ELECTRONIC SUPPORTING INFORMATION (ESI) FOR

Expanding the library of sumanene molecular receptors for caesium-selective potentiometric sensors

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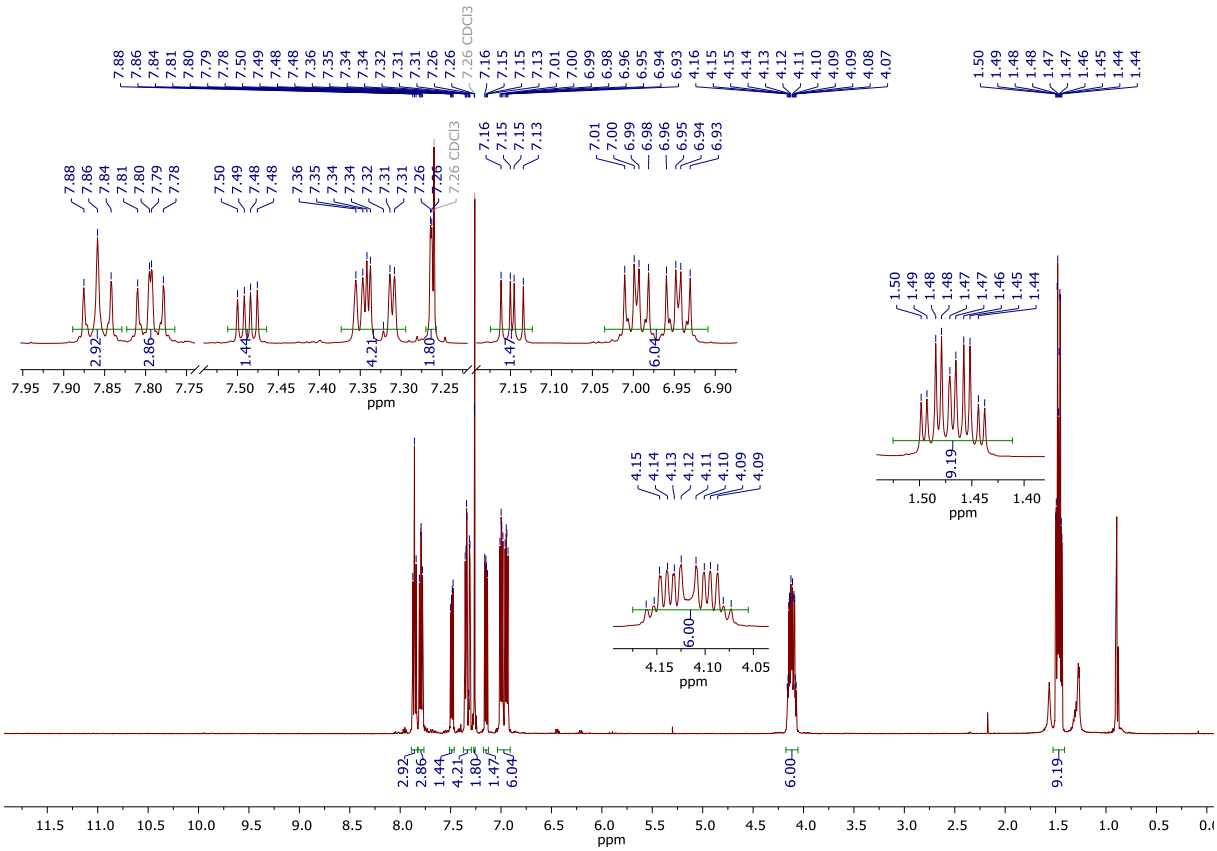

Figure S1. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **5**.

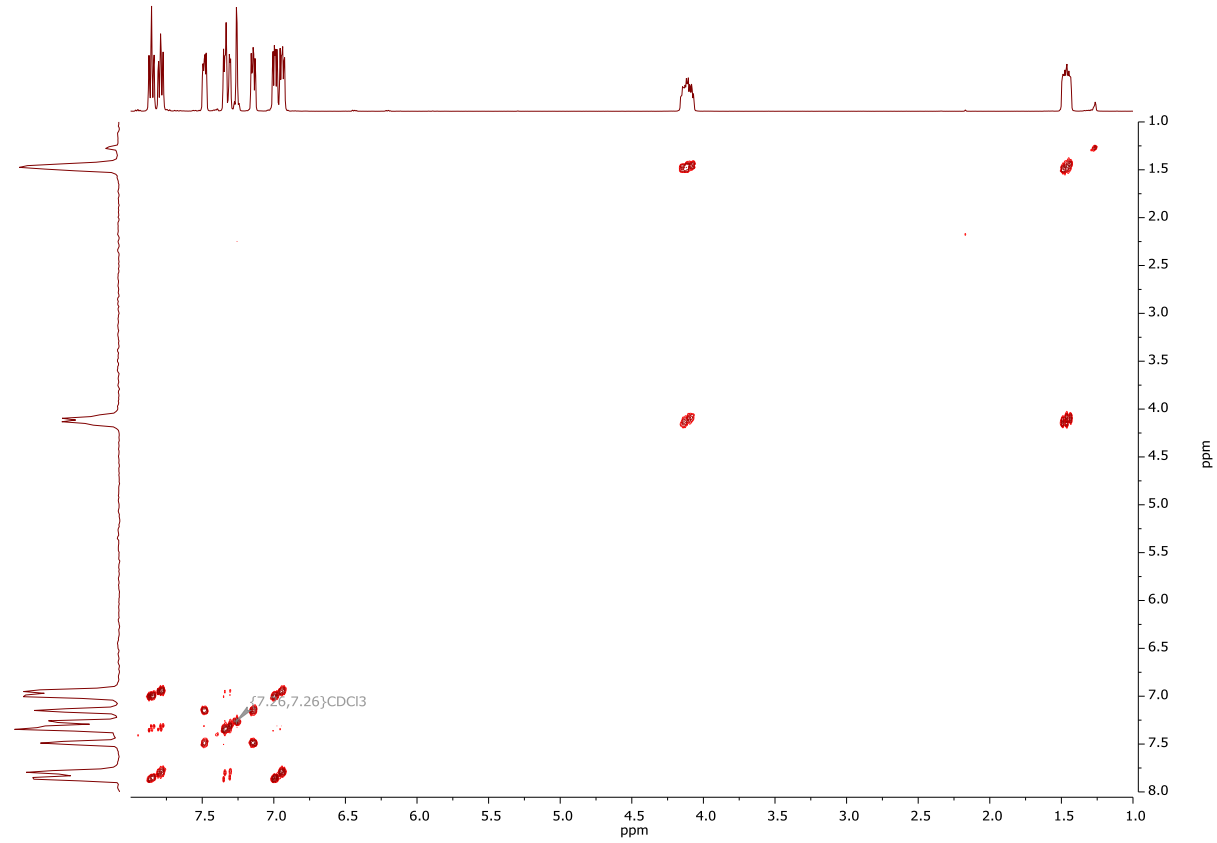

Figure S2. ^{1}H-^{1}H COSY NMR ($CDCl_3$, 500 MHz) spectrum of **5**.

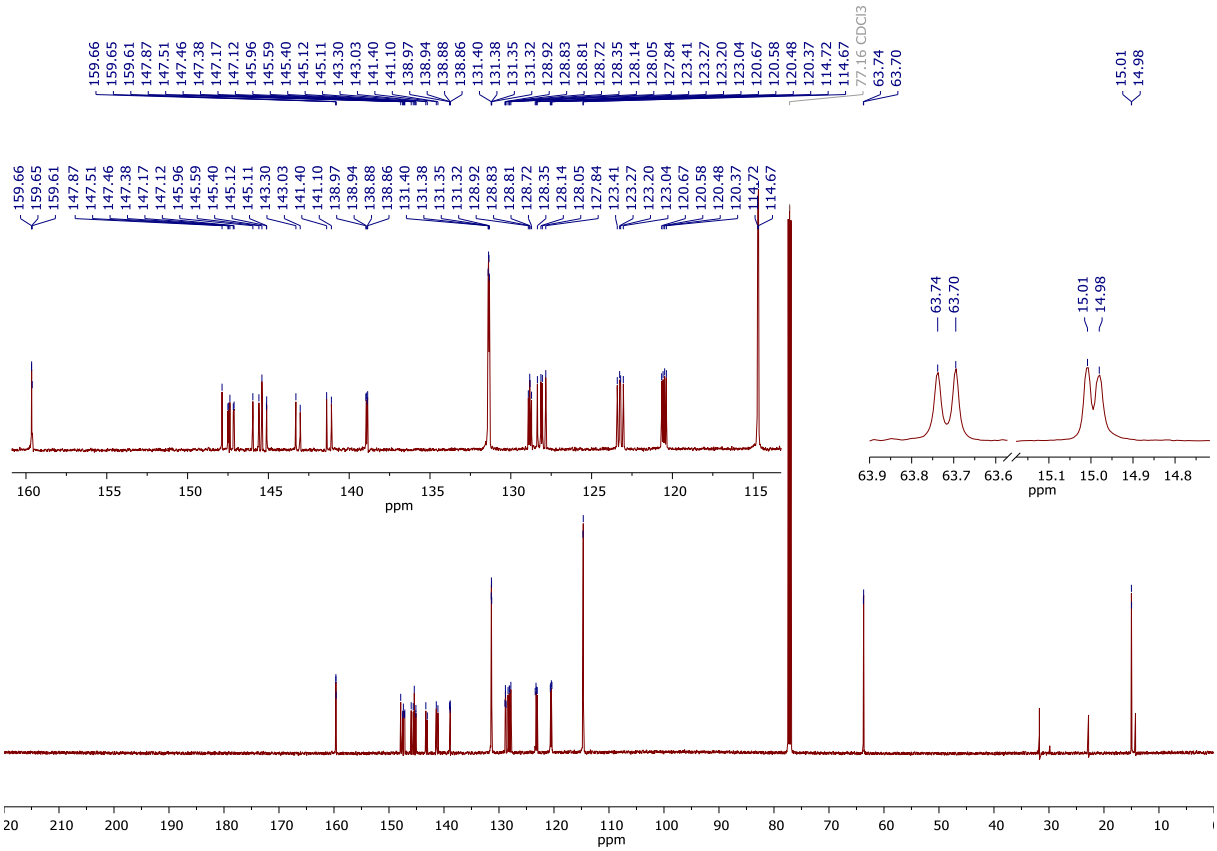

Figure S3. $\{^1H\}^{13}C$ NMR ($CDCl_3$, 125 MHz) spectrum of **5**.

