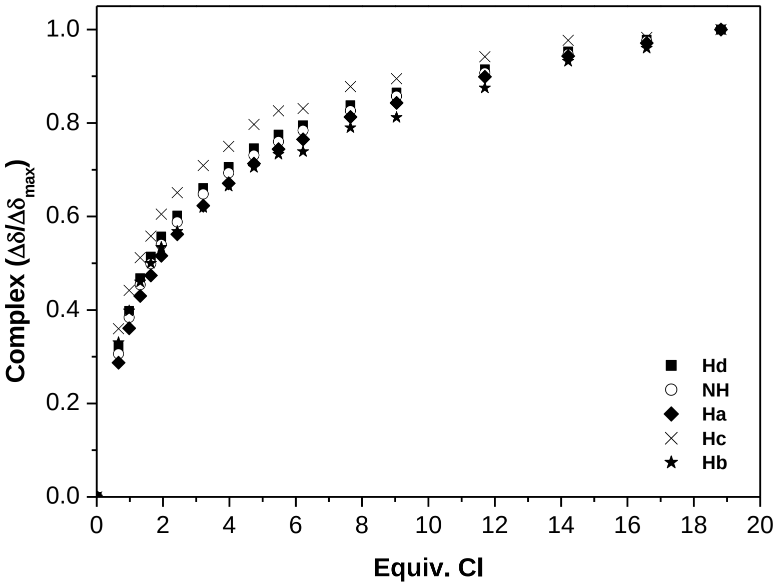


Figure S10. Plot of the chloride –induced chemical shifts of different signals for the titration of **1c**.



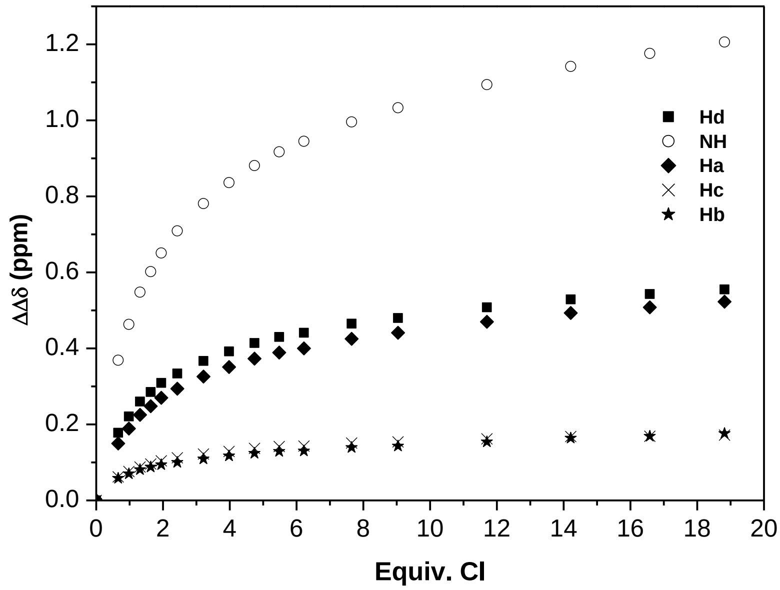
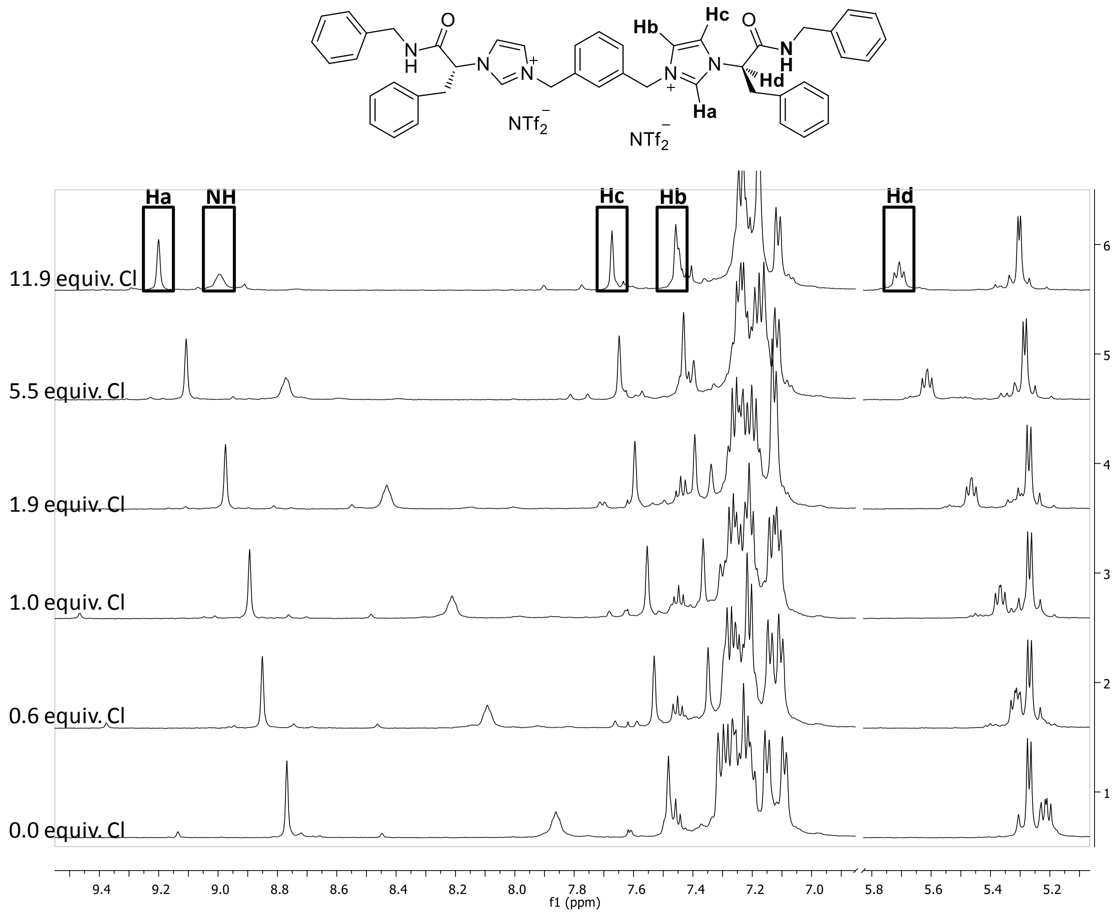


Figure S11. Stacked ^{1}H NMR spectra for the titration of **1a** with TBACl.



Data set:

Conc. Cl	equiv.Cl	Hd	Hd_fit	NH	NH_fit	Ha	Ha_fit	Hc	Hc_fit	Hb	Hb_fit
0.000	0.0	5.229	5.229	7.862	7.862	8.768	8.768	7.482	7.482	7.316	7.316
0.005	1.0	5.331	5.332	8.093	8.094	8.851	8.852	7.539	7.527	7.349	7.345
0.009	1.9	5.383	5.385	8.211	8.214	8.894	8.896	7.554	7.550	7.365	7.360
0.014	2.8	5.480	5.480	8.431	8.428	8.975	8.974	7.596	7.591	7.393	7.387
0.019	3.7	5.541	5.540	8.568	8.564	9.027	9.025	7.619	7.615	7.410	7.404
0.023	4.6	5.578	5.580	8.653	8.657	9.060	9.061	7.632	7.631	7.419	7.416
0.027	5.5	5.608	5.610	8.722	8.725	9.087	9.087	7.642	7.642	7.427	7.425
0.036	7.2	5.630	5.632	8.772	8.778	9.107	9.108	7.648	7.650	7.431	7.432
0.044	8.8	5.665	5.665	8.855	8.856	9.141	9.140	7.658	7.661	7.441	7.443
0.059	11.9	5.690	5.689	8.915	8.913	9.166	9.164	7.665	7.668	7.448	7.451
0.080	16.1	5.724	5.723	8.996	8.994	9.200	9.200	7.673	7.676	7.458	7.463
0.111	22.4	5.763	5.756	9.091	9.077	9.243	9.239	7.681	7.683	7.472	7.476
0.137	27.7	5.792	5.792	9.165	9.169	9.278	9.283	7.686	7.688	7.484	7.490
0.160	32.3	5.815	5.817	9.226	9.232	9.309	9.315	7.690	7.690	7.496	7.500
0.180	36.3	5.835	5.835	9.278	9.279	9.337	9.338	7.693	7.692	7.508	7.508
0.198	39.9	5.846	5.849	9.312	9.316	9.357	9.357	7.694	7.693	7.518	7.514

Results of the HypNMR fitting:
log β_1 = 2.16 ± 0.02 (1:1)
log β_2 = 2.61 ± 0.09 (1:2)
BC_{50} = 6.7 ± 0.3 mM = 6681 ± 291 μM

Figure S12. Plot of the experimental (symbols) and fitting (lines) data.

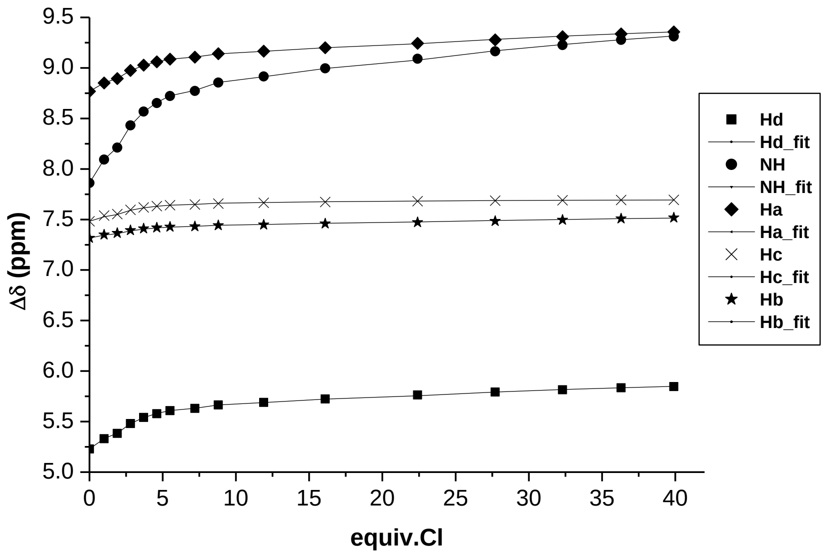


Figure S13. Species distribution as a function of the chloride (B) concentration.

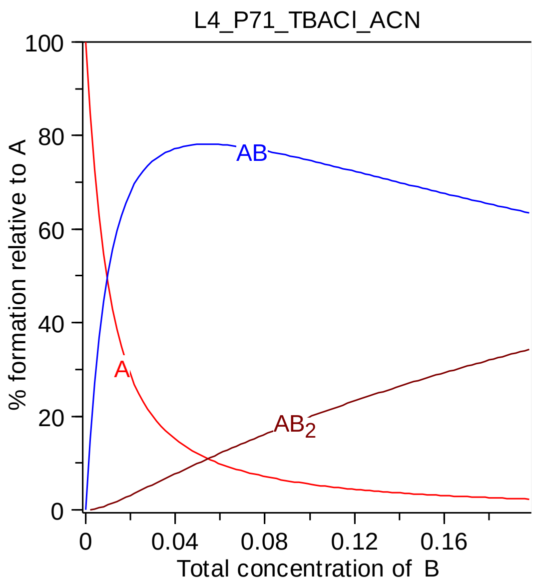
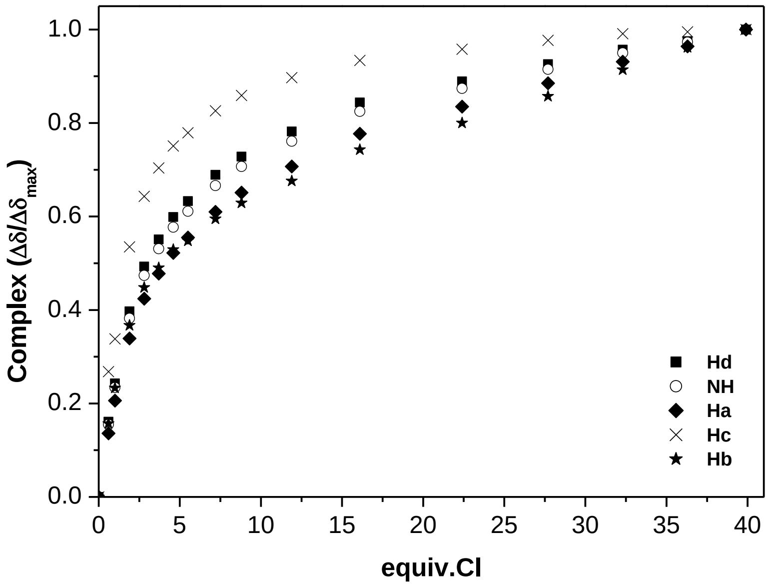


Figure S14. Plot of the chloride –induced chemical shifts of different signals for the titration of **1a**.