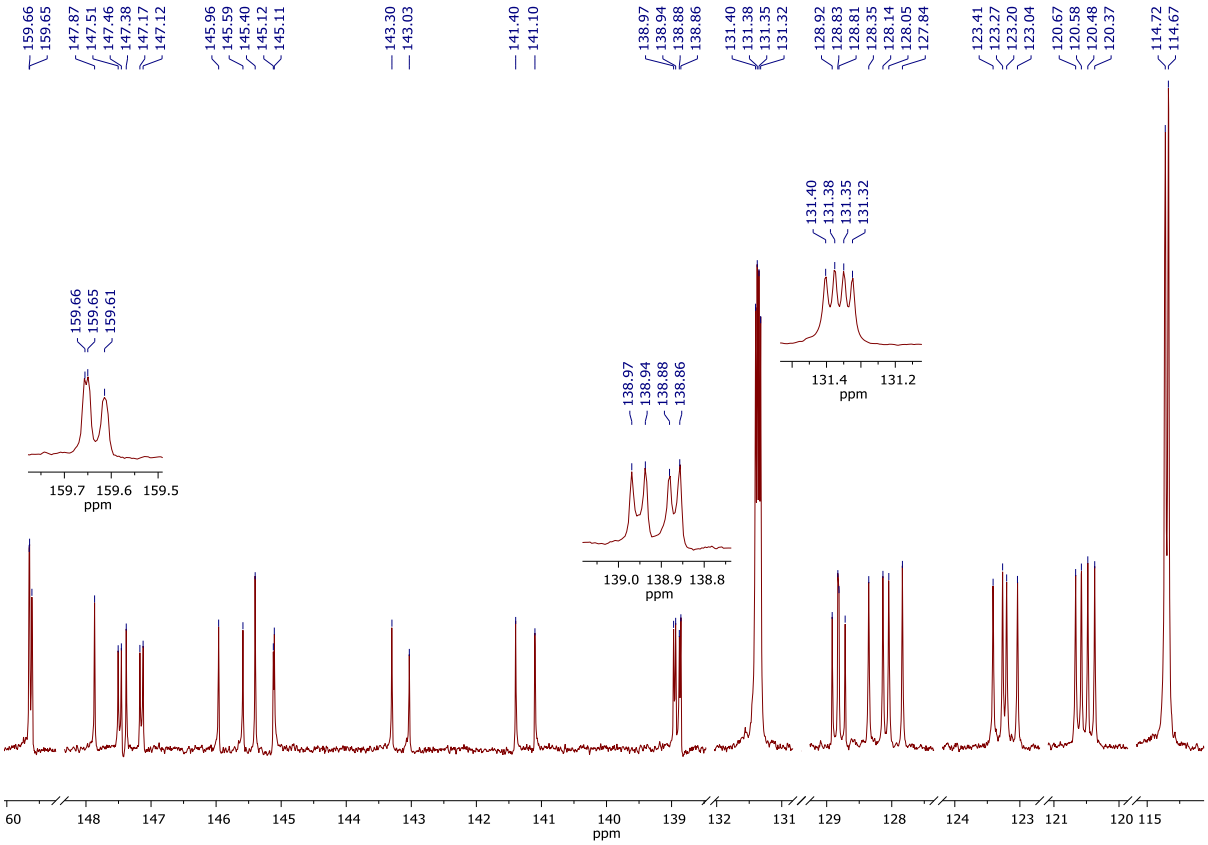

Figure S4. 160-113 ppm inset of $\{^1H\}^{13}C$ NMR ($CDCl_3$, 125 MHz) spectrum of **5**.

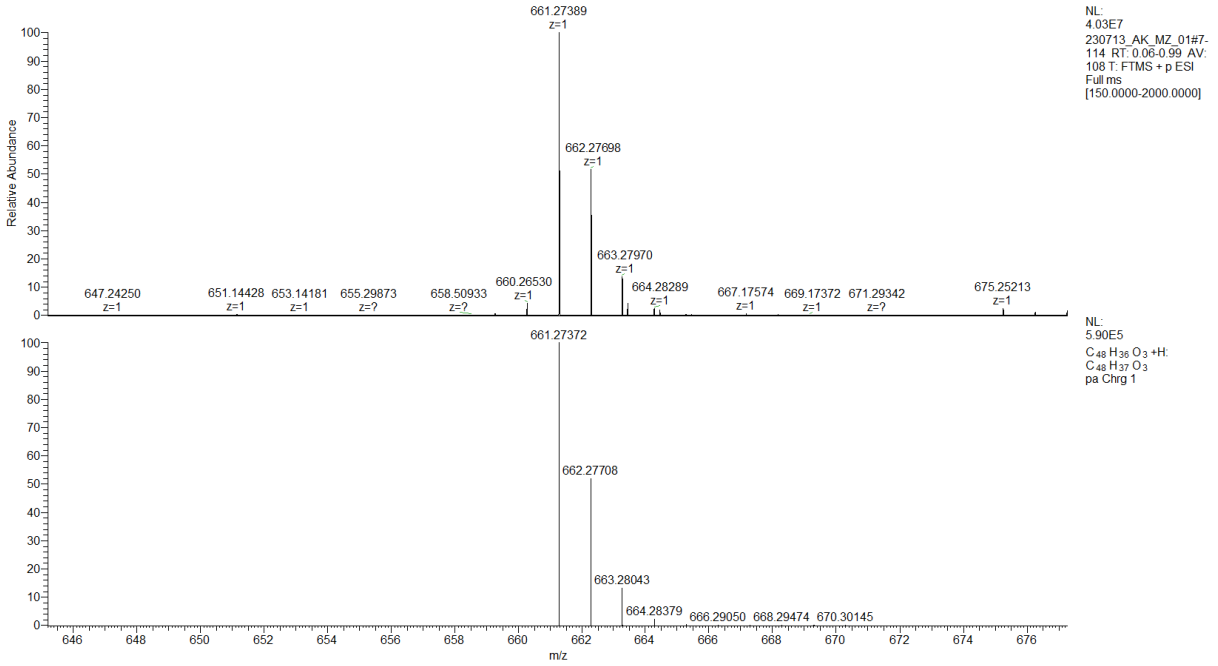

Figure S5. ESI-HRMS (TOF) spectrum of **5**.

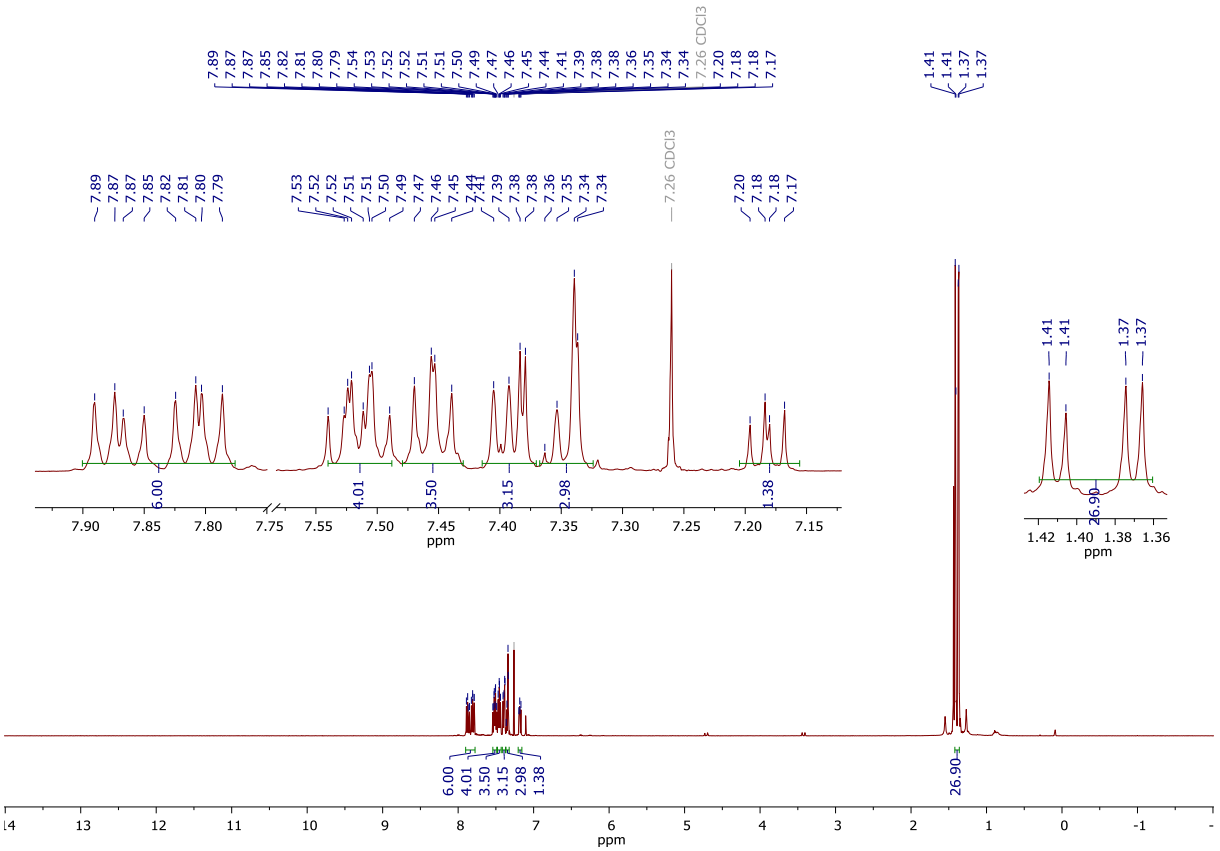

Figure S6. ^{1}H NMR ($CDCl_3$, 500 MHz) spectrum of **6**.

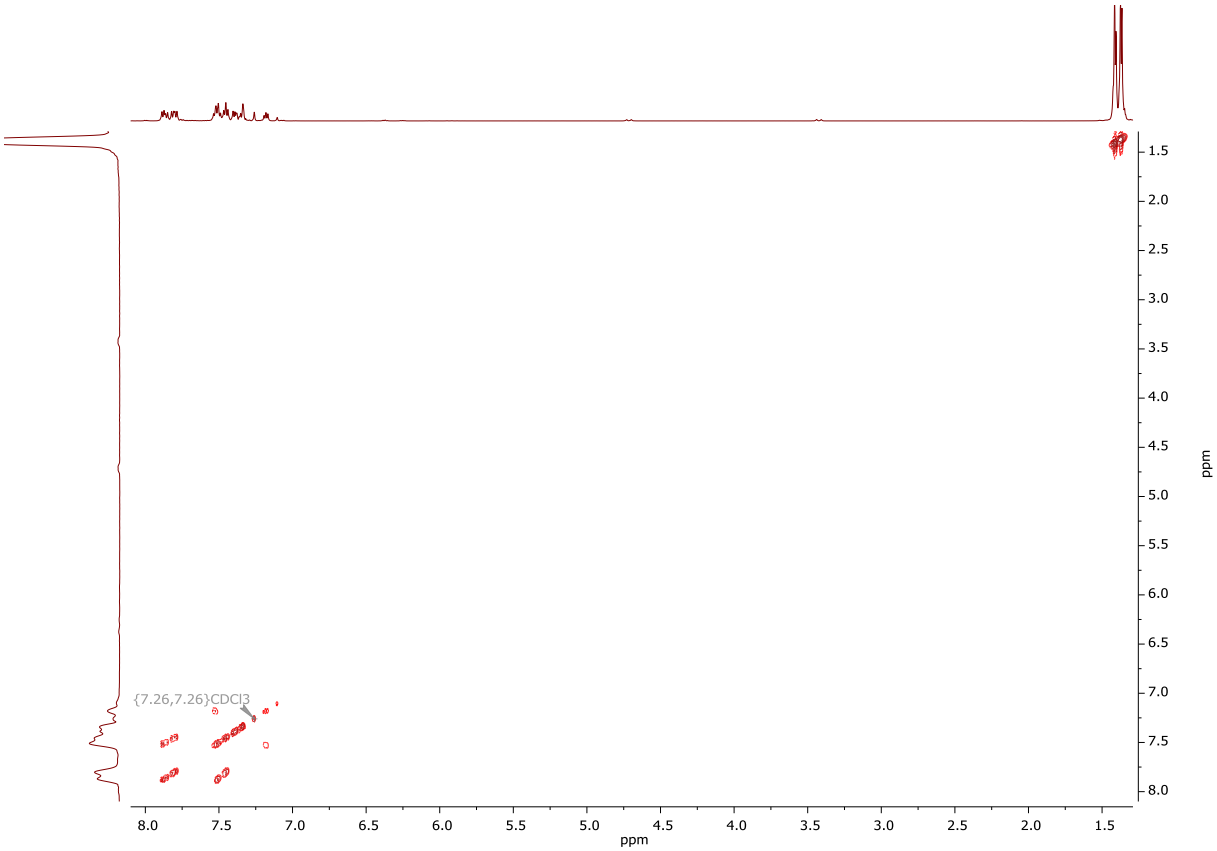

Figure S7. ^{1}H-^{1}H COSY NMR ($CDCl_3$, 500 MHz) spectrum of **6**.

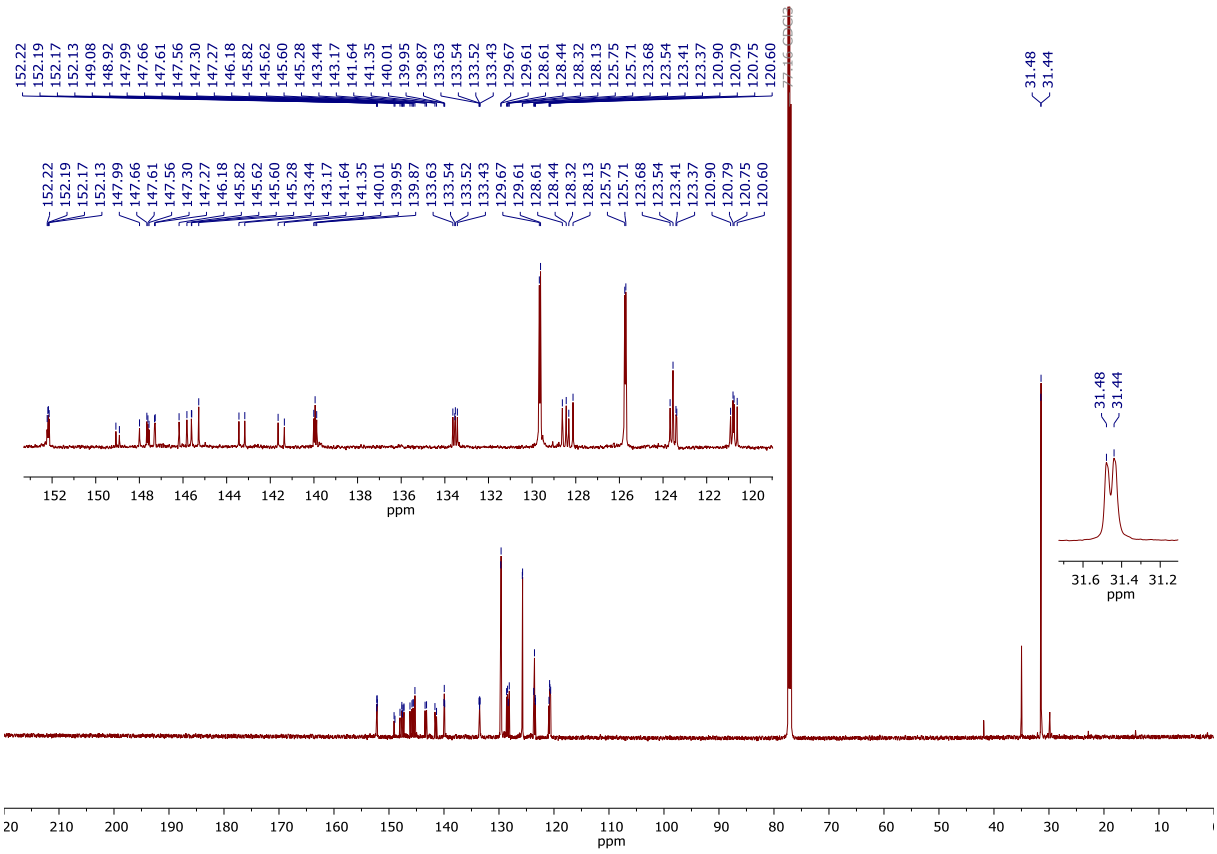

Figure S8. {^{1}H}^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of **6**.

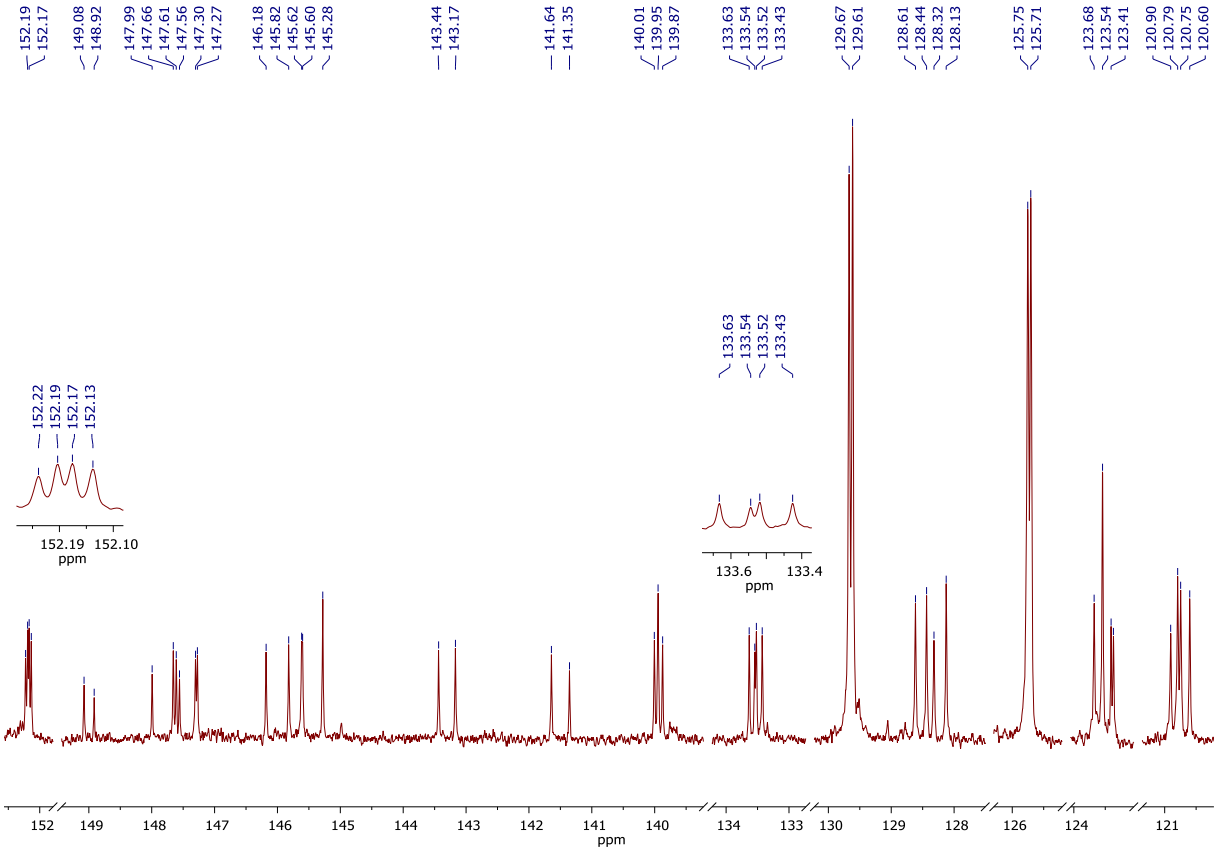

Figure S9. 153-120 ppm inset of the {^{1}H}^{13}C NMR ($CDCl_3$, 125 MHz) spectrum of **6**.

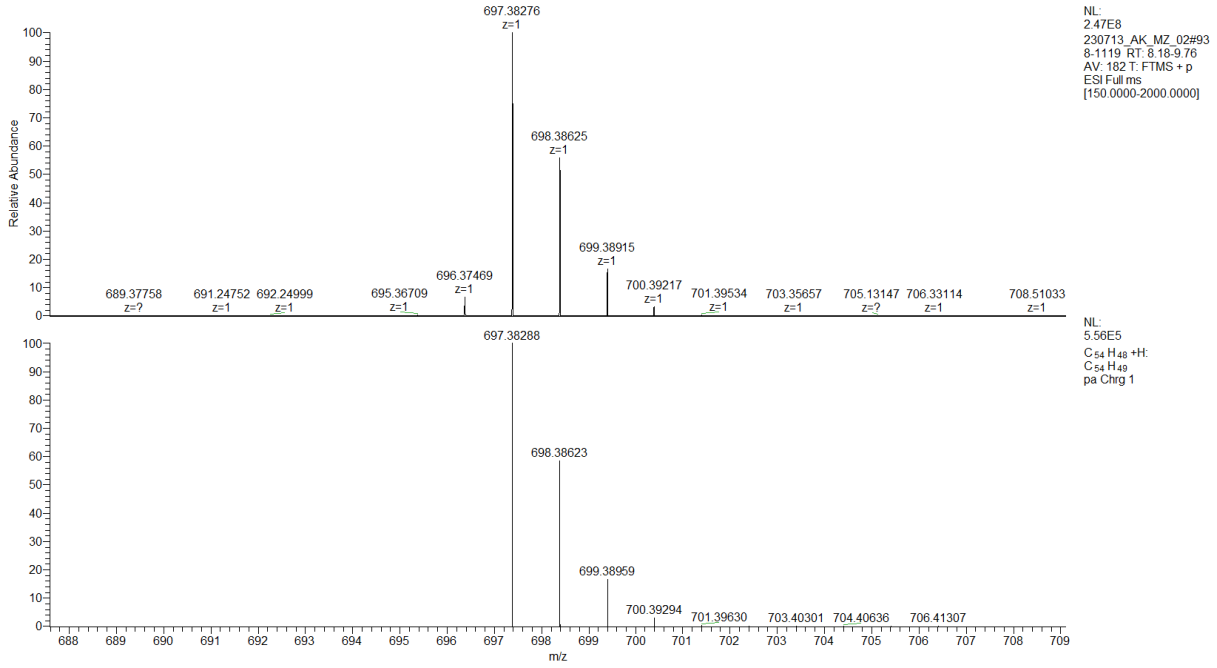

Figure S10. ESI-HRMS (TOF) spectrum of **6**.

Comparison of the caesium selectivity of sumanene derivatives with the selectivity of exemplary receptors reported in the literature

The construction of new chemical sensors (including electrochemical devices) requires the synthesis of selective molecular receptors. So far, a significant number of various receptors sensitive towards caesium cations have been proposed in the literature. Electrochemical sensors based on such ligands exhibited different selectivity pattern in terms of values of potentiometric selectivity coefficients. Generalizing, the selectivity of ion-selective electrodes containing the sumanene derivatives presented in this work are comparable (or even better) to the selectivity of the sensors based on the most frequently used for this purpose bis(benzo-18-crown-6) derivatives with various spacers [1-3] or macrocyclic diamide derivatives [4]. However, better selectivity of caesium recognition was noticed for carefully tuned structures of calix[6]arene esters [5] and calix[4]crown-ethers [6]. Finally, it should be stressed that simplified structure of the proposed sumanene receptors ensured performance of the sensors compared to the previously developed devices based on n-octyloxybenzene sumanene [7].

Supporting references:

[1] K. Kimura, A. Ishikawa, H. Tamura and T. J. Shono, *J. Chem. Soc., Perkin Trans. 2*, 1984, 447.

[2] K. W. Fung and K. H. J. Wong, *J. Electroanal. Chem*., 1980, **111**, 359.

[3] E. Luboch, A. Cygan and J. F. Biernat, *Tetrahedron*, 1991, **47**, 4101.