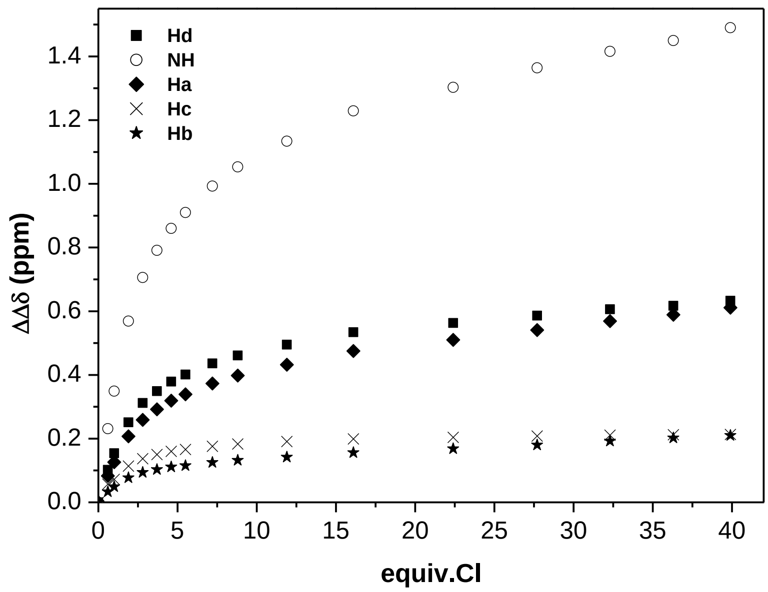
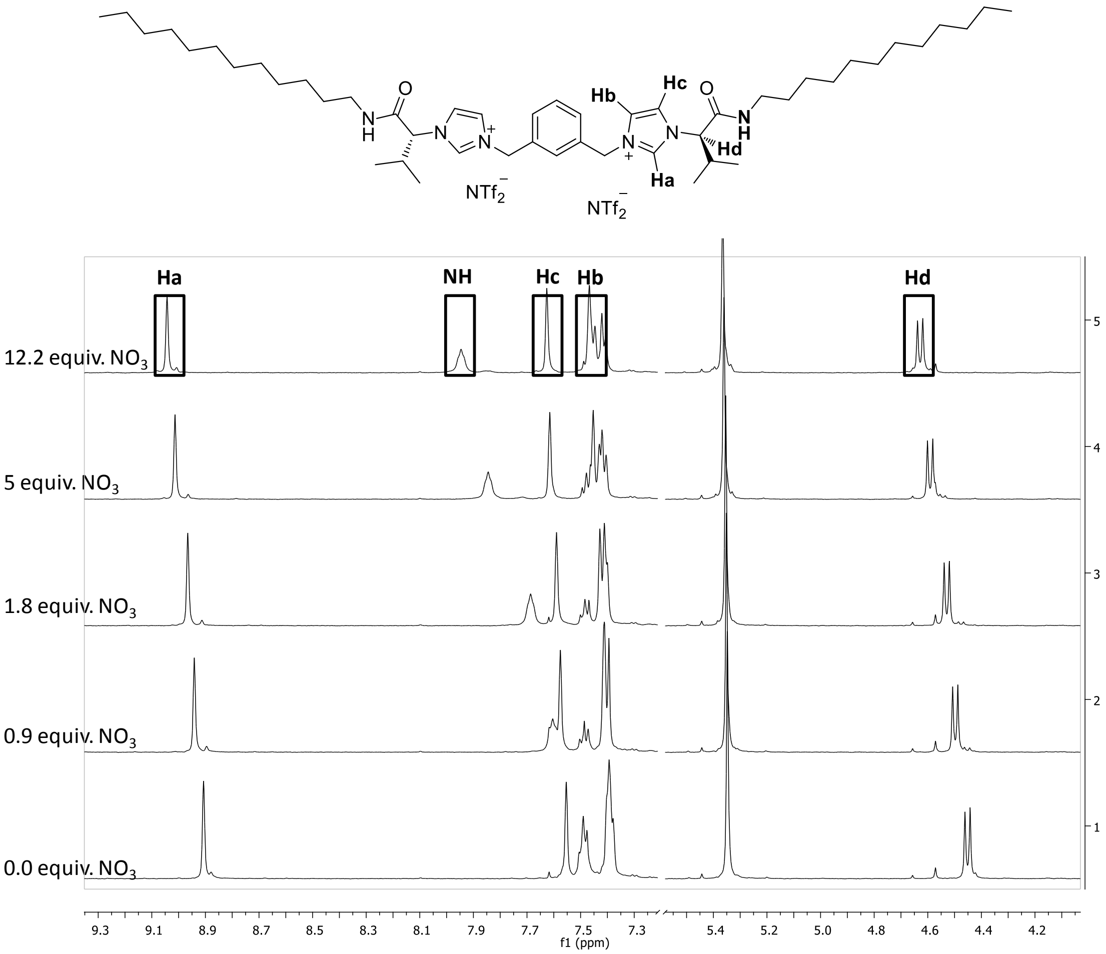


Figure S15. Stacked [1]H NMR spectra for the titration of **1c** with $TBANO_3$



Data set:

Conc. NO_3	equiv.NO_3	Hd	Hd_fit	NH	NH_fit	Ha	Ha_fit	Hc	Hc_fit	Hb	Hb_fit
0.000	0.00	4.442	4.442	7.505	7.505	8.907	8.907	7.553	7.553	7.379	7.379
0.005	0.87	4.488	4.487	7.604	7.613	8.941	8.941	7.575	7.574	7.394	7.403
0.010	1.73	4.519	4.518	7.687	7.688	8.966	8.964	7.590	7.589	7.428	7.420
0.014	2.57	4.541	4.540	7.741	7.743	8.982	8.981	7.599	7.599	7.437	7.431
0.019	3.40	4.558	4.557	7.785	7.785	8.995	8.994	7.606	7.606	7.444	7.440
0.023	4.21	4.572	4.570	7.818	7.818	9.006	9.005	7.612	7.611	7.450	7.447
0.028	5.00	4.581	4.581	7.845	7.845	9.013	9.013	7.615	7.615	7.453	7.452
0.032	5.78	4.589	4.590	7.868	7.868	9.020	9.020	7.617	7.618	7.456	7.457
0.036	6.54	4.597	4.598	7.891	7.887	9.028	9.026	7.622	7.621	7.461	7.460
0.044	8.03	4.609	4.610	7.920	7.920	9.035	9.036	7.624	7.625	7.462	7.466
0.052	9.46	4.619	4.620	7.946	7.946	9.043	9.045	7.626	7.627	7.467	7.470
0.068	12.18	4.634	4.635	7.986	7.986	9.056	9.057	7.630	7.631	7.473	7.477
0.082	14.72	4.645	4.646	8.016	8.016	9.065	9.067	7.632	7.633	7.478	7.482
0.095	17.10	4.655	4.655	8.041	8.041	9.074	9.074	7.635	7.635	7.483	7.485
0.113	20.39	4.666	4.666	8.070	8.070	9.083	9.084	7.637	7.636	7.488	7.490
0.140	25.24	4.678	4.678	8.103	8.105	9.094	9.095	7.638	7.638	7.495	7.494
0.163	29.45	4.689	4.687	8.134	8.131	9.105	9.103	7.639	7.639	7.501	7.498
0.184	33.13	4.694	4.694	8.148	8.151	9.110	9.109	7.639	7.639	7.504	7.500

Results of the HypNMR fitting:
log β_1 = 1.95 ± 0.04 (1:1)
log β_2 = 2.6 ± 0.1 (1:2)
BC_{50} = 10.3 ± 0.8 mM = 10330 ± 828 μM

Figure S16. Plot of the experimental (symbols) and fitting (lines) data.

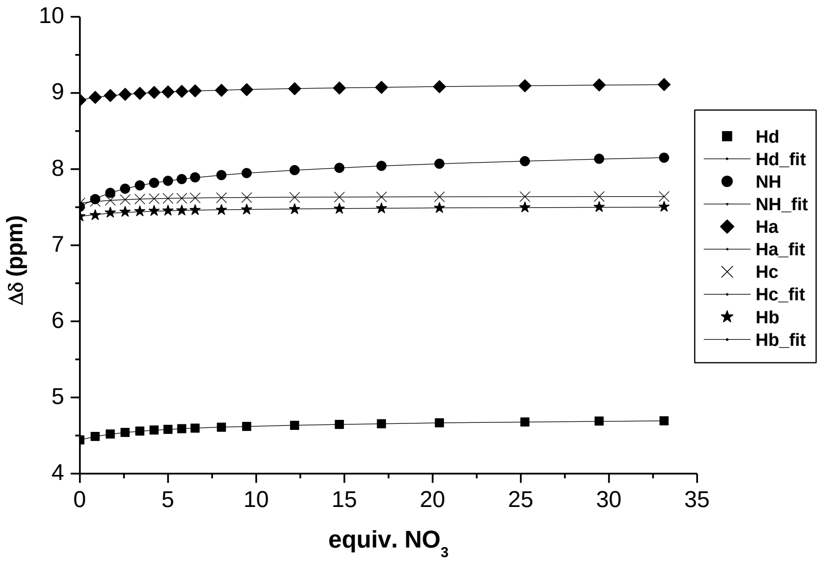


Figure S17. Species distribution as a function of the nitrate (B) concentration.

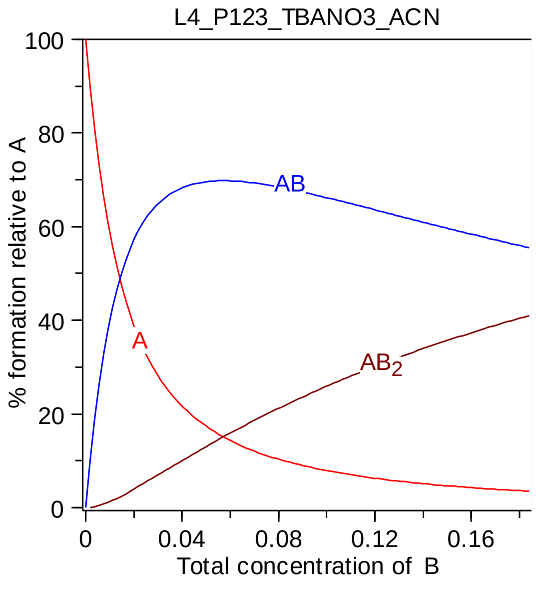
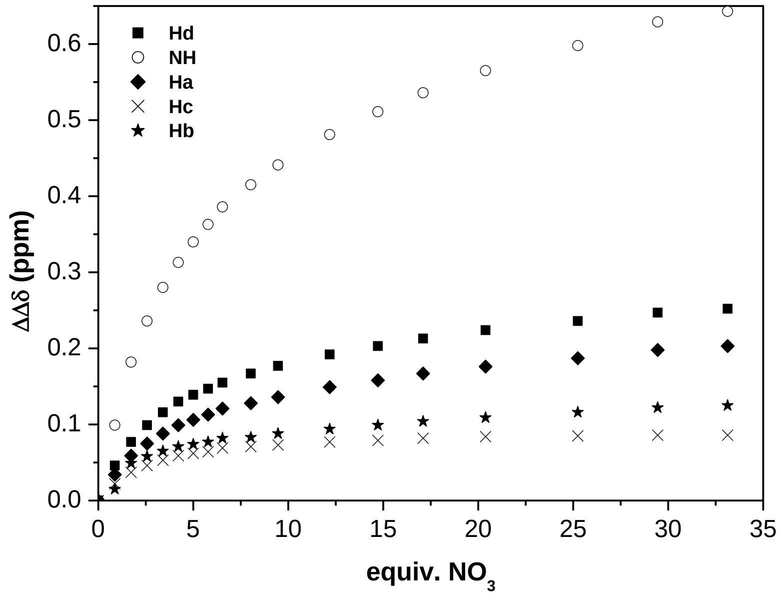


Figure S18. Plot of the nitrate –induced chemical shifts of different signals for the titration of **1c**.



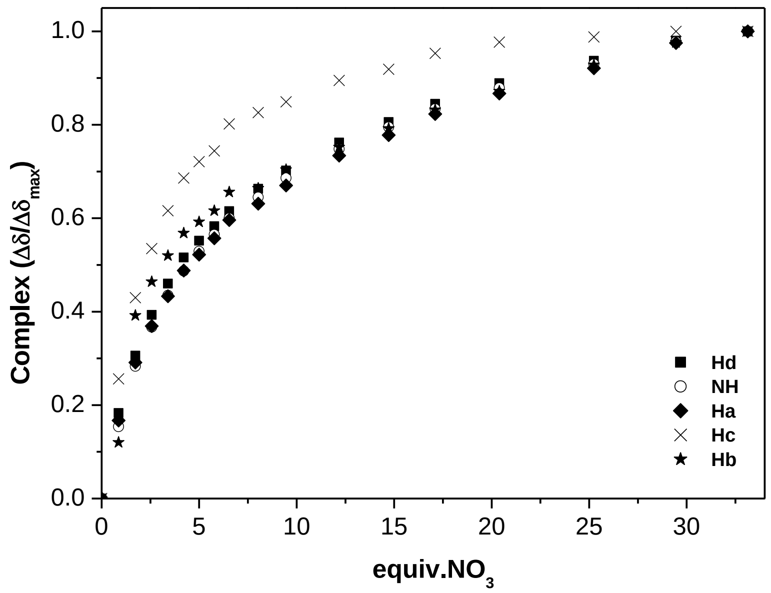
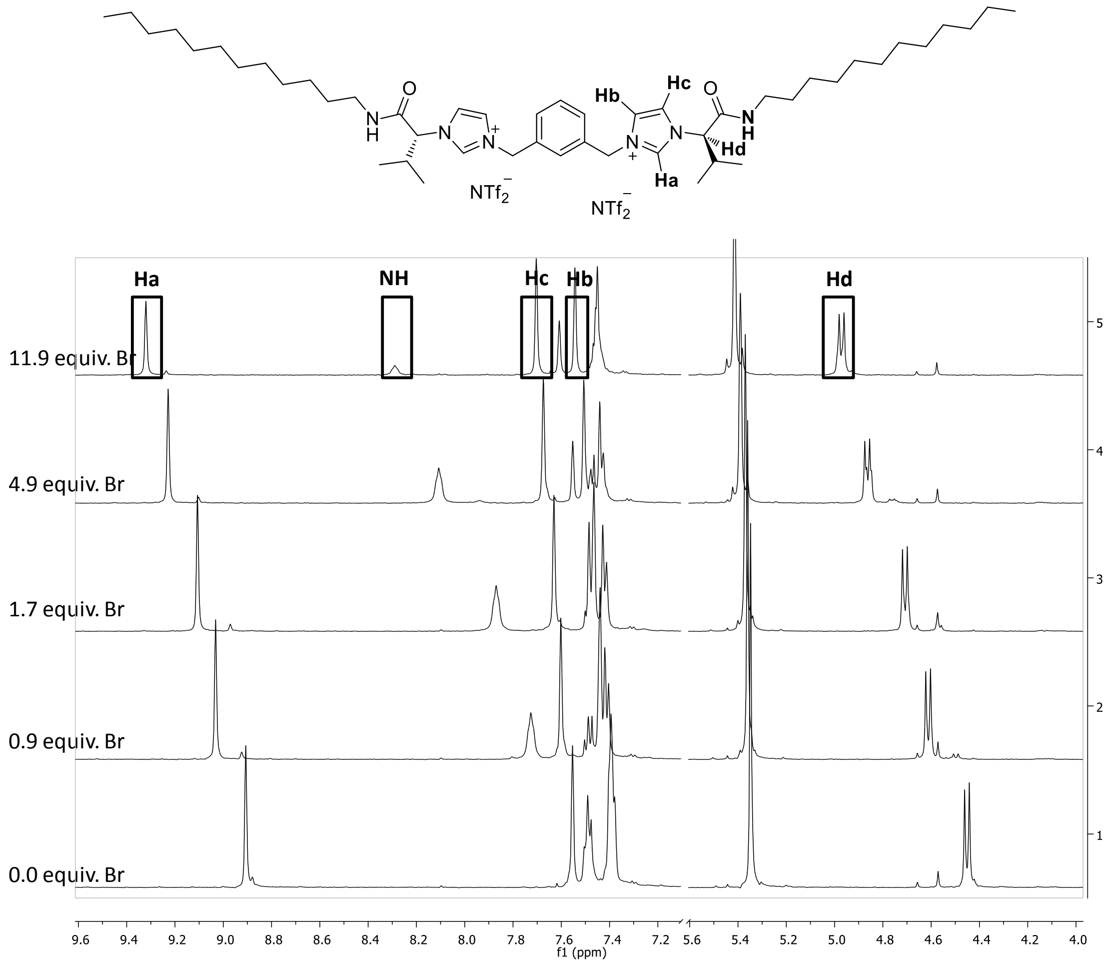


Figure S19. Stacked ^{1}H NMR spectra for the titration of **1c** with TBABr.



Data set:

Conc. Br	equiv.Br	Hd	Hd_fit	NH	NH_fit	Ha	Ha_fit	Hc	Hc_fit	Hb	Hb_fit
0.000	0.00	4.442	4.442	7.505	7.505	8.907	8.907	7.554	7.554	7.394	7.394
0.002	0.34	4.513	4.514	7.592	7.607	8.962	8.962	7.575	7.576	7.410	7.412
0.005	0.86	4.603	4.600	7.726	7.729	9.032	9.028	7.602	7.601	7.439	7.435
0.010	1.70	4.699	4.697	7.870	7.869	9.107	9.103	7.631	7.630	7.465	7.460
0.015	2.52	4.758	4.759	7.959	7.960	9.153	9.152	7.647	7.648	7.480	7.477
0.019	3.32	4.803	4.801	8.023	8.023	9.187	9.185	7.661	7.660	7.493	7.490
0.024	4.12	4.831	4.832	8.069	8.070	9.209	9.210	7.668	7.669	7.499	7.499
0.029	4.89	4.855	4.856	8.107	8.107	9.228	9.229	7.674	7.675	7.506	7.507
0.037	6.40	4.891	4.891	8.164	8.163	9.257	9.258	7.684	7.685	7.517	7.519
0.046	7.86	4.917	4.916	8.205	8.204	9.278	9.280	7.691	7.691	7.526	7.528
0.054	9.26	4.937	4.936	8.238	8.237	9.294	9.297	7.696	7.696	7.532	7.535
0.070	11.92	4.961	4.965	8.289	8.288	9.321	9.322	7.704	7.703	7.544	7.547
0.084	14.41	4.985	4.987	8.327	8.325	9.341	9.342	7.709	7.708	7.553	7.556
0.098	16.73	5.003	5.004	8.356	8.356	9.356	9.357	7.713	7.712	7.561	7.563
0.117	19.95	5.024	5.023	8.394	8.391	9.375	9.374	7.717	7.716	7.571	7.572
0.144	24.70	5.048	5.047	8.431	8.433	9.397	9.396	7.721	7.722	7.585	7.582
0.168	28.82	5.064	5.063	8.460	8.464	9.412	9.411	7.724	7.725	7.595	7.590

Results of the HypNMR fitting:
log β_1 = 2.20 ± 0.02 (1:1)
log β_2 = 2.96 ± 0.08 (1:2)
BC_{50} = 5.9 ± 0.3 mM = 5903 ± 296 µM

Figure S20. Plot of the experimental (symbols) and fitting (lines) data.

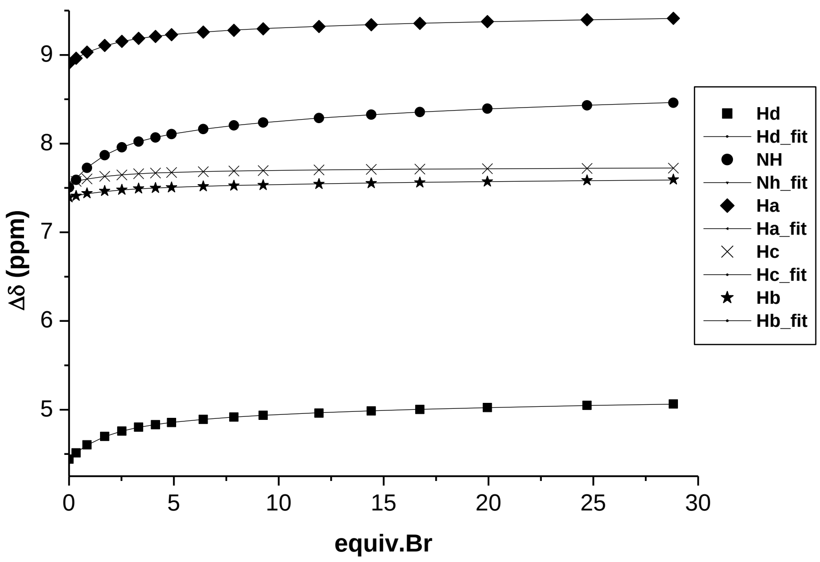


Figure S21. Species distribution as a function of the bromide (B) concentration.

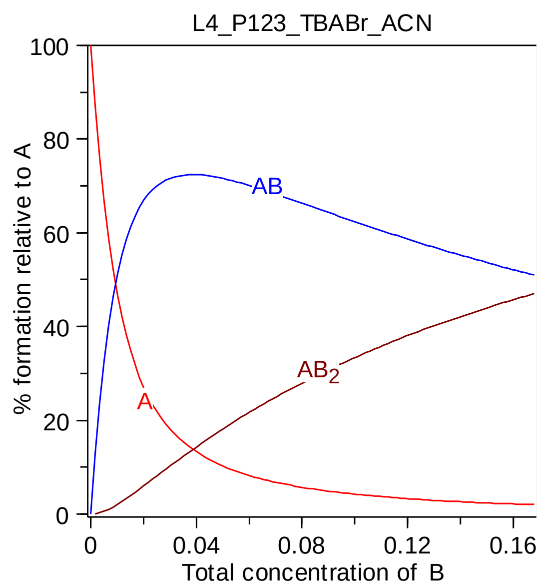
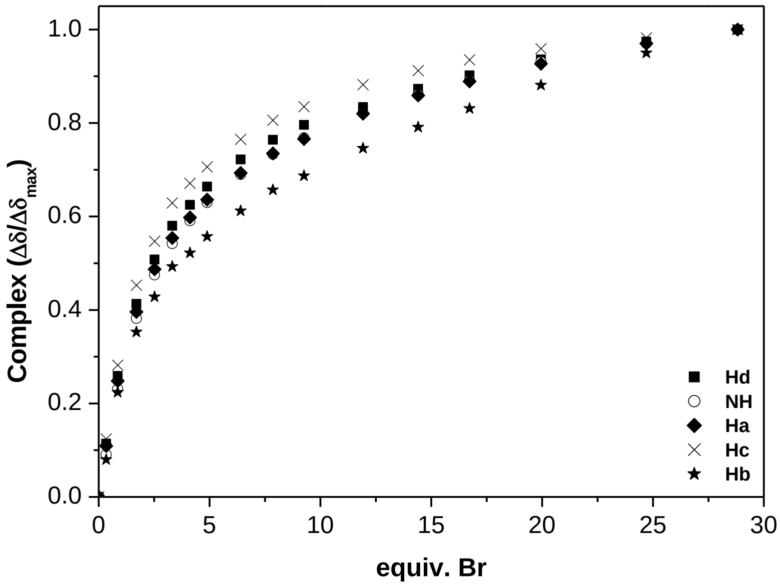


Figure S22. Plot of the bromide –induced chemical shifts of different signals for the titration of **1c**.



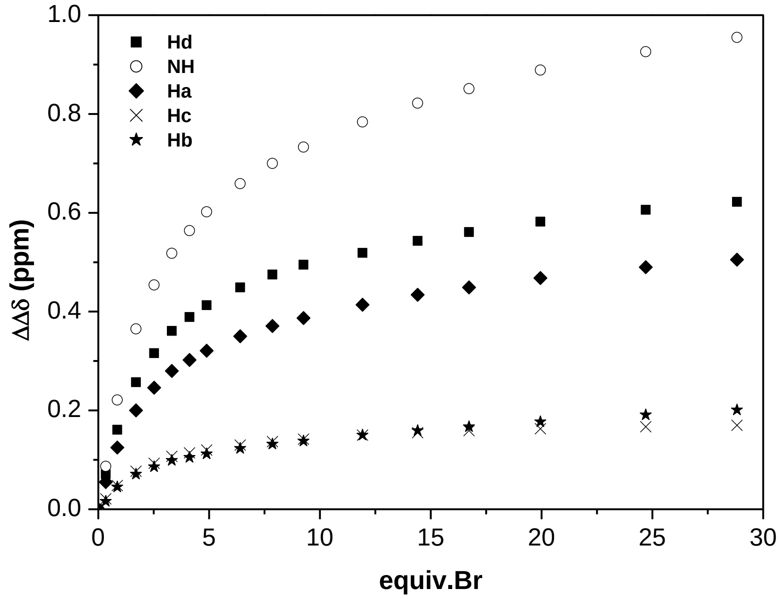
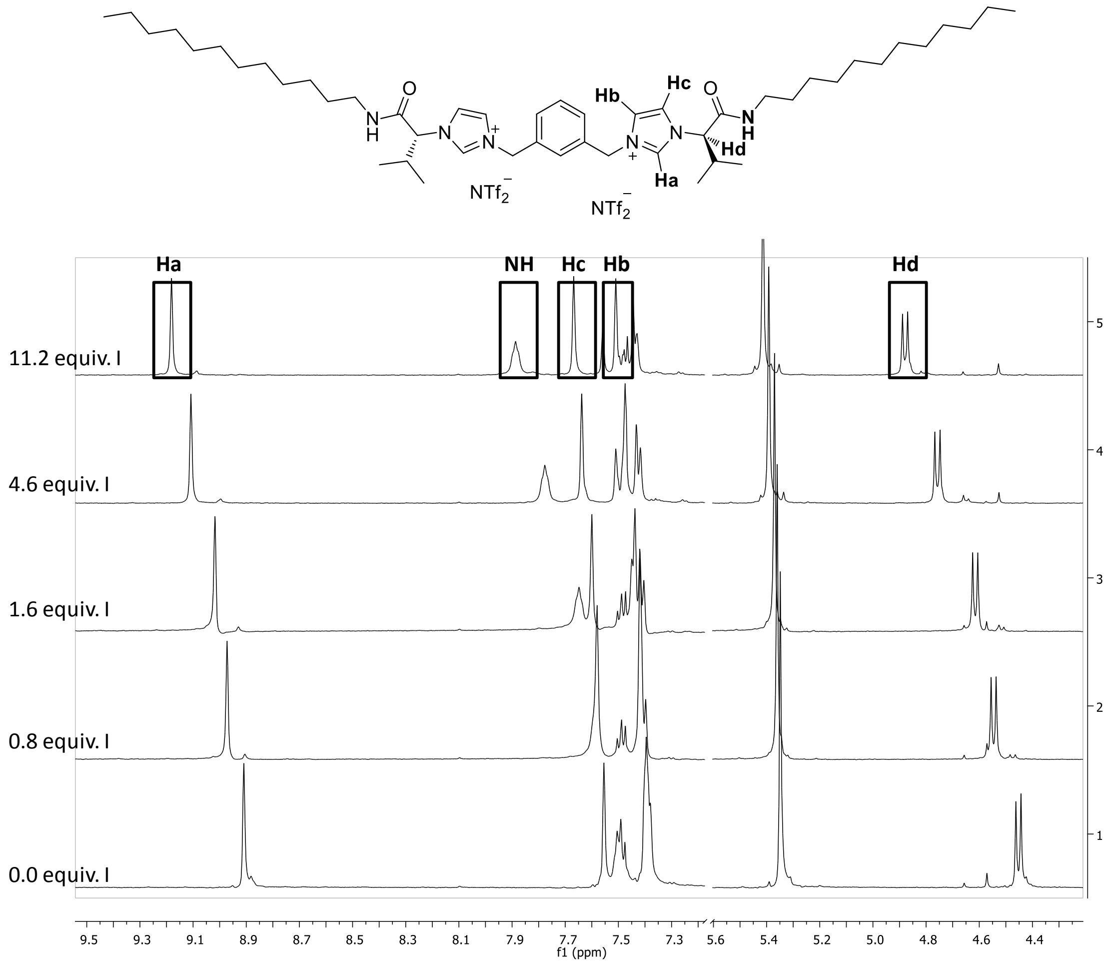


Figure S23. Stacked ^{1}H NMR spectra for the titration of **1c** with TBAI.



Data set:

Conc. I	equiv.I	Hd	Hd_fit	NH	NH_fit	Ha	Ha_fit	Hc	Hc_fit	Hb	Hb_fit
0.000	0.00	4.443	4.443	7.505	7.505	8.909	8.909	7.554	7.554	7.395	7.395
0.002	0.32	4.486	4.485	7.541	7.542	8.938	8.937	7.566	7.566	7.406	7.406
0.005	0.80	4.536	4.537	7.580	7.589	8.972	8.971	7.580	7.581	7.419	7.419
0.009	1.59	4.605	4.605	7.648	7.648	9.018	9.016	7.600	7.600	7.438	7.436
0.014	2.36	4.654	4.655	7.691	7.693	9.049	9.048	7.613	7.613	7.450	7.449
0.018	3.12	4.693	4.693	7.727	7.727	9.074	9.072	7.623	7.623	7.461	7.460
0.023	3.86	4.723	4.723	7.754	7.753	9.093	9.092	7.632	7.631	7.469	7.468
0.027	4.59	4.748	4.747	7.777	7.775	9.108	9.107	7.638	7.638	7.475	7.474
0.035	6.01	4.784	4.785	7.809	7.809	9.130	9.131	7.647	7.648	7.485	7.485
0.043	7.37	4.812	4.813	7.835	7.835	9.147	9.148	7.655	7.655	7.493	7.494
0.051	8.69	4.835	4.835	7.856	7.855	9.161	9.162	7.660	7.660	7.499	7.500
0.066	11.19	4.869	4.869	7.887	7.886	9.181	9.183	7.668	7.668	7.510	7.511
0.080	13.52	4.892	4.895	7.907	7.910	9.194	9.198	7.673	7.674	7.517	7.519
0.092	15.70	4.916	4.915	7.930	7.928	9.209	9.210	7.679	7.678	7.525	7.526
0.110	18.72	4.941	4.938	7.952	7.950	9.224	9.223	7.684	7.684	7.533	7.534
0.137	23.18	4.969	4.967	7.978	7.977	9.241	9.240	7.690	7.690	7.544	7.544
0.159	27.04	4.984	4.987	7.992	7.996	9.250	9.251	7.693	7.694	7.550	7.551
0.179	30.42	5.003	5.003	8.011	8.011	9.263	9.260	7.697	7.697	7.559	7.556

Results of the HypNMR fitting:
log β_1 = 1.92 ± 0.03 (1:1)
log β_2 = 2.5 ± 0.1 (1:2)
BC_{50} = 11.2 ± 0.2 mM = 11170 ± 225 μM

Figure S24. Plot of the experimental (symbols) and fitting (lines) data.