[4] Shamsipur, S.Y. Kazemi, H. Sharghi, K. Niknam, J. Fresenius, *Anal. Chem*., 2001, **371**, 1104-1108.

[5] A. Cadogan, D. Diamond, M. R. Smyth, G. Svehla, M. A. McKervey, E. M. Seward and S. J. Harris, *Analyst*, 1990, **115**, 1207.

[6] C. Pérez-Jiménez, L. Escriche, J. Casabó, *Anal. Chim. Acta*, 1998, **371**, 155-162.

[7] A. Kasprzak, A. Tobolska, H. Sakurai, W. Wróblewski, *Dalton Trans*., 2022, **51**, 468–472.

Table S1. Values of selectivity coefficients (log $K_{Cs, X}$) of potentiometric sensors formulated with sumanene derivative **3** and various amounts of lipophilic salt KTFPB in PVC/o-NPOE membranes (mean values calculated for 3 electrode specimens).

	log $K_{Cs, Li}$	log $K_{Cs, Na}$	log $K_{Cs, K}$	log $K_{Cs, NH4}$	log $K_{Cs, Rb}$	log $K_{Cs, Ba}$	log $K_{Cs, Ca}$
5% KTFPB	-3.10	-2.65	-1.20	-1.55	-0.50	-3.60	-3.80
20% KTFPB	-3.20	-2.70	-1.25	-1.55	-0.55	-3.30	-3.60
40% KTFPB	-3.45	-2.90	-1.35	-1.65	-0.55	-3.30	-3.60
70% KTFPB	-3.40	-2.85	-1.35	-1.65	-0.60	-3.20	-3.55

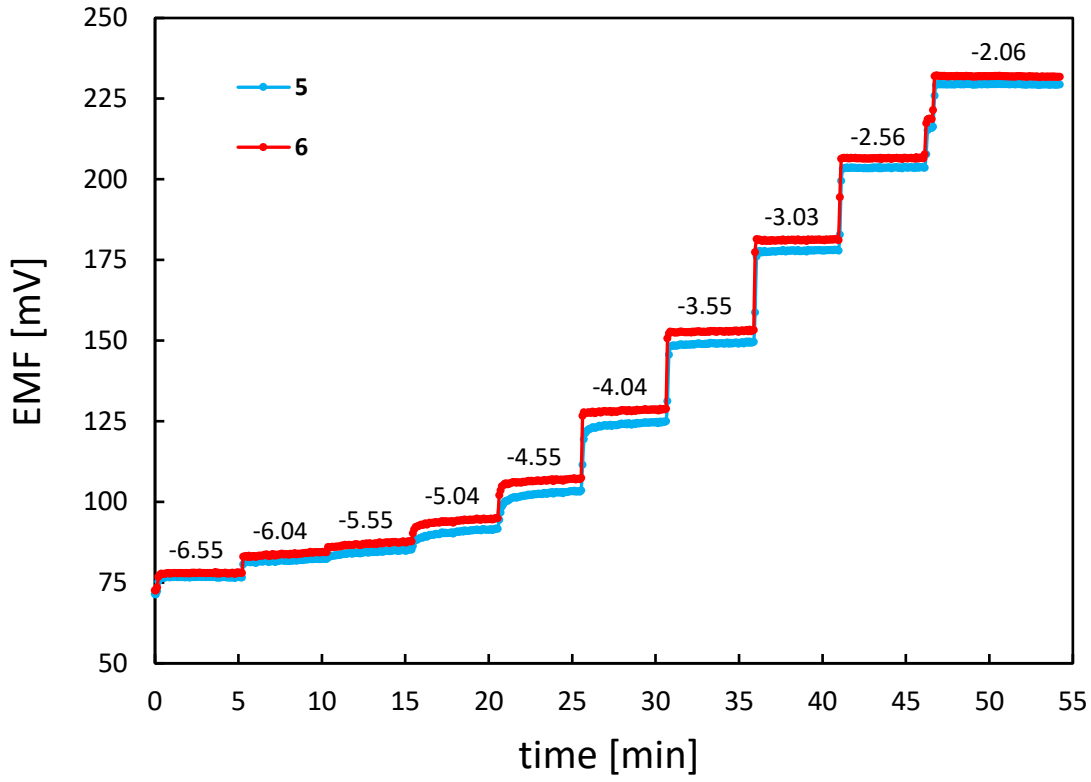

Figure S11. Dynamic responses of sensors formulated with sumanene receptor **5** and **6** (20 mol% KTFPB, PVC/o-NPOE) recorded increasing stepwise the activity of caesium cations in 0.01 M $NaNO_3$ solution.

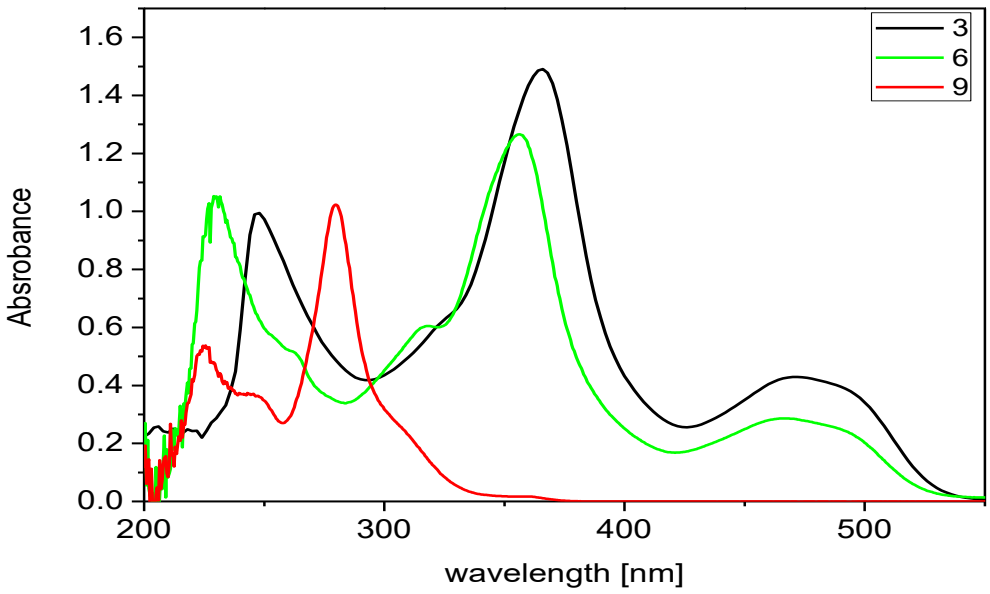

Figure S12. UV-Vis spectra of investigated sumanene derivatives **3**, **6**, **9** ($2x10^{-5}$ M) in mixture of THF and water (1:1).

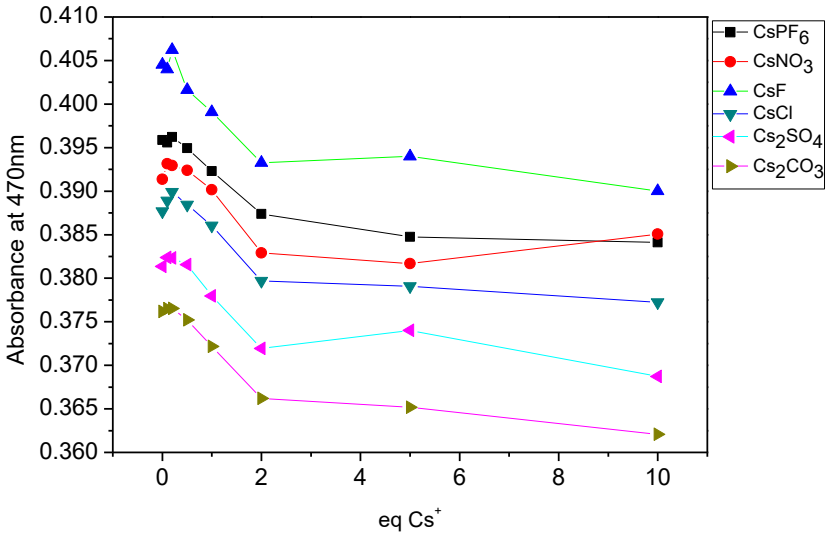

Figure S13. Titration curves of compound **3** ($2x10^{-5}$ M) with different caesium salts (absorption spectroscopy) in mixture of THF and water (1:1).

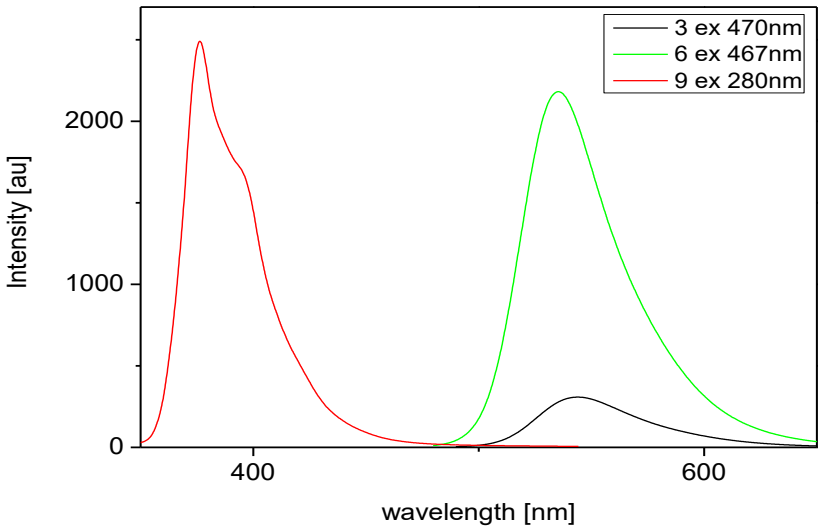

Figure S14. Emission spectra of investigated sumanene derivatives ($CHCl_3$, $2x10^{-5}$ M).

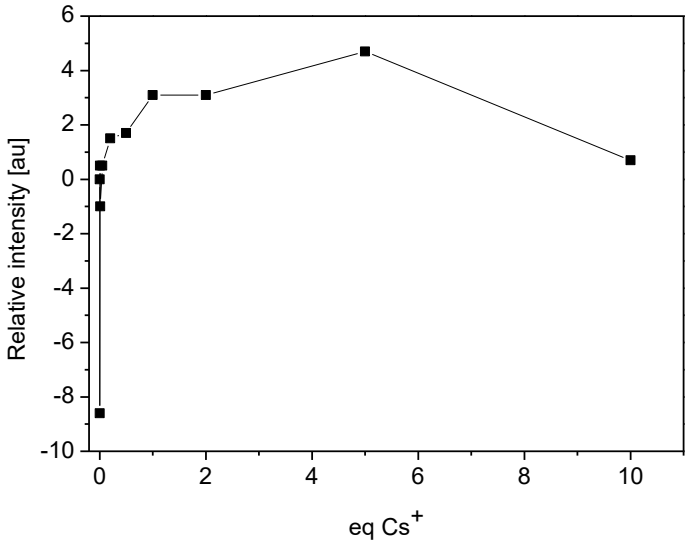

Figure S15. Titration curve of compound **3** ($2x10^{-5}$ M) with $LiPF_6$, (fluorescence spectrum), λ_{ex} = 350nm, in mixture of THF and water (1:1).