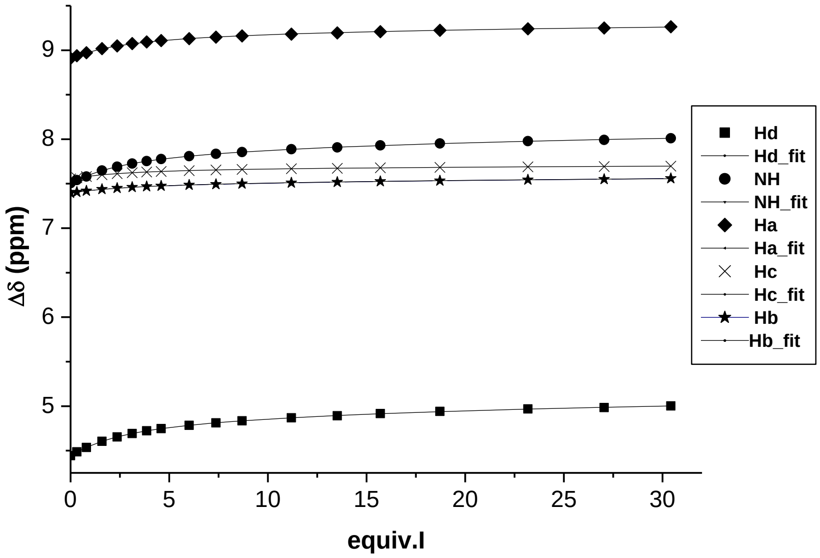


Figure S25. Species distribution as a function of the iodide (B) concentration.

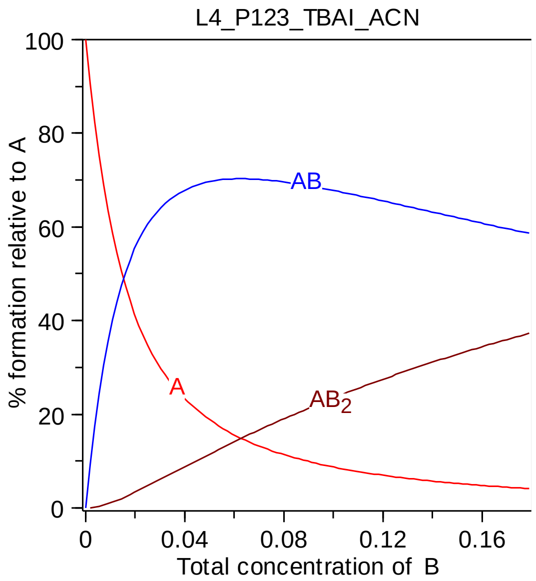
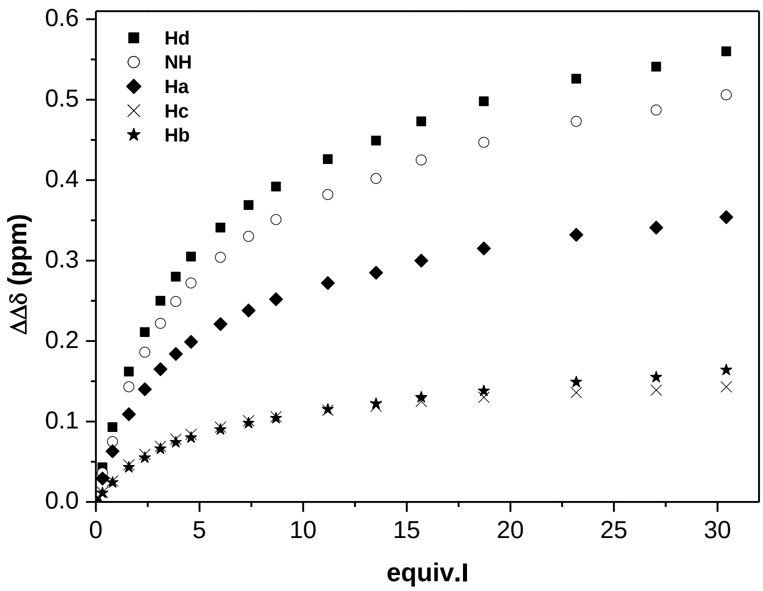


Figure S26. Plot of the iodide –induced chemical shifts of different signals for the titration of **1c**.



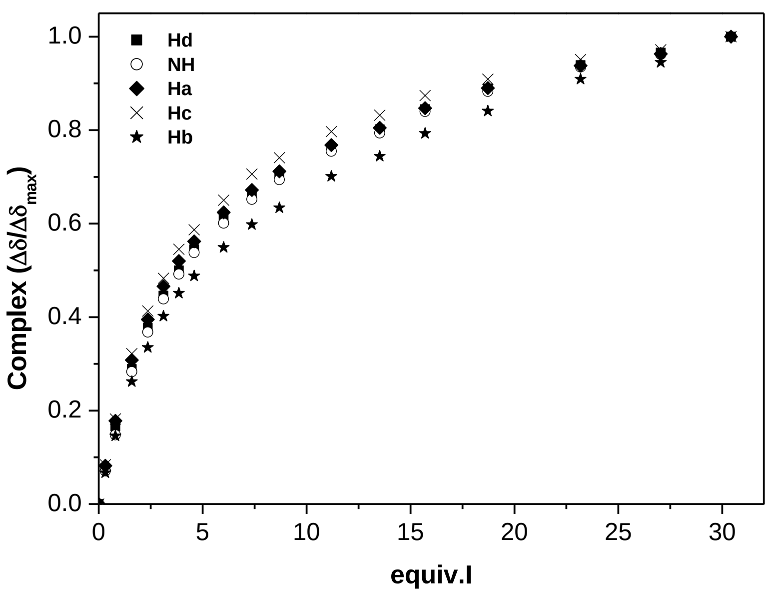
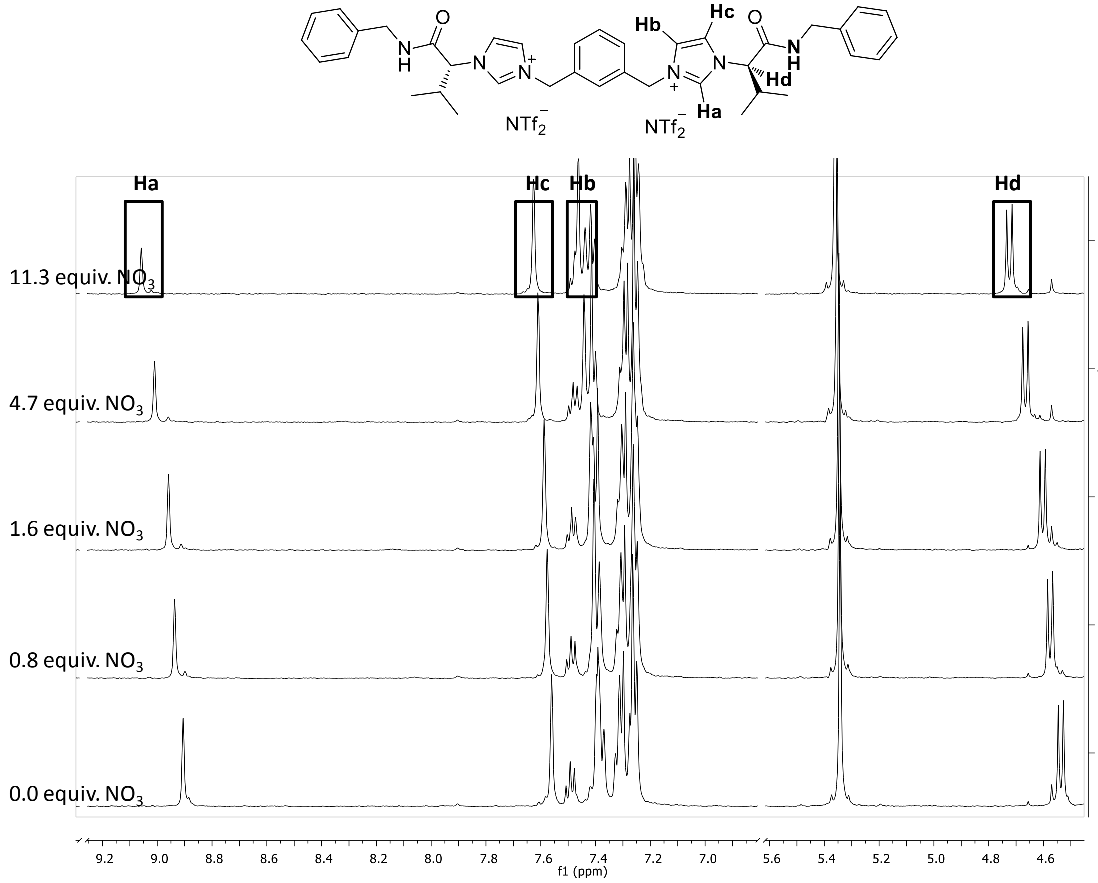


Figure S27. Selected stacked ^{1}H NMR spectra for the titration of **1b** with $TBANO_3$.



Data set:

Conc. NO_3	equiv. NO_3	Hd	Hd_fit	Ha	Ha_fit	Hc	Hc_fit	Hb	Hb_fit
0.000	0.0	4.527	4.527	8.906	8.906	7.561	7.561	7.391	7.391
0.002	0.3	4.544	4.543	8.919	8.919	7.568	7.568	7.399	7.397
0.005	0.8	4.566	4.565	8.937	8.936	7.577	7.576	7.406	7.405
0.010	1.6	4.593	4.593	8.959	8.958	7.588	7.588	7.418	7.416
0.015	2.4	4.614	4.615	8.975	8.976	7.596	7.596	7.426	7.425
0.020	3.2	4.630	4.633	8.989	8.990	7.602	7.603	7.432	7.432
0.024	3.9	4.645	4.644	9.000	8.999	7.607	7.607	7.438	7.436
0.029	4.7	4.656	4.657	9.010	9.010	7.611	7.611	7.442	7.441
0.038	6.1	4.673	4.674	9.024	9.024	7.616	7.617	7.449	7.449
0.046	7.5	4.687	4.687	9.035	9.035	7.620	7.620	7.454	7.454
0.054	8.8	4.698	4.697	9.044	9.044	7.623	7.623	7.458	7.458
0.070	11.3	4.715	4.715	9.058	9.058	7.627	7.627	7.462	7.465
0.085	13.7	4.728	4.727	9.069	9.070	7.630	7.630	7.470	7.471
0.098	15.9	4.738	4.737	9.078	9.078	7.632	7.632	7.474	7.475
0.117	19.0	4.750	4.749	9.089	9.089	7.634	7.634	7.479	7.480
0.145	23.5	4.764	4.764	9.102	9.102	7.636	7.636	7.486	7.487
0.169	27.4	4.774	4.774	9.112	9.112	7.637	7.637	7.492	7.492
0.190	30.9	4.782	4.783	9.119	9.119	7.637	7.638	7.497	7.496
0.209	33.9	4.788	4.789	9.126	9.126	7.638	7.638	7.501	7.499

Results of the HypNMR fitting:
log β_1 = 1.78 ± 0.03 (1:1)
log β_2 = 2.2 ± 0.1 (1:2)
BC_{50} = 16.5 ± 0.9 mM = 16475 ± 946 μM

Figure S28. Plot of the experimental (symbols) and fitting (lines) data.

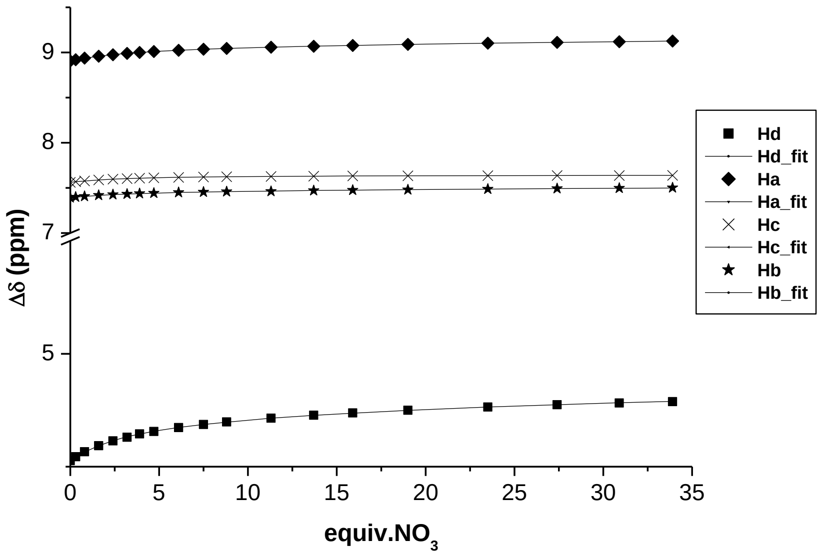


Figure S29. Species distribution as a function of the nitrate (B) concentration**.**

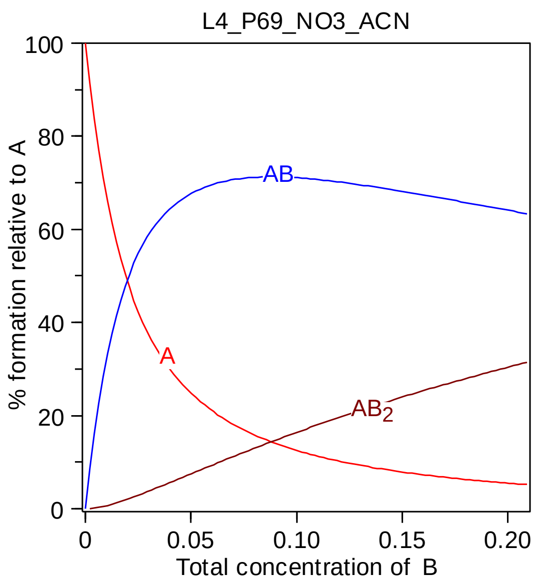
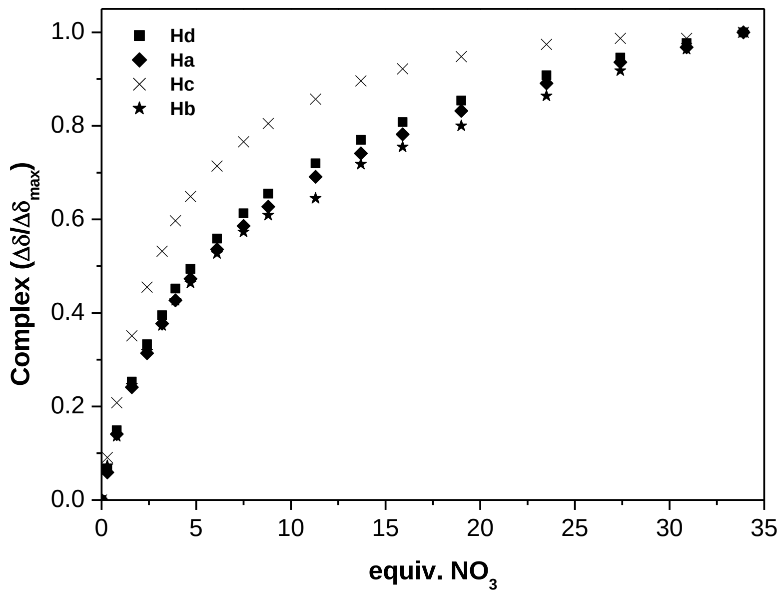


Figure S30. Plot of the nitrate –induced chemical shifts of different signals for the titration of **1b**.



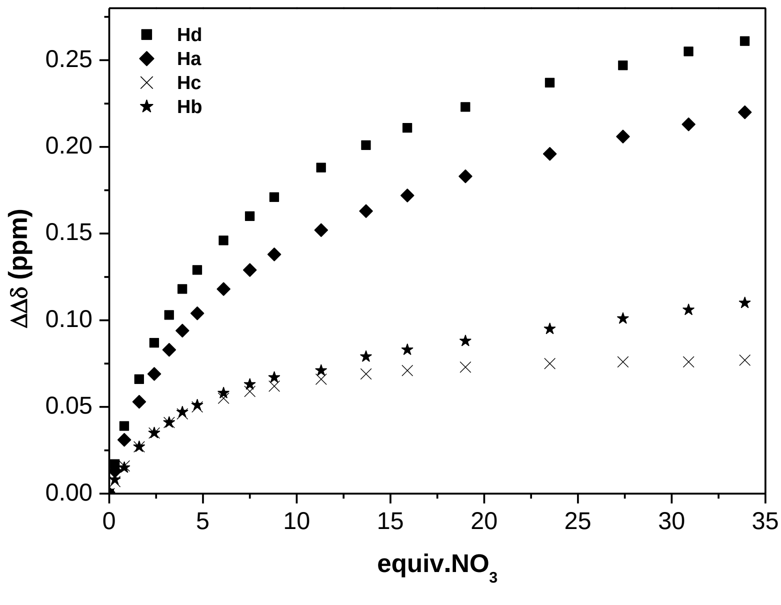
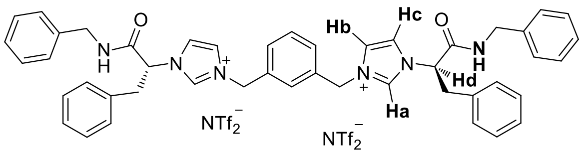
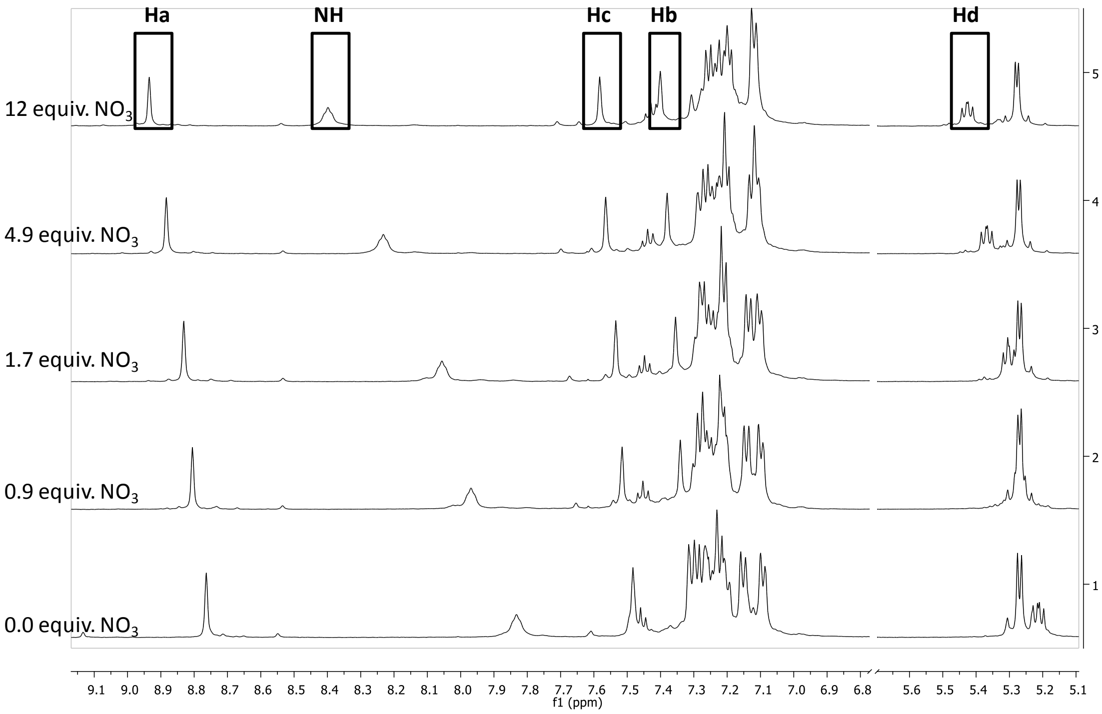


Figure S31. Stacked ^{1}H NMR spectra for the titration of **1a** with $TBANO_3$.





Data set:

Conc. NO_3	equiv. NO_3	Hd	Hd_fit	NH	NH_fit	Ha	Ha_fit	Hc	Hc_fit	Hb	Hb_fit
0.000	0.0	5.197	5.197	7.832	7.832	8.764	8.764	7.483	7.483	7.315	7.315
0.002	0.3	5.220	5.221	7.887	7.892	8.780	8.781	7.497	7.497	7.326	7.325
0.005	0.9	5.253	5.250	7.969	7.965	8.805	8.803	7.515	7.514	7.341	7.337
0.010	1.7	5.286	5.286	8.056	8.055	8.831	8.829	7.534	7.533	7.355	7.352
0.015	2.5	5.309	5.310	8.116	8.118	8.849	8.848	7.546	7.546	7.364	7.363
0.019	3.3	5.327	5.328	8.164	8.166	8.863	8.862	7.554	7.555	7.371	7.370
0.024	4.1	5.341	5.342	8.201	8.203	8.874	8.874	7.560	7.561	7.376	7.376
0.028	4.9	5.352	5.353	8.232	8.233	8.884	8.883	7.565	7.566	7.380	7.380
0.037	6.4	5.370	5.370	8.280	8.281	8.898	8.898	7.571	7.572	7.386	7.387
0.046	7.9	5.383	5.383	8.318	8.318	8.910	8.910	7.575	7.576	7.391	7.392
0.054	9.3	5.394	5.393	8.349	8.348	8.919	8.920	7.578	7.579	7.395	7.396
0.069	12.0	5.410	5.410	8.398	8.396	8.935	8.936	7.583	7.582	7.401	7.402
0.084	14.5	5.423	5.422	8.436	8.434	8.948	8.949	7.585	7.584	7.405	7.407
0.097	16.8	5.433	5.432	8.467	8.464	8.958	8.959	7.587	7.586	7.409	7.411
0.116	20.0	5.445	5.444	8.504	8.501	8.971	8.972	7.588	7.587	7.414	7.415
0.144	24.8	5.456	5.458	8.542	8.548	8.984	8.988	7.589	7.588	7.419	7.420
0.168	28.9	5.468	5.469	8.579	8.582	8.999	9.000	7.589	7.589	7.424	7.424
0.189	32.5	5.477	5.477	8.608	8.608	9.011	9.009	7.589	7.589	7.429	7.427
0.207	35.7	5.484	5.484	8.631	8.629	9.021	9.016	7.588	7.590	7.432	7.430

Results of the HypNMR fitting:
log β_1 = 2.05 ± 0.02 (1:1)
log β_2 = 2.65 ± 0.06 (1:2)
BC_{50} = 8.9 ± 0.4 mM = 8864 ± 414 µM

Figure S32. Plot of the experimental (symbols) and fitting (lines) data.

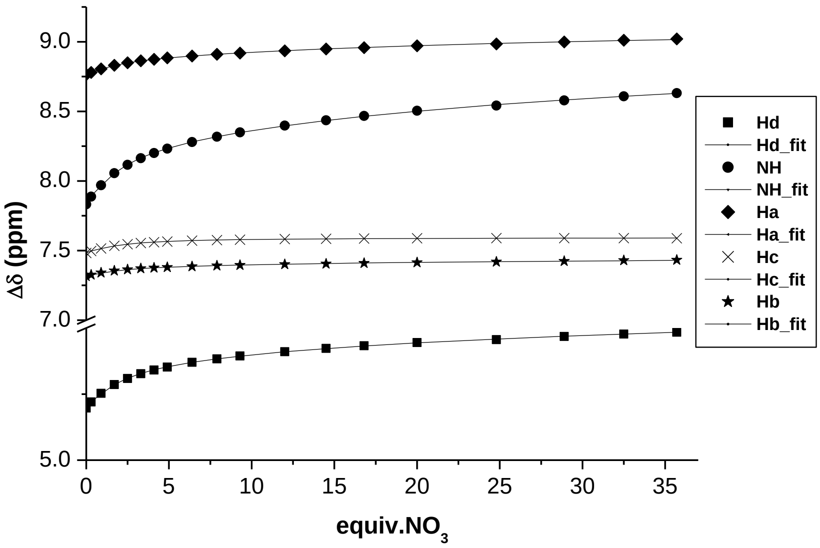


Figure S33. Species distribution as a function of the nitrate (B) concentration.

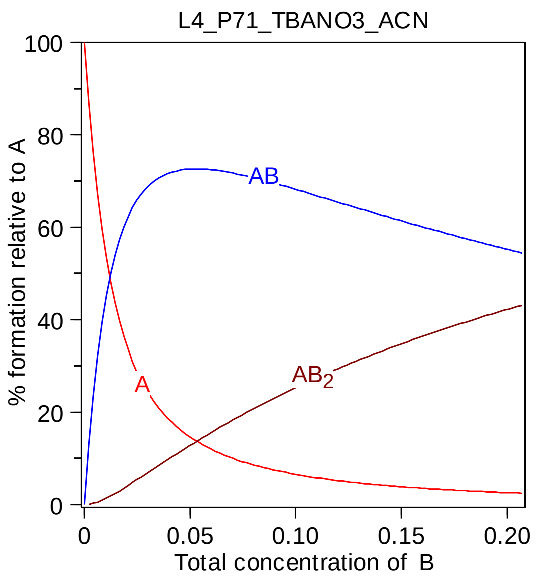
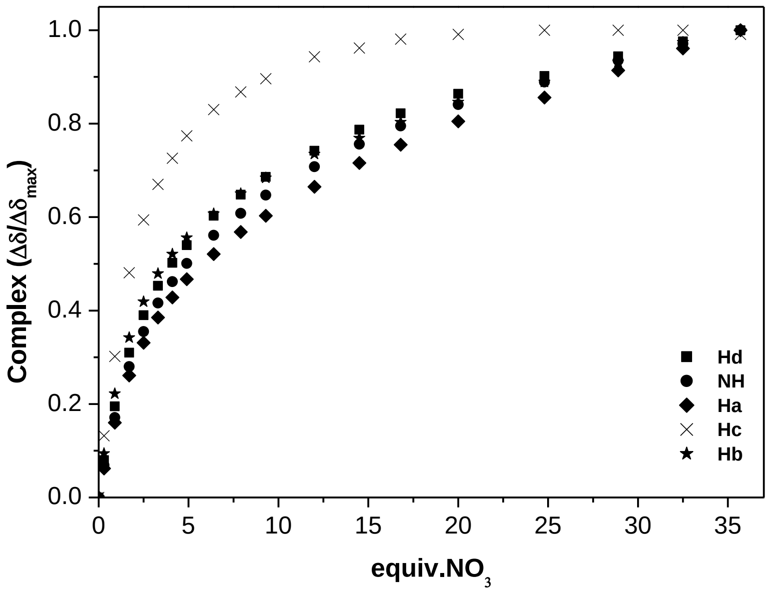
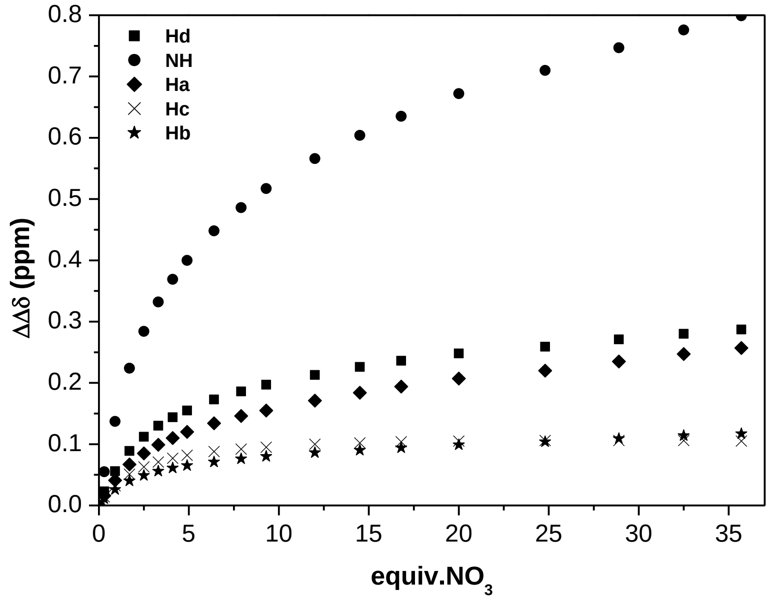


Figure S34. Plot of the nitrate –induced chemical shifts of different signals for the titration of **1a**.





Detail of ESI-MS procedures and experiments

ESI-MS represents a versatile tool to evaluate both qualitatively and quantitatively binding properties in molecular recognition processes.[1] In this work we carried out an ESI-MS study aimed to estimate the distinctive binding affinities of compound **1c** towards different anions. We initially studied equimolar solutions (1 x 10^{-5} M) of [**1c**]$(NTf_2)_2$ and (TEA)Cl (TEA = tetraethylammonium) by ESI-MS in an identical solvent (CH_3CN:H_2O (95:5)) to that used in NMR studies. The use of the corresponding TBA salts provided unsatisfactory results according to the strong footprint provided by this cation. Under these conditions, $[\mathbf{1c}]^{2+}$ was the base peak and $[\mathbf{1c}\ Cl]^+$ was barely detected whereas $[\mathbf{1c}\ NTf_2]^+$ was dominant, in contrast to what had been observed by NMR methods. When using other solvents (CH_2Cl_2 or MeOH) for the ESI-MS analysis a clear solvent-dependence of the relative intensities of the $[\mathbf{1c}\ A]^+$ (A = Cl^- and NTf_2^-) cations was observed in the resulting ESI mass spectra. In CH_2Cl_2, the adduct $[\mathbf{1c}\ Cl]^+$ was dominant over the $[\mathbf{1c}\ NTf_2]^+$ adduct, whereas in CH_3OH, the opposite trend was observed. These experimental evidences can be rationalized by considering the fundamental mechanism for gas-phase ion production upon ESI conditions.[2, 3] Because of the distinctive polarity of Cl^- and NTf_2^- anions, when a polar solvent like CH_3OH is used, the droplet partitions the less polar NTf_2^- ions preferentially at the surface and consequently its adducts are preferentially ionized upon ESI conditions. In contrast, in less polar solvents like CH_2Cl_2, the $[\mathbf{1c}\ Cl]^+$ species is dominant in the ESI mass spectrum. As identified by McIndoe in previous works on dicationic IL´s,[4] the use of MeCN as the mobile solvent provides a convenient solvent in which the effect of the distinctive polarity of ions is virtually equalized. In fact, qualitative agreement between NMR titration experiments and ESI-MS data were found only when MeCN was used as the mobile phase using equimolar solutions (1 x 10^{-5} M) of [**1c**]$(NTf_2)_2$ and (TEA)Cl. We are aware that comparison of adducts with Cl^- and NTf_2^- certainly represents two extreme situations in terms of ion size and hydrophilic character; however, we envisage that for ion adducts displaying similar size, shape and properties, such as those comprising the $[\mathbf{1c}\ X]^+$ adducts where X stands for Cl^-, Br^- I^- and NO_3^- anions, competitive ESI experiments might provide a good match between ion abundances in the ESI mass spectrum and solution concentration. To validate this hypothesis, we performed a competitive ESI mass analysis on an equimolar solution of [**1c**]$(NTf_2)_2$ and TEAX (X = Cl^-, Br^-, I^- and NO_3^-) in MeCN (see Fig. 4).