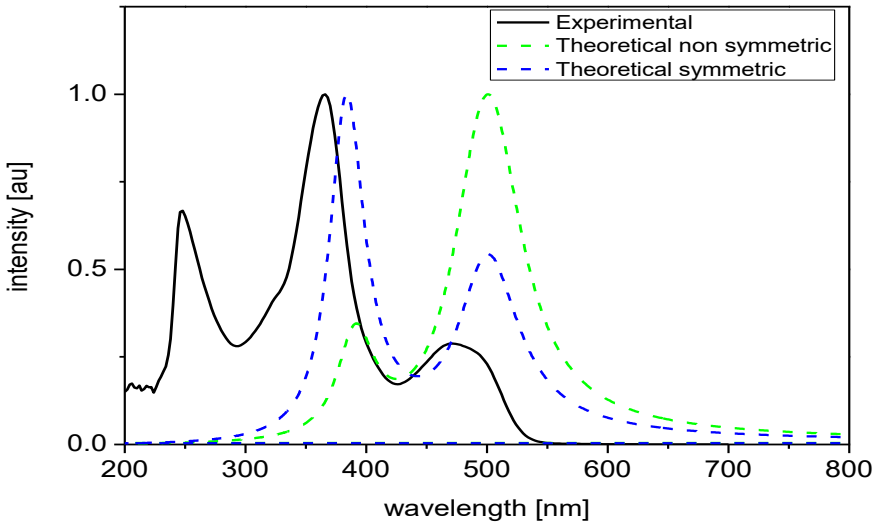

Figure S16. Computed and experimental UV-Vis spectra of compound **3**.

Table S2. Calculated values of solvation energies for different sumanene receptors using NWChem software (vs 6.8) within COSMO model, for symmetrical diastereoisomers (except compound **6**). The value of dielectric constant of o-NPOE in the PVC matrix ($\varepsilon_{NPOE/PVC}$= 14) was used for calculations (E. Bakker, P. Bühlmann, E. Pretsch, *Chem. Rev.* **1997**, *97*, 3083–3132)

Compound	Solvation energy [kJ/mol]	Solubility	Structure
1 (sumanene)	24.2	insoluble	unmodified
8 (2-nitrosumanene)	36.6	poorly soluble	mono-substituted
9 (2-iodosumanene)	26.7	soluble	
2 (tris(phenyl)methidene) sumanene)	51.6	soluble	tris-substituted
3 (tris(4-metoxyphenyl) methidene)sumanene)	75.7	soluble	
6 (tris(4-*tert*-butylphenyl) methidene)-sumanene)	56.9	soluble	

Table S3. Atomic coordinates for optimised structure of compound 3 (B3LYP/ 6-311++G(d,p))

	x	*y*	*z*		*x*	*y*	*z*		*x*	*y*	*z*
C	-0.5926	1.2780	-1.4017	C	7.7675	-2.0899	0.7523	H	0.8549	6.4172	1.7964
C	0.8308	1.1315	-1.3972	H	7.5411	-3.6089	2.2470	C	-2.0736	7.7707	0.7531
C	-1.6639	-2.0800	-0.7810	C	7.1298	-1.3473	-0.2474	H	-0.6450	8.3326	2.2486
C	0.5654	-1.2854	-1.3962	O	9.0867	-1.9833	1.0737	C	-2.3977	6.8482	-0.2476
C	-1.3950	0.1529	-1.3974	C	5.7715	-1.5338	-0.4896	O	-2.8258	8.8592	1.0759
C	1.4040	-0.1259	-1.4007	H	7.6793	-0.6365	-0.8500	C	-1.5568	5.7655	-0.4910
C	1.4218	2.2247	-0.7539	C	9.8912	-1.0525	0.3601	H	-3.2880	6.9692	-0.8501
C	-0.9690	2.4810	-0.7825	H	10.8895	-1.1356	0.7863	C	-4.0346	9.0906	0.3629
C	-0.8101	-1.1530	-1.4008	H	9.5257	-0.0281	0.4889	H	-4.4620	9.9960	0.7902
C	-2.6373	0.1187	-0.7544	C	-0.3809	5.5653	0.2457	H	-4.7384	8.2614	0.4911
C	2.6336	-0.4013	-0.7805	H	1.5786	4.6853	0.2609	C	-4.6297	-3.1123	0.2456
C	1.2161	-2.3435	-0.7521	C	-0.0611	6.5282	1.2252	H	-4.8476	-0.9753	0.2596
H	3.2352	2.7918	0.2977	H	-1.8094	5.0790	-1.2890	C	-5.6251	-3.3163	1.2236
H	-4.0354	1.4064	0.2958	C	-0.8915	7.6033	1.4865	H	-3.4918	-4.1070	-1.2867
C	0.3189	3.2212	-0.4888	C	5.0107	-2.4525	0.2471	C	-6.1416	-4.5729	1.4844
C	2.7122	2.0095	-0.2432	H	3.2689	-3.7098	0.2629	H	-5.9879	-2.4673	1.7938
C	-2.2772	2.5057	-0.2595	C	5.6855	-3.2116	1.2256	C	-5.6944	-5.6806	0.7523
H	9.9312	-1.2952	-0.7071	H	5.3025	-0.9713	-1.2869	H	-6.8978	-4.7236	2.2454
C	0.5449	4.4617	0.0036	C	7.0320	-3.0302	1.4857	C	-4.7318	-5.5006	-0.2468
H	4.2482	0.6041	0.2694	H	5.1319	-3.9497	1.7968	O	-6.2620	-6.8760	1.0745
H	-1.6014	-3.9806	0.2697	C	-2.9491	-1.3346	-0.4883	C	-4.2140	-4.2312	-0.4899
C	2.6306	-1.8867	-0.4865	C	-4.1367	-1.7588	0.0033	H	-4.3906	-6.3324	-0.8484
C	0.3842	-3.3533	-0.2417	C	-1.0313	-3.2247	-0.2567	C	-5.8576	-8.0389	0.3624
C	3.3086	0.7194	-0.2572	C	-3.0963	1.3442	-0.2448	H	-6.4292	-8.8614	0.7889
H	0.7998	-4.1972	0.2998	H	-2.6471	3.3775	0.2665	H	-4.7879	-8.2344	0.4922
C	3.5919	-2.7026	0.0056	H	-3.8448	9.2479	-0.7041	H	-6.0870	-7.9532	-0.7051

Table S4. Atomic coordinates for optimised structure of compound 1 (PSPW/Vosko)

	x	*y*	*z*
C	2.309534	-1.250662	0.043861
C	1.261298	-0.591078	0.654935
C	1.150589	0.777242	0.654313
C	2.081820	1.594236	0.043376
C	-0.120446	1.382960	0.655284
C	-0.071382	2.619607	0.043016
C	-1.249535	0.607229	0.656879
C	-2.418587	1.006281	0.043026
C	-1.137455	-0.798016	0.657504
C	-2.234996	-1.371277	0.046218
C	0.099951	-1.387474	0.656778
C	0.341177	-2.599232	0.041941
H	4.176231	-0.877458	-0.962162
H	-2.849830	-3.178570	-0.951750
C	1.394713	2.928517	-0.209735
C	-1.276130	3.103716	-0.437446
C	3.209994	0.959694	-0.445639
H	1.766597	3.715565	0.457509
H	1.561745	3.284119	-1.229400
H	-0.676161	-4.211674	-0.953109
H	-1.332509	4.063351	-0.940841
C	-2.436333	2.303917	-0.439622
C	-3.230196	-0.252328	-0.213378
C	-2.049298	-2.654661	-0.440776
H	-4.114038	-0.319094	0.438310
H	-3.612250	-0.287140	-1.237079
H	2.068320	-3.009157	-1.221750
H	-3.311881	2.689926	-0.950808
C	1.840071	-2.676867	-0.206240
C	3.326666	-0.445956	-0.443098
H	3.978346	1.522166	-0.965501
C	-0.775786	-3.258633	-0.443330
H	2.330113	-3.389834	0.468826

Table S5. Atomic coordinates for optimised structure of 1:1 complex of compound 1 and caesium ion at concave site (PSPW/Vosko)

	x	*y*	*z*
C	2.614815	0.110480	0.600407
C	1.399467	0.170253	1.263368
C	0.618862	1.298606	1.260178
C	0.999978	2.455799	0.598128
C	-0.791725	1.183284	1.268161
C	-1.363193	2.264388	0.615303
C	-1.374289	-0.060640	1.277009
C	-2.573457	-0.320177	0.632715
C	-0.572023	-1.224929	1.294093
C	-1.228774	-2.280735	0.681712
C	0.798404	-1.108543	1.287042
C	1.612744	-2.043731	0.667420
H	3.976409	1.312546	-0.551920
H	-0.861844	-4.146284	-0.324752
C	-0.257498	3.274526	0.375501
C	-2.613737	2.051674	0.061294
C	2.256746	2.448792	0.019929
H	-0.321226	4.117786	1.079377
H	-0.304957	3.717309	-0.623389
H	1.548841	-3.944354	-0.336059
H	-3.117797	2.836005	-0.493049
C	-3.210554	0.772944	0.070623
C	-2.657960	-1.825976	0.440163
C	-0.425248	-3.293998	0.186547
H	-3.341002	-2.280341	1.170521
H	-3.040404	-2.115616	-0.542226
H	3.342749	-1.577216	-0.589186
H	-4.141459	0.647540	-0.473279
C	2.943011	-1.358144	0.404811
C	3.054414	1.285998	0.019699
H	2.605135	3.301024	-0.553812
C	0.982490	-3.175686	0.179608
H	3.709144	-1.691443	1.116386
Cs	-0.022112	-0.038882	-1.928198

Table S6. Atomic coordinates for optimised structure of 1:1 complex of compound 1 and caesium ion at convex site (PSPW/Vosko)

	x	*y*	*z*
C	-1.365026	-0.113491	0.360801
C	-0.409523	-1.027276	0.859490
C	0.651741	2.681192	-0.410317
C	1.356046	0.424425	0.086214
C	-0.951207	1.043667	-0.254741
C	0.933368	-0.762542	0.725548
C	-0.918760	-1.715042	1.943259
C	-2.533237	-0.180305	1.097319
C	0.427788	1.315120	-0.397127
C	-1.676526	2.218354	-0.184006
C	1.868294	-1.164098	1.665174
C	2.578035	0.832809	0.587043
H	-0.305365	-2.804279	3.690042
H	-0.896749	3.825534	-1.440736
C	-2.386803	-1.347177	2.056431
C	0.015210	-2.255812	2.809921
C	-3.343573	0.941694	1.053304
H	-2.647351	-1.051953	3.076726
H	-3.050845	-2.185324	1.809516
H	2.174966	4.143451	0.002975
H	2.053685	-2.324073	3.465057
C	1.391226	-1.977209	2.678871
C	3.085427	-0.272998	1.489837
C	2.878290	2.173835	0.438461
H	3.440188	0.117814	2.447145
H	3.935895	-0.812015	1.050193
H	-3.536074	3.010303	0.543936
H	-4.259959	0.985939	1.632339
C	-0.706874	3.354071	-0.467513
C	-2.920276	2.126396	0.419530
C	1.923066	3.089678	-0.045820
H	-0.790667	4.149011	0.278347
H	3.808001	2.577862	0.825187
Cs	0.014250	-1.358608	-2.618306