1 R. Bini, O. Bortolini, C. Chiappe, D. Pieraccini, C. Siciliano, *J. Phys. B.* 2007, **111**, 598.
2 A. M. Fernández et *al*., *J. Phys. B.*, 2011, **115**, 4033.
3 J. M. Daniel, S. Friess, S. D. Rajagopalan, S. Wendt, R. Zenobi, *Int. J. Mass Spectrom*. 2002, **216**, 1.
4 J. Pape, K. L. Vikse, E. Janusson, N. Taylor, J. S. McIndoe, *Int. J. Mass Spectrom*. 2014, **373**, 66.

Chloride transport studies. Data regarding the transport experiments, with the anion efflux measured and the corresponding Hill plots, along with CF leakage experiments.

Figure S35. Chloride efflux upon addition of **1a** (25-100 µM, 5-20% mol carrier to lipid concentration molar) to vesicles composed of POPC. The vesicles contained NaCl (488 mM NaCl and 5 mM phosphate buffer, pH 7.2) and were immersed in $NaNO_3$ (494 mM $NaNO_3$ and 5 mM phosphate buffer, pH 7.2).

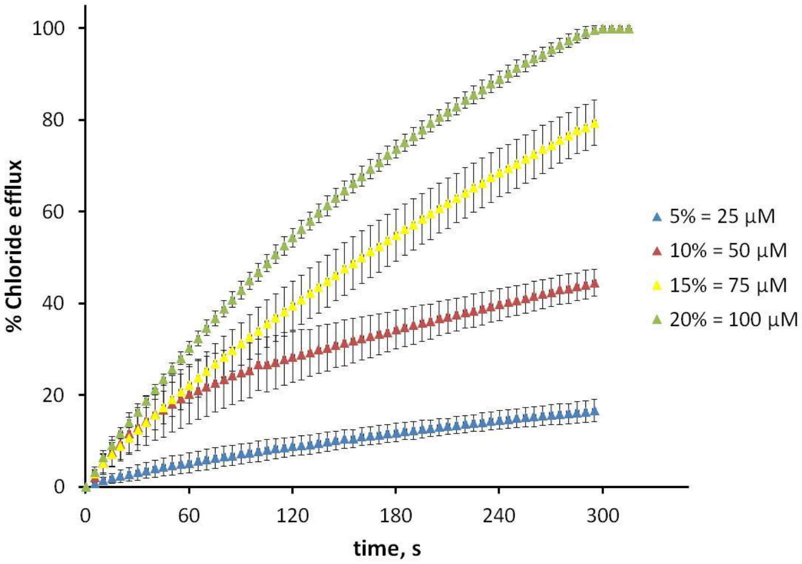


Figure S36. Hill plot corresponding to the chloride release (t = 300 s) mediated by receptor **1a** from POPC vesicles loaded with 489 mM NaCl buffered to pH 7.2 dispersed in 489 mM NaNO3 buffered to pH 7.2.

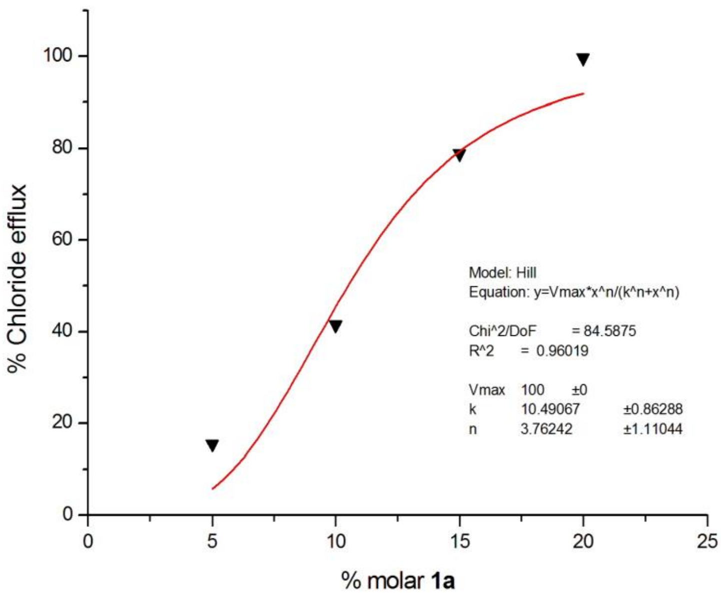


Figure S37. Chloride efflux upon addition of **1b** (25-100 µM, 5-20% mol carrier to lipid concentration molar) to vesicles composed of POPC. The vesicles contained NaCl (488 mM NaCl and 5 mM phosphate buffer, pH 7.2) and were immersed in $NaNO_3$ (494 mM $NaNO_3$ and 5 mM phosphate buffer, pH 7.2).

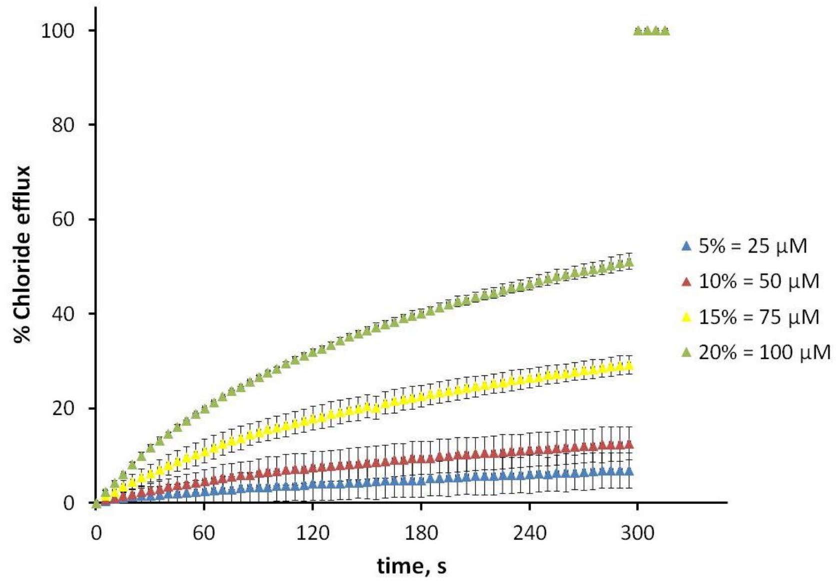


Figure S38 Chloride efflux upon addition of **1c** (25-100 µM, 5-20 % mol carrier to lipid concentration molar) to vesicles composed of POPC. The vesicles contained NaCl (488 mM NaCl and 5 mM phosphate buffer, pH 7.2) and were immersed in $NaNO_3$ (494 mM $NaNO_3$ and 5 mM phosphate buffer, pH 7.2).

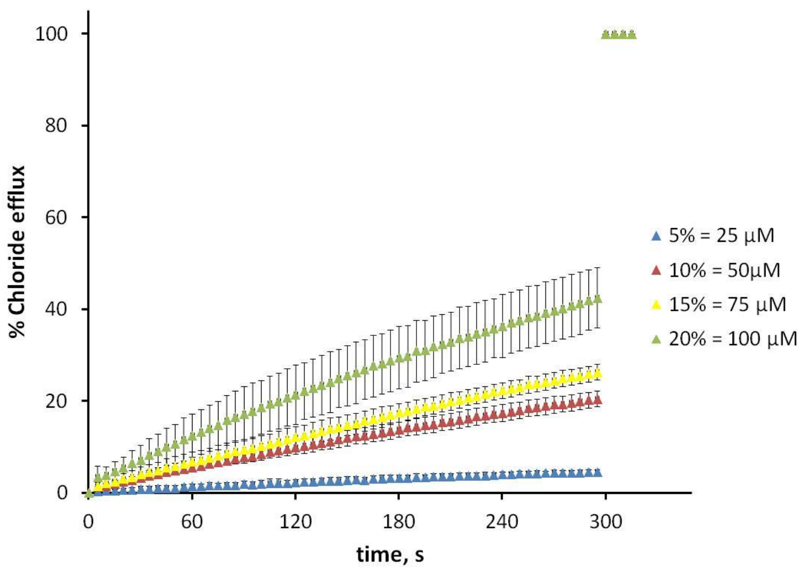


Figure S39. Chloride efflux upon addition of **1a-c** (75 µM, 15 % mol carrier to lipid concentration) to unilamellar POPC vesicles. Vesicles loaded with 450 mM NaCl buffered at pH 7.2 with 20 mM phosphate dispersed in 150 mM Na_2SO_4 buffered at pH 7.2. Each trace represents the average of at least different three trials.

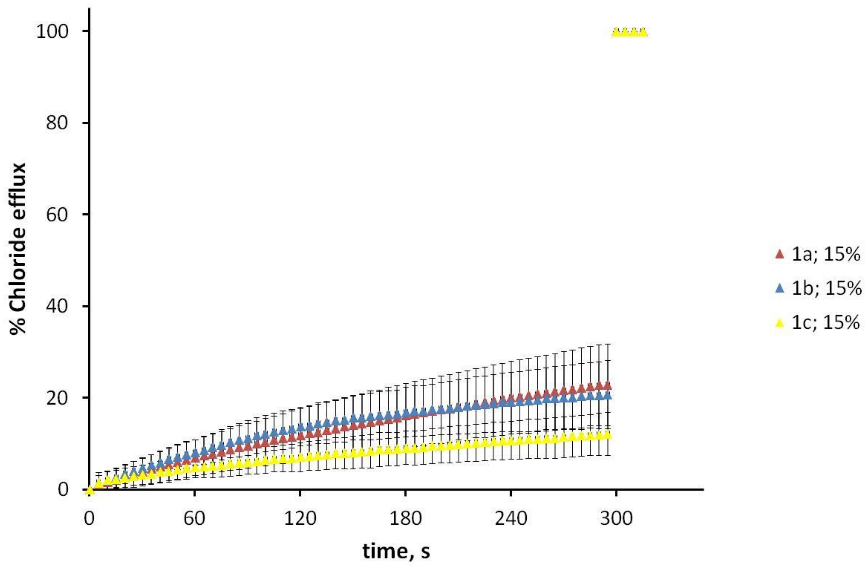


Figure S40. CF leakage induced by **1a** (15 mol% carrier to lipid) from unilamellar POPC (0.025mM) vesicles loaded with 50 mM CF and 451 mM NaCl, buffered to pH 7.2 with 20 mM sodium phosphate salts. The vesicles were dispersed in 150 mM Na_2SO_4 buffered to pH 7.2 with 20 mM sodium phosphate salts. At t = 60 s, a DMSO solution of the transporter was added to start the experiment. At the end of the experiment (6 min), detergent was added to lyse the vesicles. Each trace represents the average of three trials.

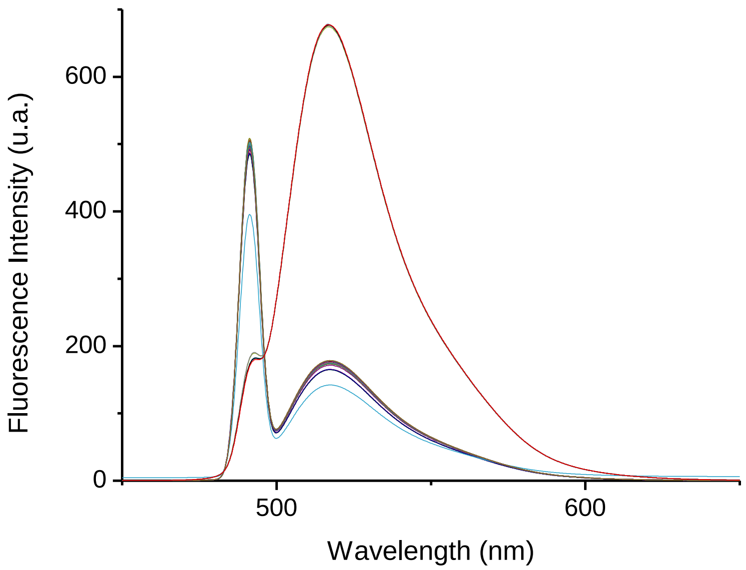


Figure S41. CF leakage induced by **1b** (15 mol% carrier to lipid) from unilamellar POPC (0.025mM) vesicles loaded with 50 mM CF and 451 mM NaCl, buffered to pH 7.2 with 20 mM sodium phosphate salts. The vesicles were dispersed in 150 mM Na_2SO_4 buffered to pH 7.2 with 20 mM sodium phosphate salts. At t = 60 s, a DMSO solution of the transporter was added to start the experiment. At the end of the experiment (6 min), detergent was added to lyse the vesicles. Each trace represents the average of three trials.

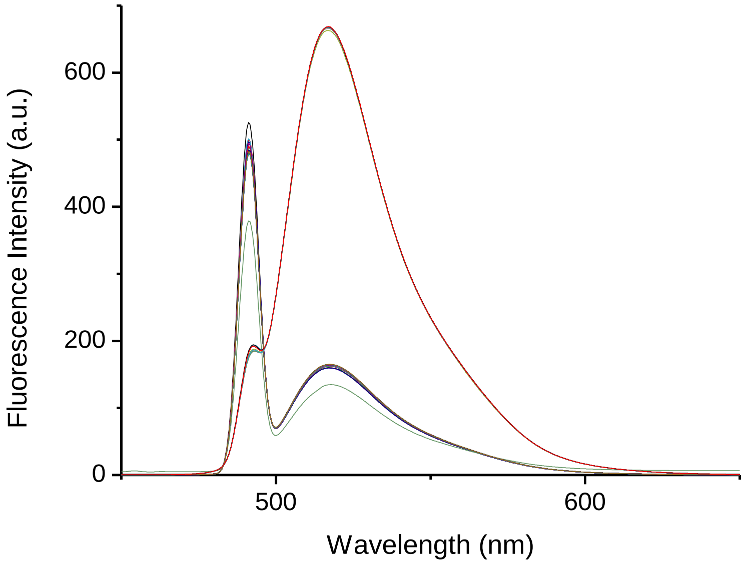


Figure S42. CF leakage induced by **1c** (15 mol% carrier to lipid) from unilamellar POPC (0.025mM) vesicles loaded with 50 mM CF and 451 mM NaCl, buffered to pH 7.2 with 20 mM sodium phosphate salts. The vesicles were dispersed in 150 mM Na_2SO_4 buffered to pH 7.2 with 20 mM sodium phosphate salts. At t = 60 s, a DMSO solution of the transporter was added to start the experiment. At the end of the experiment (6 min), detergent was added to lyse the vesicles. Each trace represents the average of three trials.

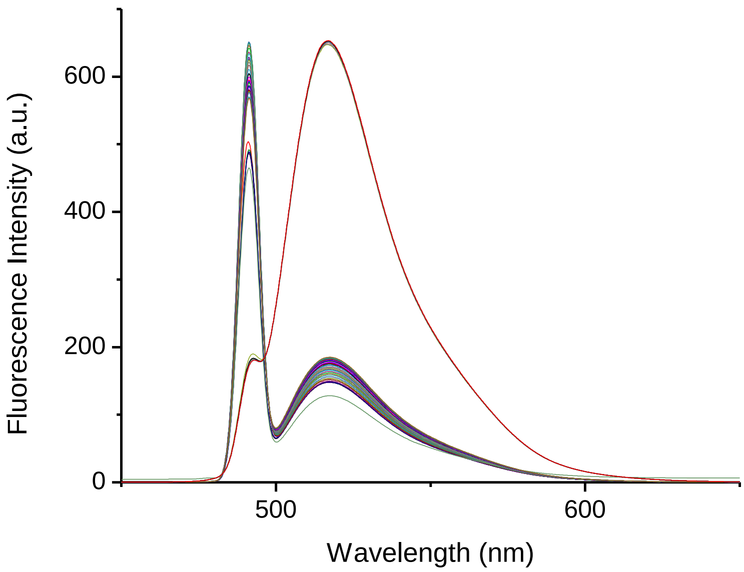


Figure S43. CF leakage induced by **1a-c** (15 mol% carrier to lipid) from unilamellar POPC vesicles (0.025mM) loaded with 50 mM CF and 451 mM NaCl, buffered to pH 7.2 with 20 mM sodium phosphate salts. The vesicles were suspended in 150 mM Na_2SO_4 buffered to pH 7.2 with 20 mM sodium phosphate salts. At t = 60 s, a DMSO solution of the transporter was added to start the experiment. At the end of the experiment (t=360 s), detergent was added to lyse the vesicles and induce the release of all encapsulated CF.

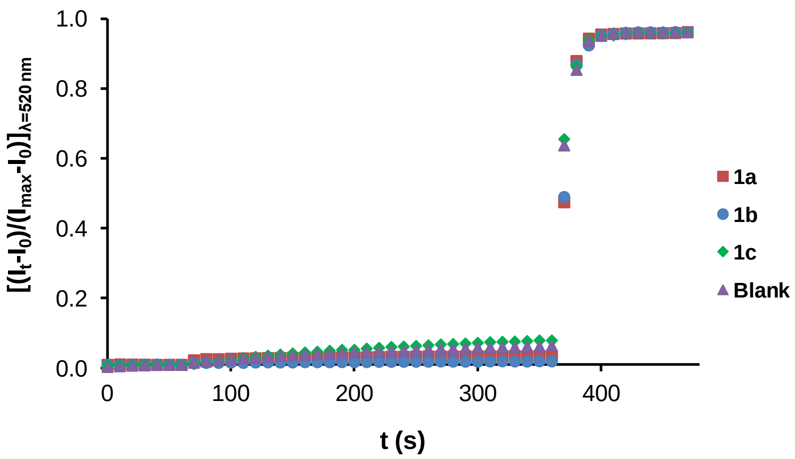


Figure S44. CF lekeage induced by **1a** (15 mol% carrier to lipid) from unilamellar POPC (0.05mM) vesicles loaded with 50 mM CF and 451 mM NaCl, buffered to pH 7.2 with 20 mM sodium phosphate salts. The vesicles were dispersed in 150 mM Na_2SO_4 buffered to pH 7.2 with 20 mM sodium phosphate salts. At t = 60 s, a DMSO solution of the transporter was added to start the experiment. At the end of the experiment (6 min), detergent was added to lyse the vesicles. Each trace represents the average of three trials.

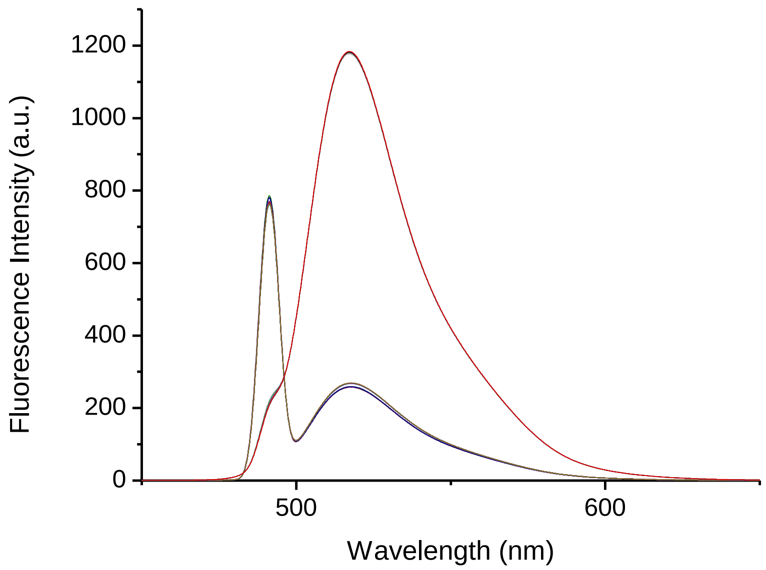


Figure S45. CF lekeage induced by **1b** (15 mol% carrier to lipid) from unilamellar POPC (0.05mM) vesicles loaded with 50 mM CF and 451 mM NaCl, buffered to pH 7.2 with 20 mM sodium phosphate salts. The vesicles were dispersed in 150 mM Na_2SO_4 buffered to pH 7.2 with 20 mM sodium phosphate salts. At t = 60 s, a DMSO solution of the transporter was added to start the experiment. At the end of the experiment (6 min), detergent was added to lyse the vesicles. Each trace represents the average of three trials**.**

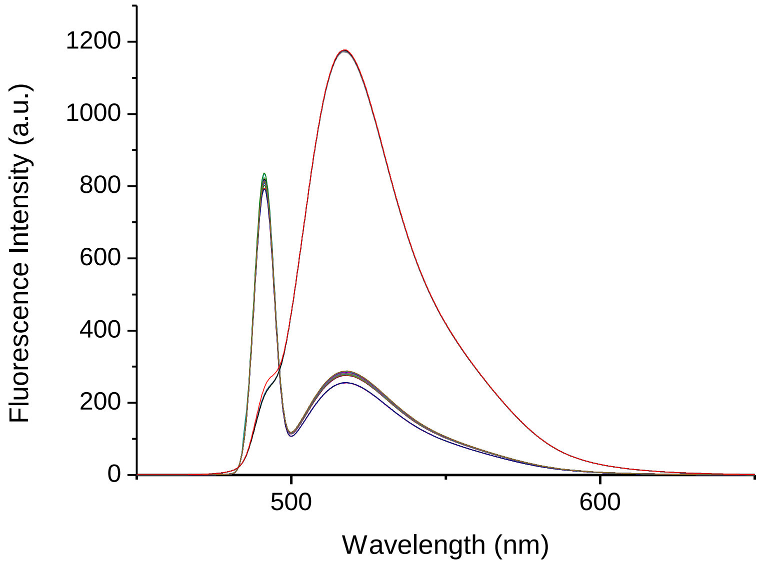
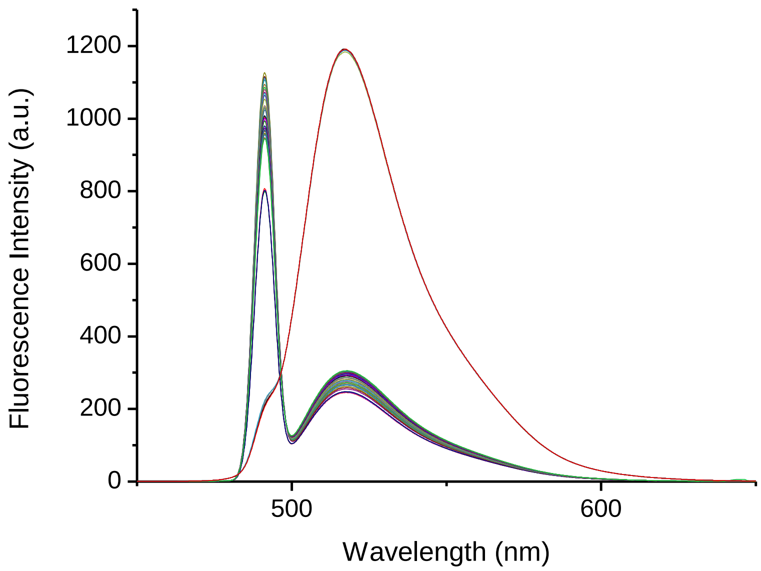
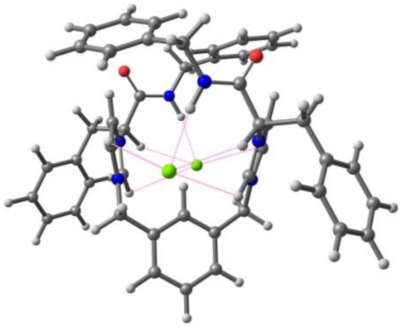


Figure S46. CF lekeage induced by **1c** (15 mol% carrier to lipid) from unilamellar POPC (0.05mM) vesicles loaded with 50 mM CF and 451 mM NaCl, buffered to pH 7.2 with 20 mM sodium phosphate salts. The vesicles were dispersed in 150 mM Na_2SO_4 buffered to pH 7.2 with 20 mM sodium phosphate salts. At t = 60 s, a DMSO solution of the transporter was added to start the experiment. At the end of the experiment (6 min), detergent was added to lyse the vesicles. Each trace represents the average of three trials.



Molecular modeling. Optimized geometries and geometric parameters obtained from computational calculations

Figure S47. Optimized structure for **3a**-2Cl



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C	1.360304097	-2.632840495	-2.247166196
H	0.578570807	-2.263837635	-2.925073156
H	2.123994427	-3.174869775	-2.814264166
N	1.980325697	-1.417181295	-1.672120456
N	3.002885357	-0.054504215	-0.321212026
N	-1.972404823	-1.640127075	1.494347014
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C	2.023150137	-0.181345145	-2.294667966
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H	2.626719027	-2.071793655	0.288560954
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H	-2.935582963	-2.144801715	-0.372187166
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H	-2.534730923	1.584903775	1.561955544
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C	-0.578475153	-5.035829845	0.755374904
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H	-0.127031763	-1.814329215	-0.194653116
H	0.270201397	-6.738934645	-0.250022026
H	-1.077959783	-5.636743955	1.511575524
Cl	-1.537450254	-0.847726770	-3.035120655
Cl	1.525596480	-1.342444350	2.959367020
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H	5.378025337	1.354906365	-0.123960306
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H	1.889418567	4.029510735	-0.718756556
H	3.034612917	4.548109245	-2.859165886
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C	0.031844937	3.954027385	2.246554994
C	-0.257219703	2.607191925	4.224693234
C	-1.627580603	2.876532535	4.209821084
C	-1.338254843	4.221251895	2.223789764
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H	0.162221757	1.979327415	5.007917084
H	-2.267472213	2.461181635	4.984490704
H	-1.758348273	4.840693925	1.436872084
H	-3.236662653	3.900568535	3.194971604

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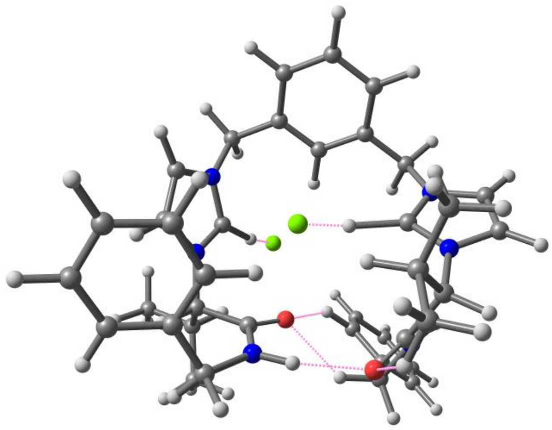
C	-6.897664783	-3.413896515	0.236818694	C	7.076349587	-3.140966695	-0.689939496
C	-5.989293013	-1.776176755	-1.295530806	C	6.279255287	-0.910580935	-1.180832356
C	-6.229620423	-1.232269195	1.040113434	C	6.107448997	-1.780407845	1.060055664
C	-6.755808753	-2.503060485	1.284052524	C	6.693896607	-2.975086585	0.643438494
C	-6.512753243	-3.046447445	-1.055211276	C	6.868544997	-2.105089325	-1.601098436
H	-5.691090003	-1.498970585	-2.304320936	H	6.124537897	-0.104424795	-1.894605936
H	-6.122868033	-0.524468765	1.859187394	H	5.812591497	-1.659466075	2.100261084
H	-7.056215483	-2.778392755	2.291730054	H	6.854804307	-3.774992035	1.361163084
H	-6.622470503	-3.748152385	-1.877698936	H	7.166967637	-2.223085695	-2.639595826
H	-7.308069483	-4.402577745	0.423881684	H	7.536705607	-4.070287335	-1.014515686

Figure S48. Optimized structure for **3b**-2Cl



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H	-1.688265000	5.277492000	-0.290750000	H	0.938517000	2.963728000	-1.201157000
C	1.770215000	2.068484000	-3.617375000	H	-2.527977000	3.581763000	-4.725902000
H	2.596481000	2.656435000	-3.131418000	H	-2.968975000	4.364275000	-2.410734000
H	1.973590000	2.075043000	-4.711359000	C	2.435158000	-1.865401000	-0.577984000
N	1.825165000	0.683922000	-3.109110000	H	2.464520000	-2.939648000	-0.897577000
N	2.120990000	-1.038144000	-1.759009000	C	-3.291133000	0.209219000	1.941942000
N	-2.141037000	3.358381000	0.516504000	C	-2.005393000	-0.397801000	2.573440000
N	-3.033221000	1.593069000	1.491863000	C	1.321516000	-1.615579000	0.470090000
C	1.444459000	-0.476586000	-3.834337000	N	0.419632000	-2.630322000	0.761712000
H	1.073054000	-0.442976000	-4.839531000	H	-0.365229000	-2.391938000	1.397817000
C	1.631928000	-1.553143000	-2.991446000	N	-1.188506000	0.463130000	3.270522000
H	1.441886000	-2.600389000	-3.154424000	H	-1.400489000	1.449164000	3.391598000
C	2.233231000	0.328876000	-1.845630000	O	-1.770174000	-1.600660000	2.510457000
H	2.709129000	1.237241000	-0.895727000	O	1.242448000	-0.570465000	1.096530000
C	-2.050167000	1.992751000	0.608796000	C	0.098509000	-0.003940000	3.860032000
H	-1.163123000	1.034450000	-0.193676000	H	-0.109217000	-0.586262000	4.784377000
C	-3.224079000	3.827303000	1.313999000	H	0.593749000	-0.707463000	3.134724000
H	-3.491838000	4.864215000	1.385318000	C	0.448445000	-4.007738000	0.237394000
C	-3.780346000	2.724902000	1.926277000	H	-0.260681000	-4.622927000	0.847443000
H	-4.611837000	2.654607000	2.600740000	H	1.458413000	-4.451055000	0.407360000
C	0.435479000	2.701636000	-3.293465000	C	3.812264000	-1.483006000	0.046934000
C	-2.014899000	3.902976000	-2.656229000	H	3.761412000	-0.404161000	0.368960000
C	-0.541603000	2.866314000	-4.282597000	C	-3.807715000	-0.686415000	0.769530000
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C	-1.033506000	3.739417000	-1.668101000	H	-4.075346000	0.231085000	2.747125000