Table S7. Atomic coordinates for optimised structure of 2:1 complex of compound 1 and caesium ion (PSPW/Vosko)

	x	*y*	*z*
C	1.183971	-3.613753	-0.272161
C	1.045212	-3.422220	1.079549
C	-0.233247	-3.191770	1.630895
C	-1.335947	-3.153521	0.814431
C	-1.195871	-3.347920	-0.577880
C	0.047321	-3.578217	-1.110574
C	2.021123	-2.811208	1.847386
C	-0.135304	-2.420031	2.776239
C	1.340684	-2.333193	3.121107
H	1.648801	-1.325211	3.411624
H	1.589033	-2.981913	3.971787
C	-2.419032	-2.331708	1.079751
C	-2.174248	-2.648664	-1.263492
C	-3.165858	-2.142435	-0.230011
H	-4.100314	-2.724551	-0.249737
H	-3.458740	-1.101207	-0.406662
C	2.310769	-3.206034	-0.965531
C	0.398528	-3.140967	-2.376669
C	1.915232	-3.108112	-2.427921
H	2.299216	-2.203076	-2.907970
H	2.317998	-3.948153	-3.009227
C	3.207137	-2.519656	1.195520
C	3.351540	-2.714951	-0.195955
H	4.257511	-2.343847	-0.665730
H	4.016982	-2.020577	1.717555
C	-1.263932	-1.702391	3.132423
C	-2.393959	-1.658628	2.290021
H	-3.196845	-0.979774	2.561003
H	-1.261410	-1.054026	4.002926
C	-0.612853	-2.565841	-3.129993
C	-1.885586	-2.316881	-2.575369
H	-2.590947	-1.747452	-3.172636
H	-0.415945	-2.184548	-4.127929
C	1.247850	3.485526	0.210309
C	1.078600	3.278002	-1.136452
C	-0.221163	3.164251	-1.678086
C	-1.314069	3.256240	-0.854439
C	-1.140872	3.475487	0.528923
C	0.121250	3.592126	1.054907
C	1.979623	2.544231	-1.889932
C	-0.209832	2.348162	-2.797165
C	1.249035	2.108694	-3.148820
H	1.455659	1.070667	-3.423035
H	1.552123	2.717063	-4.012093
C	-2.481726	2.549391	-1.091194
C	-2.186374	2.912333	1.240513
C	-3.231624	2.484074	0.225798
H	-4.107225	3.150362	0.228878
H	-3.624629	1.481784	0.431536
C	2.325592	2.967804	0.906687
C	0.428499	3.154280	2.331765
C	1.931222	2.951039	2.373679
H	2.214069	2.022137	2.877969
H	2.430911	3.755714	2.929380
C	3.298595	2.336822	0.150500

C	3.129848	2.130628	-1.236609
H	3.871407	1.528420	-1.750932
H	4.157182	1.876337	0.628956
C	-1.408640	1.736065	-3.123210
C	-2.535537	1.842363	-2.280988
H	-1.475469	1.057315	-3.967794
H	-3.407277	1.246011	-2.532343
C	-0.633413	2.716593	3.106055
C	-1.926982	2.586578	2.560418
H	-2.689284	2.118537	3.175118
H	-0.474301	2.344806	4.113942
Cs	0.010587	0.073294	0.122652

Table S8. Atomic coordinates for optimised structure compound 2 (PSPW/Vosko)

	x	y	z
C	2.465451	-0.847123	-0.904901
C	1.269976	-0.483146	-1.514476
C	0.176946	-1.302493	-1.521498
C	0.184233	-2.550972	-0.924572
C	-1.122216	-0.756433	-1.466596
C	-1.990487	-1.633490	-0.826039
C	-1.289740	0.599566	-1.429309
C	-2.329496	1.191190	-0.726258
C	-0.167411	1.452947	-1.438249
C	-0.455086	2.630808	-0.761255
C	1.091114	0.912606	-1.465182
C	2.159778	1.492538	-0.799404
H	3.410083	-2.511865	0.087078
H	0.501870	4.218890	0.338897
C	-1.222589	-2.882769	-0.617004
C	-3.127284	-1.062833	-0.259119
C	1.403003	-2.987563	-0.430917
C	-1.463766	5.539758	-0.415327
C	-1.641177	-4.076824	-0.191291
H	2.698891	3.244215	0.331457
H	-3.836198	-1.678279	0.284034
C	-3.290589	0.330663	-0.210537
C	-1.900192	2.567363	-0.419130
C	0.642021	3.302564	-0.222361
C	5.495224	-1.491044	-0.493681
C	-2.669865	3.488298	0.189475
C	4.312187	0.587973	0.100090
H	-4.116380	0.717966	0.377713
C	3.142511	0.420456	-0.542925
C	2.526513	-2.153138	-0.426041
H	1.474565	-3.932912	0.097454
C	1.923019	2.739861	-0.235208
C	5.263807	-0.446927	0.393422
H	4.539261	1.582936	0.478809
C	5.959772	-0.442684	1.594088
H	6.502028	-3.328443	-0.879393
H	4.986174	-1.483329	-1.449978
C	6.798062	-1.483047	1.922832
H	5.809275	0.375135	2.289723
C	6.986066	-2.531841	1.048180
H	7.311236	-1.478996	2.876260
C	6.343509	-2.522381	-0.173342
H	7.643473	-3.350858	1.312113
C	-2.299002	4.847142	0.450804
H	-3.652788	3.171767	0.534683
C	-2.754383	5.496334	1.591056
H	-0.394712	7.338659	-0.804166
H	-1.142171	5.057897	-1.330309
C	-2.330061	6.769024	1.893785
H	-3.426050	4.972476	2.262044
C	-1.467057	7.427243	1.044926
H	-2.671888	7.252056	2.800397
C	-1.049638	6.813774	-0.119272
H	-1.128103	8.428065	1.281074
C	-2.989710	-4.404153	0.223473
H	-0.903085	-4.876716	-0.138543

C	-3.836125	-5.123524	-0.600967
H	-5.032183	-4.072212	2.891222
H	-2.770517	-3.460703	2.125145
C	-5.103378	-5.456708	-0.178380
H	-3.494795	-5.415349	-1.586475
C	-5.533650	-5.083109	1.076332
H	-5.764829	-6.009435	-0.833640
C	-4.696183	-4.369316	1.905046
H	-6.529104	-5.346840	1.411500
C	-3.433202	-4.025490	1.479688

Table S9. Atomic coordinates for optimised structure of complex of compound 2 and caesium ion at concave site (PSPW/Vosko)

	x	*y*	*z*
C	2.407530	-0.906272	-0.859741
C	1.232353	-0.537640	-1.498181
C	0.113248	-1.328705	-1.495979
C	0.062809	-2.546310	-0.832122
C	-1.170589	-0.747852	-1.510187
C	-2.090608	-1.585443	-0.886381
C	-1.292423	0.615981	-1.508911
C	-2.337254	1.266198	-0.869923
C	-0.148176	1.439169	-1.511436
C	-0.426258	2.656928	-0.902562
C	1.095917	0.865996	-1.492531
C	2.172579	1.445513	-0.832810
H	3.301372	-2.564508	0.192048
H	0.566828	4.295285	0.096937
C	-1.359471	-2.835306	-0.568736
C	-3.225703	-0.949784	-0.379887
C	1.270030	-2.993992	-0.299990
C	-1.429619	5.644435	-0.808602
C	-1.794590	-3.986706	-0.014096
H	2.739072	3.265636	0.179170
H	-3.994172	-1.526295	0.123725
C	-3.347066	0.446456	-0.370439
C	-1.883717	2.646244	-0.620986
C	0.683671	3.332237	-0.387600
C	5.460077	-1.562408	-0.811649
C	-2.669551	3.622591	-0.129191
C	4.349650	0.467217	0.013970
H	-4.198111	0.870930	0.151924
C	3.131109	0.350281	-0.550540
C	2.419708	-2.194703	-0.320108
H	1.323417	-3.932613	0.242788
C	1.952598	2.734087	-0.347132
C	5.306057	-0.591262	0.171529
H	4.652132	1.450369	0.371827
C	6.140847	-0.632621	1.281569
H	6.515075	-3.297411	-1.451525
H	4.852986	-1.508205	-1.707233
C	7.054236	-1.648971	1.436238
H	6.058754	0.140223	2.037628
C	7.186470	-2.610723	0.457455
H	7.689366	-1.678307	2.312383
C	6.390325	-2.560375	-0.667954
H	7.924167	-3.396348	0.563791
C	-2.324205	4.998755	0.038463
H	-3.674309	3.338697	0.181775
C	-2.906912	5.720293	1.072609
H	-0.399217	7.452969	-1.266978
H	-1.014718	5.100990	-1.648946
C	-2.548109	7.026073	1.297060
H	-3.626396	5.232064	1.720804
C	-1.639763	7.645515	0.465362
H	-2.982820	7.571658	2.124805
C	-1.090575	6.957475	-0.597526
H	-1.363783	8.677116	0.642376
C	-3.138641	-4.414521	0.215870
H	-1.022823	-4.689461	0.300870

C	-4.202221	-3.996767	-0.578288
H	-4.846492	-6.442823	2.311454
H	-2.558048	-5.677852	1.842497
C	-5.476374	-4.441780	-0.328026
H	-4.006505	-3.342477	-1.419307
C	-5.712472	-5.308887	0.719588
H	-6.292997	-4.125875	-0.964192
C	-4.665247	-5.746653	1.502384
H	-6.716114	-5.663417	0.915049
C	-3.387544	-5.316919	1.243623
Cs	-0.039783	0.043930	1.642496

Table S10. Atomic coordinates for optimised structure of complex of compound 2 and caesium ion at convex site (PSPW/Vosko)

	x	y	z
C	2.067278	-1.549794	-0.123569
C	1.061849	-0.889264	-0.821453
C	-0.226942	-1.358290	-0.880892
C	-0.635495	-2.506271	-0.215751
C	-1.312350	-0.462182	-0.981957
C	-2.458734	-1.023551	-0.422420
C	-1.072774	0.888881	-0.973684
C	-1.945296	1.788983	-0.381915
C	0.246603	1.381780	-0.874178
C	0.258325	2.612752	-0.224692
C	1.297786	0.503204	-0.809619
C	2.450561	0.775515	-0.083371
H	2.412281	-3.353191	1.003351
H	1.559159	3.881810	0.935223
C	-2.094312	-2.398071	-0.023118
C	-3.420237	-0.105930	0.003822
C	0.380865	-3.243330	0.382238
C	0.031503	5.773807	0.429973
C	-2.823741	-3.361024	0.580254
H	3.389646	2.340245	1.060076
H	-4.336595	-0.452912	0.467421
C	-3.169162	1.268943	0.024748
C	-1.157258	2.970403	0.001852
C	1.469689	2.955404	0.380326
C	4.815296	-3.021074	0.437610
C	-1.704117	4.029595	0.633192
C	4.235300	-0.664801	0.900736
H	-3.902902	1.900446	0.514465
C	3.069667	-0.523078	0.238297
C	1.700568	-2.782538	0.418181
H	0.149204	-4.135311	0.955157
C	2.540825	2.058346	0.446194
C	4.907116	-1.884335	1.232902
H	4.710080	0.249030	1.255279
C	5.705572	-1.939493	2.369426
H	5.366153	-5.061961	0.166550
H	4.248166	-2.973584	-0.484080
C	6.321114	-3.112195	2.741534
H	5.813397	-1.051234	2.982011
C	6.184661	-4.240972	1.962155
H	6.915505	-3.146147	3.645453
C	5.444340	-4.187147	0.800059
H	6.672582	-5.162810	2.252294
C	-1.092106	5.246784	1.055431
H	-2.762692	3.939652	0.875243
C	-1.665947	5.956760	2.104673
H	1.449255	7.364101	0.357863
H	0.447092	5.258686	-0.427218
C	-1.103181	7.129732	2.546648
H	-2.559293	5.565109	2.578960
C	0.022345	7.629569	1.927856
H	-1.551022	7.664292	3.374618
C	0.582698	6.955200	0.861368
H	0.457838	8.559391	2.270451
C	-4.233699	-3.444544	0.795822
H	-2.257841	-4.208846	0.965111

C	-5.171325	-2.788536	0.002496
H	-6.384409	-5.112545	2.810474
H	-3.978379	-4.835517	2.398072
C	-6.517168	-2.962257	0.219467
H	-4.830518	-2.177235	-0.824283
C	-6.959131	-3.785850	1.236948
H	-7.233633	-2.465808	-0.423086
C	-6.043746	-4.450394	2.024877
H	-8.020218	-3.925081	1.399090
C	-4.698256	-4.292250	1.795918
Cs	0.221468	-0.020762	-4.049968

Table S11. Atomic coordinates for optimised structure of 2:1 complex of compound 2 and caesium ion (PSPW/Vosko)

	x	*y*	*z*
C	1.658494	-2.402874	-2.155860
C	1.127147	-1.403304	-2.966882
C	-0.216850	-1.263257	-3.188787
C	-1.153031	-2.088500	-2.579721
C	-0.773927	0.016932	-3.399537
C	-2.091577	0.046209	-2.946921
C	0.038872	1.122456	-3.375908
C	-0.385810	2.349285	-2.879102
C	1.426648	0.987651	-3.146919
C	1.928347	2.124577	-2.519293
C	1.949422	-0.257265	-2.929302
C	3.003788	-0.476177	-2.051779
H	1.058342	-4.140839	-1.018687
H	3.488387	2.764291	-1.176531
C	-2.425835	-1.340495	-2.550617
C	-2.565062	1.306368	-2.573807
C	-0.639881	-3.177068	-1.880240
C	3.163854	5.122754	-2.342532
C	-3.586024	-1.873697	-2.111647
H	4.399500	0.564505	-0.781507
H	-3.568350	1.417080	-2.177292
C	-1.731416	2.432435	-2.541933
C	0.823900	3.104317	-2.489030
C	3.066834	1.932909	-1.734570
C	3.596963	-4.859527	-1.739273
C	0.806672	4.391353	-2.085784
C	3.990202	-2.529984	-1.060312
H	-2.137114	3.344756	-2.115926
C	2.973785	-1.904978	-1.692639
C	0.737663	-3.338296	-1.677811
H	-1.302619	-3.857543	-1.353591
C	3.594367	0.656168	-1.504854
C	4.220224	-3.931618	-0.910638
H	4.793876	-1.889219	-0.696752
C	5.192798	-4.387424	-0.026074
H	3.464849	-6.886523	-2.365940
H	2.882656	-4.514911	-2.476182
C	5.521927	-5.719240	0.031858
H	5.709471	-3.671317	0.604348
C	4.898634	-6.620728	-0.802557
H	6.288384	-6.056361	0.718094
C	3.936578	-6.185075	-1.689130
H	5.179212	-7.666435	-0.777045
C	1.888072	5.283385	-1.810789
H	-0.180619	4.842261	-1.988017
C	1.621791	6.429405	-1.068059
H	5.096792	5.973807	-2.606605
H	3.380653	4.257322	-2.956734
C	2.582754	7.387557	-0.866188
H	0.625034	6.569215	-0.663018
C	3.831751	7.226212	-1.426396
H	2.355709	8.271260	-0.283578
C	4.118136	6.092557	-2.157594
H	4.588189	7.990321	-1.294233
C	-4.900853	-1.319099	-2.115729
H	-3.519450	-2.887169	-1.716093

C	-5.284167	-0.280649	-2.959805
H	-7.902849	-1.897792	-0.654007
H	-5.588573	-2.733973	-0.666855
C	-6.579352	0.171745	-2.964990
H	-4.562956	0.134185	-3.652662
C	-7.521287	-0.401988	-2.133516
H	-6.868156	0.964661	-3.643759
C	-7.164934	-1.440858	-1.300241
H	-8.543749	-0.045682	-2.148816
C	-5.870940	-1.898441	-1.300078
Cs	-0.170904	0.175166	-0.050340
C	0.723162	2.341199	2.648715
C	0.026346	1.271456	3.202088
C	-1.334596	1.152819	3.109863
C	-2.116629	2.079851	2.431626
C	-1.936719	-0.119733	3.030285
C	-3.136830	-0.044915	2.329430
C	-1.151402	-1.239288	3.036548
C	-1.480475	-2.374272	2.311160
C	0.249977	-1.128802	3.142556
C	0.861533	-2.216736	2.523753
C	0.829290	0.111593	3.201797
C	2.053972	0.391568	2.605583
H	0.400301	4.221104	1.641312
H	2.699635	-2.766368	1.532777
C	-3.372832	1.392138	2.072090
C	-3.547949	-1.227278	1.709714
C	-1.457733	3.223999	1.993400
C	1.949754	-5.283278	2.499738
C	-4.444774	2.004913	1.533331
H	3.688703	-0.580872	1.582849
H	-4.451598	-1.245669	1.106622
C	-2.730427	-2.364764	1.697443
C	-0.231887	-3.142063	2.136695
C	2.158533	-1.985809	2.061799
C	2.782242	4.823454	2.718845
C	-0.217045	-4.411675	1.681881
C	3.184852	2.508862	1.939681
H	-3.046125	-3.202123	1.081344
C	2.095287	1.851352	2.386105
C	-0.065645	3.358363	2.106693
H	-1.991481	3.991362	1.442189
C	2.739564	-0.707720	2.095867
C	3.440174	3.912486	1.896067
H	4.023715	1.883527	1.632475
C	4.485400	4.375309	1.101836
H	2.676091	6.829702	3.418571
H	2.003014	4.471370	3.384092
C	4.863850	5.693691	1.121948
H	5.024508	3.665872	0.480974
C	4.210558	6.577956	1.951294
H	5.685757	6.030685	0.504040
C	3.170401	6.139571	2.746598
H	4.524522	7.613281	1.995734
C	0.842240	-5.366282	1.661808
H	-1.174518	-4.792484	1.325083
C	0.717352	-6.482200	0.838989
H	3.744930	-6.208713	3.175415
H	2.036424	-4.444945	3.180678
C	1.680012	-7.460253	0.826943

H	-0.156908	-6.571086	0.201997
C	2.769953	-7.365349	1.664581
H	1.572415	-8.315423	0.171182
C	2.899060	-6.276091	2.503075
H	3.519751	-8.146458	1.668728
C	-5.757774	1.482375	1.314799
H	-4.320248	3.056260	1.274637
C	-6.285774	0.427142	2.056227
H	-8.516650	2.229904	-0.491392
H	-6.202823	2.969672	-0.153919
C	-7.589173	0.029069	1.884549
H	-5.668405	-0.050565	2.807403
C	-8.395489	0.669573	0.965260
H	-7.988585	-0.775111	2.489725
C	-7.886829	1.714644	0.223113
H	-9.426649	0.363628	0.837376
C	-6.589697	2.125632	0.407186

Table S12. Atomic coordinates for optimised structure of two molecules of 2 (PSPW/Vosko)

	x	*y*	*z*
C	2.047100	-2.007846	-2.240498
C	1.331362	-1.100103	-3.016997
C	-0.019922	-1.197062	-3.216525
C	-0.782745	-2.190584	-2.616992
C	-0.799963	-0.032270	-3.385136
C	-2.093215	-0.249639	-2.913787
C	-0.196861	1.199753	-3.343037
C	-0.824159	2.318753	-2.807672
C	1.196691	1.309517	-3.136891
C	1.499210	2.502397	-2.485941
C	1.936824	0.173129	-2.959996
C	3.029242	0.125081	-2.103275
H	1.787192	-3.851789	-1.142232
H	2.944667	3.378085	-1.148110
C	-2.167710	-1.682835	-2.550285
C	-2.776735	0.896393	-2.500490
C	-0.071098	-3.186445	-1.954123
C	2.183755	5.667916	-2.245794
C	-3.206074	-2.425027	-2.109845
H	4.240254	1.367562	-0.824873
H	-3.776248	0.816613	-2.087361
C	-2.156632	2.152148	-2.449885
C	0.238609	3.268128	-2.414174
C	2.667832	2.498393	-1.722406
C	4.399592	-4.088069	-1.916758
C	-0.000270	4.521359	-1.976323
C	4.383844	-1.742693	-1.180986
H	-2.710512	2.966874	-1.993991
C	3.260900	-1.294295	-1.782243
C	1.316608	-3.103863	-1.775093
H	-0.592207	-3.986759	-1.436851
C	3.418540	1.331262	-1.534337
C	4.862638	-3.083889	-1.072177
H	5.067017	-0.977595	-0.811462
C	5.916927	-3.379730	-0.213651
H	4.619292	-6.090467	-2.595736
H	3.621914	-3.859010	-2.634239
C	6.479101	-4.632353	-0.196034
H	6.309211	-2.598173	0.428590
C	6.011210	-5.610411	-1.045683
H	7.305820	-4.843512	0.470280
C	4.970823	-5.332467	-1.906902
H	6.474044	-6.589503	-1.052121
C	0.909741	5.585333	-1.692404
H	-1.050143	4.786220	-1.852893
C	0.457193	6.647244	-0.915578
H	3.928944	6.856575	-2.513530
H	2.539984	4.870084	-2.885936
C	1.235591	7.756498	-0.701316
H	-0.540924	6.597048	-0.493236
C	2.482859	7.834278	-1.282808
H	0.865447	8.571230	-0.092120
C	2.953195	6.787843	-2.048052
H	3.093337	8.717808	-1.140614
C	-4.598532	-2.114230	-2.080923
H	-2.952737	-3.419497	-1.742596
C	-5.176165	-1.141014	-2.891455

H	-7.422046	-3.254606	-0.594043
H	-4.996443	-3.663477	-0.661217
C	-6.531106	-0.927213	-2.866649
H	-4.553246	-0.587568	-3.582797
C	-7.340324	-1.679697	-2.037979
H	-6.968976	-0.182593	-3.519844
C	-6.789339	-2.657882	-1.237882
H	-8.410017	-1.511462	-2.029620
C	-5.434737	-2.876880	-1.267831
C	0.369731	2.376426	2.702133
C	-0.115054	1.186490	3.236136
C	-1.434537	0.828949	3.159518
C	-2.381546	1.617389	2.517251
C	-1.801636	-0.528402	3.054109
C	-3.008526	-0.652351	2.372116
C	-0.829420	-1.489529	3.019495
C	-0.964245	-2.647327	2.268501
C	0.531552	-1.133114	3.109113
C	1.315715	-2.079195	2.452960
C	0.881566	0.189020	3.193646
C	2.025615	0.697416	2.588347
H	-0.301356	4.192033	1.750104
H	3.203842	-2.267817	1.422357
C	-3.501489	0.725196	2.156723
C	-3.213689	-1.873937	1.726604
C	-1.945213	2.870981	2.100862
C	2.932298	-4.900617	2.331640
C	-4.675164	1.149406	1.649428
H	3.788416	0.057347	1.517451
H	-4.110510	-2.038965	1.135743
C	-2.206934	-2.846505	1.672539
C	0.397755	-3.175381	2.056302
C	2.542115	-1.609345	1.979547
C	1.954501	5.184108	2.810501
C	0.630235	-4.410664	1.567407
C	2.748724	2.997973	1.964008
H	-2.379627	-3.711780	1.038591
C	1.802128	2.145941	2.407588
C	-0.597503	3.249050	2.198532
H	-2.617171	3.543665	1.577856
C	2.886641	-0.249225	2.039906
C	2.749016	4.425265	1.954578
H	3.679808	2.540049	1.628597
C	3.680299	5.086210	1.158733
H	1.505427	7.121795	3.565230
H	1.262816	4.682685	3.476728
C	3.818085	6.450119	1.209015
H	4.325707	4.499541	0.511681
C	3.033014	7.183367	2.070722
H	4.555316	6.943187	0.589111
C	2.102383	6.547340	2.868226
H	3.158239	8.256753	2.138611
C	1.842113	-5.159983	1.507122
H	-0.250445	-4.947691	1.213739
C	1.902987	-6.260227	0.656441
H	4.875732	-5.506484	2.957433
H	2.880683	-4.076841	3.033582
C	3.024128	-7.050057	0.604881
H	1.047018	-6.488535	0.029397
C	4.094898	-6.782117	1.429669