C	0.982262000	1.188441000	4.121661000
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C	1.011963000	1.782242000	5.392335000
C	1.775315000	1.707012000	3.088639000
C	2.598090000	2.811290000	3.327636000
C	1.836859000	2.885432000	5.625804000
H	0.400242000	1.383025000	6.197495000
H	1.760683000	1.247628000	2.087938000
H	3.216105000	3.200672000	2.513436000
H	1.864958000	3.342294000	6.612091000
H	3.274370000	4.257746000	4.779504000
C	0.050628000	-4.124286000	-1.217802000
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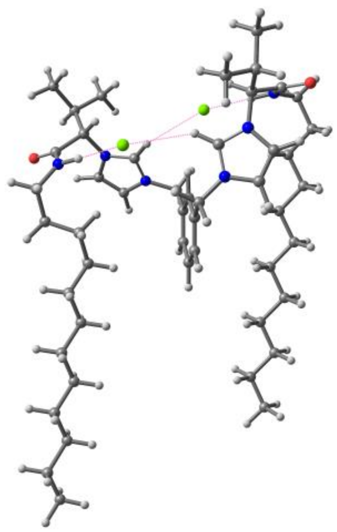
C	-0.973064000	-3.331431000	-1.753551000
C	0.699289000	-5.066172000	-2.030990000
C	0.323844000	-5.211622000	-3.369170000
C	-1.340481000	-3.476625000	-3.094134000
H	-1.471940000	-2.583552000	-1.130008000
H	1.490194000	-5.692667000	-1.624005000
H	0.824695000	-5.947793000	-3.995386000
H	-2.130209000	-2.849074000	-3.506227000

H	-0.987325000	-4.532181000	-4.945187000
Cl	3.315524000	2.378408000	-0.179805000
Cl	-0.665354000	0.046837000	-1.057475000
C	4.937053000	-1.646655000	-0.975294000
H	5.906186000	-1.391845000	-0.526742000
H	4.805785000	-0.974164000	-1.832145000
H	5.010655000	-2.669157000	-1.356856000
C	4.066493000	-2.351091000	1.281997000
H	5.036431000	-2.102152000	1.732443000
H	4.081707000	-3.419450000	1.050033000
H	3.312592000	-2.177916000	2.061142000
C	-4.402170000	-1.976804000	1.338818000
H	-3.660530000	-2.518428000	1.949826000
H	-4.702344000	-2.656359000	0.533050000
H	-5.283588000	-1.796587000	1.960002000
C	-4.847378000	0.049481000	-0.078861000
H	-4.398613000	0.875103000	-0.645349000
H	-5.664727000	0.457237000	0.523061000
H	-5.292954000	-0.629070000	-0.817135000

Figure S49. Optimized structure for **3c**-2Cl



C	0.663594000	-0.133211000	2.469995000
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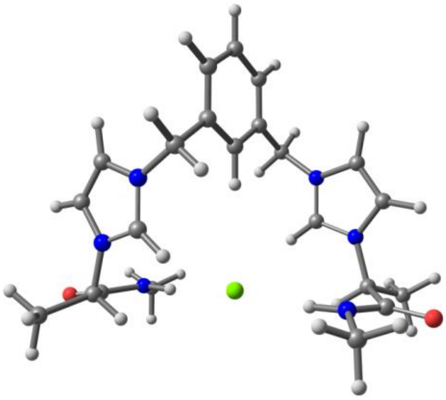
H	0.192686000	0.313606000	3.353757000
C	1.013024000	0.636342000	-2.501726000
H	0.523111000	1.187184000	-3.314307000
H	1.019297000	-0.411489000	-2.797181000
N	2.383986000	1.138563000	-2.396608000
N	4.536129000	1.150084000	-2.166285000
N	0.438849000	-1.576550000	2.490602000
N	0.725643000	-3.686929000	2.109195000
C	2.808933000	2.420704000	-2.684476000
H	2.082162000	3.164555000	-2.956897000
C	4.167021000	2.425721000	-2.558639000
H	4.922917000	3.180688000	-2.691168000

C	3.439323000	0.382184000	-2.039328000
H	3.421938000	-0.655912000	-1.728394000
C	1.202620000	-2.463265000	1.824262000
H	2.042978000	-2.244243000	1.177771000
C	-0.545864000	-2.246555000	3.189331000
H	-1.254223000	-1.682662000	3.768546000
C	-0.365512000	-3.577529000	2.952379000
H	-0.880221000	-4.468920000	3.267155000
C	0.265558000	0.836578000	-1.205350000
C	-1.190031000	1.045308000	1.196497000
C	-1.001341000	1.434134000	-1.188641000
C	0.782667000	0.347878000	0.002258000
C	0.072601000	0.443552000	1.208264000
C	-1.721378000	1.540525000	0.004301000

H	-1.450948000	1.805708000	-2.107087000
H	1.753067000	-0.142684000	0.005362000
H	-2.706736000	2.001275000	0.001302000
H	-1.773123000	1.129393000	2.110344000
Cl	4.449265000	-0.608418000	1.528845000
Cl	1.762061000	-3.083735000	-1.890354000
C	5.915290000	0.679071000	-1.839138000
H	5.830685000	-0.230393000	-1.235828000
C	1.257283000	-4.938227000	1.497018000
C	0.059392000	-5.661356000	0.823198000
C	6.613977000	1.783574000	-0.997355000
N	6.355267000	1.731657000	0.351883000
H	5.749987000	0.980215000	0.722137000
N	-0.219630000	-5.239037000	-0.456102000
H	0.396160000	-4.542904000	-0.907034000
O	-0.657876000	-6.455548000	1.434844000
O	7.251510000	2.701978000	-1.516423000
C	-1.445728000	-5.569838000	-1.145021000
H	-1.672569000	-6.626762000	-0.967503000
C	6.680413000	2.808087000	1.260544000
H	7.696661000	3.154750000	1.043661000
H	6.669263000	2.396418000	2.274991000
C	6.706511000	0.356642000	-3.129326000
H	6.855463000	1.277663000	-3.707256000
C	1.953637000	-5.822755000	2.556291000
H	1.219008000	-6.153341000	3.301386000
H	1.988608000	-4.662894000	0.731553000
H	-1.270359000	-5.433723000	-2.217103000
C	5.702485000	3.981010000	1.145688000
H	5.780670000	4.428602000	0.147353000
H	5.994468000	4.754595000	1.865830000
C	4.249294000	3.567102000	1.397436000
H	3.946407000	2.811775000	0.663610000
H	4.161936000	3.108743000	2.389818000
C	-2.622246000	-4.708011000	-0.675785000
H	-2.791838000	-4.864194000	0.396400000
C	-2.403655000	-3.213733000	-0.941421000
H	-2.281010000	-3.042928000	-2.017678000
H	-1.473740000	-2.888617000	-0.460634000
H	-3.522483000	-5.050455000	-1.197644000
C	-3.528617000	-2.326065000	-0.402575000
H	-3.649297000	-2.497972000	0.673970000
H	-3.221588000	-1.279884000	-0.521602000
C	3.296659000	4.758847000	1.298503000
H	3.523899000	5.478475000	2.094007000
H	3.446183000	5.273655000	0.341634000
C	-4.865857000	-2.535207000	-1.114709000
H	-4.728819000	-2.419783000	-2.196590000
H	-5.230578000	-3.553263000	-0.938852000
C	-5.914573000	-1.535268000	-0.622021000
H	-6.049561000	-1.648590000	0.460563000
H	-5.558886000	-0.512732000	-0.798291000
C	-7.254783000	-1.739651000	-1.330136000
H	-7.611948000	-2.761412000	-1.152919000
H	-7.119044000	-1.627627000	-2.412727000
C	-8.301549000	-0.738453000	-0.838710000
H	-7.944151000	0.283280000	-1.015755000
H	-8.437242000	-0.850539000	0.243890000

C	1.840344000	4.303432000	1.405857000
H	1.690784000	3.758678000	2.346066000
H	1.617317000	3.605173000	0.589800000
C	0.876402000	5.488573000	1.341981000
H	1.056051000	6.062539000	0.424832000
H	1.064769000	6.160920000	2.187612000
C	-0.577016000	5.015447000	1.370409000
H	-0.752694000	4.414954000	2.271205000
H	-0.762222000	4.367493000	0.506211000
C	-1.553397000	6.191216000	1.339195000
H	-1.373945000	6.794886000	0.441275000
H	-1.376808000	6.839337000	2.206106000
C	-3.003478000	5.703866000	1.348214000
H	-3.182367000	5.099787000	2.246089000
H	-3.177834000	5.053959000	0.481921000
C	-3.985449000	6.875799000	1.314947000
H	-3.806237000	7.480138000	0.417336000
H	-3.812156000	7.525281000	2.181654000
C	-5.433693000	6.387115000	1.322449000
H	-5.613100000	5.740329000	0.455720000
H	-5.619286000	5.785762000	2.220026000
C	-6.413848000	7.548842000	1.289081000
H	-7.443094000	7.176645000	1.295049000
H	-6.282352000	8.198240000	2.160473000
C	-9.641938000	-0.942175000	-1.546843000
H	-9.506180000	-0.830221000	-2.629452000
H	-9.999440000	-1.963843000	-1.369664000
C	-10.688570000	0.059219000	-1.055570000
H	-10.824361000	-0.052507000	0.027089000
H	-10.331114000	1.080976000	-1.232527000
C	-12.027965000	-0.144342000	-1.763237000
H	-11.898578000	-0.029590000	-2.845732000
H	-12.391857000	-1.163112000	-1.586049000
C	-13.071240000	0.849289000	-1.277661000
H	-12.751973000	1.878629000	-1.469661000
H	-13.248000000	0.738818000	-0.203003000
H	-14.020876000	0.685787000	-1.796669000
H	-6.276123000	8.152534000	0.386350000
C	3.051917000	-5.048114000	3.293442000
H	3.797076000	-4.654400000	2.593780000
H	3.569624000	-5.695121000	4.009851000
H	2.637044000	-4.207210000	3.857773000
C	2.569896000	-7.069859000	1.911834000
H	3.308776000	-6.797950000	1.150169000
H	1.807751000	-7.694524000	1.436140000
H	3.073126000	-7.686429000	2.664519000
C	8.085813000	-0.225090000	-2.796557000
H	8.638678000	-0.459901000	-3.712625000
H	7.995649000	-1.147012000	-2.211787000
H	8.693198000	0.481363000	-2.222772000
C	5.952267000	-0.635121000	-4.021987000
H	6.550759000	-0.901165000	-4.900063000
H	5.014713000	-0.206780000	-4.389587000
H	5.718138000	-1.557878000	-3.480310000

Figure S50. Optimized structure for **CIL**-Cl



C	-0.455601000	-1.097170000	3.174589000
H	-0.922621000	-1.821334000	3.851727000
H	0.446114000	-1.561718000	2.760200000
C	1.576627000	3.542757000	3.108938000
H	0.927382000	3.879317000	2.292960000
H	1.771729000	4.404767000	3.756944000
N	-1.403885000	-0.811924000	2.100245000
N	-2.215483000	-0.615825000	0.102893000
N	2.856247000	3.089543000	2.568574000
N	4.373487000	2.535727000	1.127106000
C	-2.695237000	-0.325830000	2.236764000
H	-3.081277000	-0.123787000	3.220690000
C	-3.203504000	-0.191437000	0.976209000
H	-4.142812000	0.158776000	0.581987000
C	-1.130761000	-0.986875000	0.796597000
C	3.120181000	2.992238000	1.254963000
H	2.446335218	3.253230495	0.447243252
C	3.971398000	2.692773000	3.290743000
H	3.934867000	2.704948000	4.366139000
C	4.924888000	2.332678000	2.381577000
H	5.928527000	1.949854000	2.462298000
C	-0.089799000	0.179517000	3.892982000
C	0.618745000	2.548772000	5.229075000
C	-0.360390000	0.334138000	5.258531000
C	0.546441000	1.229927000	3.210339000
C	0.908312000	2.419426000	3.864790000
C	-0.009613000	1.511813000	5.920174000
H	-0.845195000	-0.459036000	5.825726000
H	0.764015000	1.119630000	2.150031000
H	-0.227368000	1.622202000	6.981368000
H	0.875861000	3.457370000	5.771486000
Cl	1.368603782	0.813139505	-0.796326252
H	-0.206568000	-1.374778000	0.384293000
C	5.006404000	2.222119000	-0.179555000
H	4.250616000	2.328007000	-0.965606000
C	-2.275771000	-0.592506000	-1.38106100
H	-1.278346000	-0.820889000	-1.77258300
C	-3.239697000	-1.659735000	-1.88649700
H	-4.258534000	-1.486882000	-1.52346600
H	-2.929572000	-2.651663000	-1.54188300
H	-3.272479000	-1.668522000	-2.98092400
C	6.133509000	3.206626000	-0.469344000
H	5.754086000	4.233684000	-0.476246000
H	6.590598000	3.000315000	-1.442702000
H	6.922354000	3.150366000	0.288455000
C	5.505080000	0.759735000	-0.189172000
O	6.696104000	0.467036000	-0.100206000
N	4.502483000	-0.189543000	-0.227228000
H	3.548842000	0.107198000	-0.472970000
C	4.810159000	-1.590686000	-0.361065000
H	5.649198000	-1.859108000	0.286331000
H	5.074601000	-1.792740000	-1.402325000
H	3.925963000	-2.169299000	-0.084154000
C	-2.671521000	0.817701000	-1.873029000
O	-3.790096000	1.073673000	-2.315065000
N	-1.695790000	1.780598000	-1.704046000
H	-0.734671000	1.480066000	-1.494752000
C	-1.869884000	3.114023000	-2.221201000
H	-1.140877000	3.771308000	-1.741825000
H	-2.883268000	3.470828000	-2.018958000
H	-1.699134000	3.095460000	-3.300773000