H	3.058616	-7.894735	-0.072057
C	4.043213	-5.707719	2.295244
H	4.971824	-7.416631	1.402515
C	-5.877830	0.406163	1.435057
H	-4.744729	2.211980	1.417360
C	-6.195665	-0.743857	2.155093
H	-8.758418	0.692008	-0.312235
H	-6.607636	1.824817	0.013067
C	-7.410203	-1.364080	1.990764
H	-5.489381	-1.121482	2.884597
C	-8.334470	-0.856040	1.100197
H	-7.648762	-2.240927	2.579578
C	-8.033865	0.280547	0.379435
H	-9.296784	-1.338072	0.978364
C	-6.827566	0.912058	0.556587

Table S13. Atomic coordinates for optimised structure of compound 8 (PSPW/Vosko)

	x	*y*	*z*
C	-1.327471	-0.395501	0.960029
C	-0.260119	0.522554	1.107964
C	0.404144	-3.196433	-0.287335
C	1.331120	-1.263743	0.808408
C	-1.047341	-1.707768	0.676397
C	1.043702	0.095387	1.027131
C	-0.661412	1.753603	0.623500
C	-2.438680	0.236088	0.429869
C	0.291927	-2.143519	0.600889
C	-1.846541	-2.464172	-0.165652
C	2.058259	0.887729	0.494519
C	2.548210	-1.396205	0.157767
H	-4.171685	-0.080554	-0.781558
H	-1.074073	-3.658333	-1.790877
C	-2.137599	1.705810	0.367577
C	0.346054	2.556019	0.123197
C	-3.323950	-0.543753	-0.286533
H	-2.362847	2.148092	-0.606891
H	-2.685230	2.333696	1.081918
H	1.781698	-4.198329	-1.578007
H	-3.671226	-2.391307	-1.296477
C	1.701952	2.141411	0.070566
C	3.205269	-0.031519	0.140572
C	2.720734	-2.528711	-0.613139
H	3.633706	0.203186	-0.837114
H	4.033307	0.039292	0.860148
H	2.383792	2.787876	-0.468422
H	3.631482	-2.676069	-1.183584
C	-3.025405	-1.882067	-0.590370
C	-0.996500	-3.584261	-0.702507
C	1.654014	-3.414412	-0.841341
H	-1.292907	-4.577572	-0.343923
N	-0.024860	3.668795	-0.673457
O	0.889085	4.274074	-1.294558
O	-1.247751	4.004507	-0.818392

Table S14. Atomic coordinates for optimised structure of complex compound 8 and caesium ion (PSPW/Vosko)

	x	*y*	*z*
C	-1.353938	-0.198495	0.974366
C	-0.287294	0.720329	1.107386
C	0.370076	-3.021521	-0.210841
C	1.304550	-1.072219	0.848465
C	-1.074406	-1.525621	0.761235
C	1.019464	0.286526	1.071387
C	-0.671979	1.950517	0.604062
C	-2.460597	0.415801	0.409944
C	0.268567	-1.956305	0.666560
C	-1.889302	-2.326247	-0.022241
C	2.055419	1.074427	0.583788
C	2.519043	-1.198793	0.185339
H	-4.241263	0.008275	-0.725370
H	-1.206950	-3.726756	-1.561498
C	-2.146141	1.887625	0.293873
C	0.376719	2.768203	0.206193
C	-3.366939	-0.408268	-0.235194
H	-2.355491	2.295610	-0.700424
H	-2.731414	2.525726	0.969156
H	1.724806	-3.989756	-1.556384
H	-3.761054	-2.339920	-1.074635
C	1.725444	2.348093	0.203640
C	3.194850	0.155394	0.217723
C	2.668278	-2.311903	-0.616965
H	3.655112	0.422962	-0.737081
H	4.001969	0.186541	0.962908
H	2.432142	3.026502	-0.259477
H	3.566689	-2.453842	-1.208422
C	-3.084176	-1.770125	-0.446198
C	-1.044093	-3.477136	-0.509465
C	1.601539	-3.206163	-0.821181
H	-1.279809	-4.411623	0.014676
N	0.102642	3.965297	-0.507193
O	1.077776	4.681794	-0.858967
O	-1.089965	4.227515	-0.841733
Cs	-0.062699	-0.304541	-2.357560

Table S15. Atomic coordinates for optimised structure of compound 9 (PSPW/Vosko)

	x	*y*	*z*
C	0.203774	-0.233281	1.108546
C	1.296962	-1.088259	0.868232
C	-2.485303	-2.165046	-0.078092
C	-0.232755	-2.887246	0.390016
C	-1.076892	-0.709634	0.995058
C	1.082178	-2.397278	0.520241
C	2.382664	-0.373761	0.401278
C	0.547793	1.072478	0.806333
C	-1.297522	-2.053651	0.622497
C	-2.116995	0.090435	0.557349
C	1.941792	-3.084520	-0.315831
C	-0.276187	-3.891407	-0.560132
H	-2.587046	2.121936	0.009833
H	-3.567927	-0.496626	-0.949475
C	2.027784	1.094798	0.503386
C	3.328787	-1.085674	-0.313784
C	-0.516235	1.898882	0.512901
H	2.221809	1.634528	-0.429336
H	2.601067	1.620299	1.277438
H	-3.467565	-3.367134	-1.561824
H	3.816785	-2.893502	-1.347084
C	3.110072	-2.430767	-0.666675
C	1.156944	-4.238741	-0.906836
C	-1.493862	-4.093229	-1.181845
H	1.306870	-4.324801	-1.986113
H	1.457136	-5.204241	-0.479502
H	-1.597160	-4.831698	-1.969695
H	4.191025	-0.587222	-0.742098
C	-1.838220	1.434289	0.384835
C	-3.195099	-0.831261	0.021487
C	-2.586297	-3.238447	-0.942523
H	-4.067979	-0.877360	0.685364
I	-0.116688	3.892442	-0.045227

Table S15. Atomic coordinates for optimised structure of complex of compound 9 and caesium ion (PSPW/Vosko)

	x	*y*	*z*
C	0.168205	0.022373	1.388844
C	1.265011	-0.846608	1.186286
C	-2.517784	-1.926095	0.191114
C	-0.273852	-2.641983	0.714995
C	-1.114084	-0.444026	1.247252
C	1.045317	-2.159077	0.852682
C	2.353523	-0.142256	0.697867
C	0.524841	1.315815	1.035291
C	-1.337250	-1.795824	0.905164
C	-2.137790	0.346204	0.741265
C	1.900021	-2.867591	0.022567
C	-0.313761	-3.678924	-0.201952
H	-2.569789	2.339230	0.047011
H	-3.675513	-0.289693	-0.687351
C	2.017790	1.329590	0.811222
C	3.280368	-0.863782	-0.031376
C	-0.511530	2.132374	0.629871
H	2.290045	1.913791	-0.074369
H	2.544741	1.811339	1.645347
H	-3.505341	-3.194881	-1.235580
H	3.762614	-2.694972	-1.035009
C	3.054870	-2.215044	-0.368218
C	1.121073	-4.058583	-0.499138
C	-1.525087	-3.901036	-0.829697
H	1.302605	-4.268376	-1.555977
H	1.403536	-4.976711	0.033897
H	-1.632839	-4.687955	-1.567976
H	4.145873	-0.374339	-0.463334
C	-1.836607	1.669141	0.481397
C	-3.230055	-0.592950	0.263125
C	-2.617461	-3.030441	-0.634728
H	-4.062982	-0.625901	0.978876
I	-0.060038	4.052850	-0.097586
Cs	0.038581	-0.522354	-2.047541

Table S16. Atomic coordinates for optimised structure of 2:1 complex of compound 9 and caesium ion (PSPW/Vosko).

	x	*y*	*z*
C	2.757014	-2.108093	-0.764471
C	3.154478	-1.609708	0.496393
C	2.177661	0.867340	-2.547619
C	3.348473	0.601175	-0.451816
C	2.661811	-1.258999	-1.837949
C	3.450967	-0.276380	0.650471
C	2.582087	-2.356788	1.512753
C	1.919777	-3.200810	-0.599878
C	2.951510	0.115709	-1.676418
C	1.701708	-1.437769	-2.821059
C	3.206827	0.400353	1.835829
C	3.013063	1.874459	-0.016165
H	0.164754	-2.798404	-3.481369
H	0.474847	0.134558	-3.717929
C	1.931235	-3.567133	0.867024
C	2.464911	-1.732161	2.743178
C	1.070435	-3.459823	-1.656278
H	0.919078	-3.764163	1.238953
H	2.493138	-4.491249	1.057354
H	1.297794	2.818840	-2.778743
H	2.543190	0.093638	3.858301
C	2.773270	-0.367350	2.903510
C	3.156653	1.879401	1.494588
C	2.347261	2.678058	-0.923052
H	2.334676	2.399846	1.996634
H	4.072534	2.396796	1.808189
H	2.004746	3.671836	-0.650370
H	2.016622	-2.248205	3.585874
C	0.942726	-2.590177	-2.755923
C	1.522215	-0.102127	-3.515001
C	1.928103	2.175000	-2.172474
H	2.025674	-0.092336	-4.490823
I	-0.247072	-5.093809	-1.519773
Cs	0.041707	-0.008855	0.149282
C	-2.534031	0.138400	2.449077
C	-3.074757	-0.628624	1.390056
C	-1.854503	3.203521	0.850080
C	-3.193341	1.362682	0.034213
C	-2.331430	1.486046	2.288907
C	-3.391527	-0.025399	0.196208
C	-2.591997	-1.926505	1.447083
C	-1.685541	-0.642117	3.218749
C	-2.674274	2.107001	1.064902
C	-1.269813	2.147875	2.886266
C	-3.245478	-0.672817	-1.022753
C	-2.919110	1.658594	-1.291093
H	0.028862	-0.527938	4.509650
H	-4.110054	0.461977	-2.664214
C	-1.873498	-2.079531	2.771637
C	-2.561208	-2.626516	0.254469
C	-0.693170	0.023124	3.916808
H	-0.924310	-2.617918	2.680799
H	-2.471162	-2.650814	3.493657
H	-2.709950	-2.582119	-1.874204
H	0.379216	1.853125	4.232881
C	-1.700750	3.581105	-0.467525

C	-1.054082	3.430236	2.109682
C	-0.487487	1.408471	3.755001
H	-0.000744	3.628393	1.879901
H	-1.400875	4.315282	2.658884
H	-2.152826	-3.632286	0.207746
I	-0.478079	5.227881	-0.931917
C	-3.174330	0.398426	-2.094304
C	-2.207771	2.816788	-1.536093
C	-2.885135	-2.007389	-0.969424
H	-2.391793	0.202328	-2.833313
H	-1.931752	3.103399	-2.544812