The Anionic Recognition Mechanism based in Polyol and Boronic Acid Receptors

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Supplementary Material

Table S1. Optimized Cartesian coordinates of the compounds investigated in this study.

Complex	**1**–Cl [Computational Model = B97D3/6–31+G(d); Solvent = CD_3CN]		
Atom	X	Y	Z
C	–0.578317	–0.773567	0.707117
C	–0.433708	–0.438219	–0.785536
C	–0.000103	1.015693	–1.114410
O	0.657071	–0.762004	1.402762
O	–0.614406	2.017387	–0.325497
Cl	0.034248	1.949959	2.789702
C	–1.202945	–2.167172	0.897784
F	–2.430403	–2.261171	0.294962
F	–1.391554	–2.458259	2.217657
F	–0.429494	–3.168761	0.378867
C	1.528078	1.252850	–1.194844
F	2.150033	0.286255	–1.941712
F	2.161505	1.303114	0.006335
F	1.786623	2.448692	–1.815873
H	–1.287459	–0.073438	1.175691
H	0.259471	–1.144801	–1.260102
H	–1.413562	–0.576629	–1.261937
H	–0.332929	1.209303	–2.143795
H	0.640759	0.049533	1.975399
H	–0.333000	1.943741	0.626439
Complex	**1**–Cl [Computational Model = B97D3/Def2–TZVP; Solvent = CD_3CN]		
Atom	X	Y	Z
C	–0.581916	–0.772730	0.711829
C	–0.407393	–0.448288	–0.775287
C	–0.001087	1.010833	–1.101260

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O	0.631256	–0.756622	1.434520
O	–0.611652	1.996113	–0.300088
Cl	0.070688	1.947030	2.762241
C	–1.214537	–2.159928	0.895121
F	–2.424794	–2.250023	0.274912
F	–1.424621	–2.442432	2.205745
F	–0.438533	–3.159623	0.395648
C	1.520195	1.257644	–1.209146
F	2.117064	0.330142	–2.011203
F	2.181892	1.253200	–0.030978
F	1.756503	2.473618	–1.779716
H	–1.300200	–0.069840	1.155283
H	0.314077	–1.140076	–1.219586
H	–1.366275	–0.618142	–1.274595
H	–0.345981	1.203628	–2.124739
H	0.609301	0.073038	1.976839
H	–0.314080	1.924964	0.643470

Complex	**2**–Cl [Computational Model = B97D3/6–31+G(d); Solvent = CD_3CN]		
Atom	X	Y	Z
C	–0.601527	–0.804519	0.951456
C	–0.209936	–0.386167	–0.512855
C	0.660791	0.885002	–0.827311
O	–0.912390	0.200731	1.864667
O	1.714212	1.192688	0.031147
Cl	1.204163	2.121368	2.868369
C	0.497414	–1.764635	1.555561
F	0.632979	–2.918517	0.837879
F	0.217608	–2.114082	2.835783
F	1.711557	–1.159677	1.564972
C	–1.961963	–1.592537	0.819873
F	–2.950693	–0.741190	0.434708
F	–2.353136	–2.157124	1.987901
F	–1.901316	–2.582843	–0.112338
C	1.395965	0.570695	–2.187380
F	0.537201	0.155088	–3.158523
F	2.301097	–0.427594	–2.000202
F	2.073756	1.638421	–2.673658
C	–0.267785	2.147811	–1.019939
F	–1.007754	2.374918	0.093975

F	–1.144009	1.997367	–2.056392
F	0.450116	3.274015	–1.256329
H	0.297853	–1.250607	–0.950896
H	–1.136748	–0.268676	–1.082310
H	–0.123200	0.753759	2.146573
H	1.421586	1.518806	0.934699

Complex	**2**–Cl [Computational Model = B97D3/Def2–TZVP; Solvent = CD_3CN]		
Atom	X	Y	Z
C	–0.597252	–0.802022	0.953858
C	–0.207466	–0.380524	–0.505366
C	0.659638	0.886980	–0.822760
O	–0.901302	0.195340	1.870082
O	1.706788	1.200989	0.032628
Cl	1.195552	2.111778	2.849341
C	0.499357	–1.766945	1.549656
F	0.634399	–2.908400	0.825895
F	0.217501	–2.125188	2.819813
F	1.707509	–1.166373	1.567572
C	–1.957919	–1.585724	0.816542
F	–2.937035	–0.734052	0.431396
F	–2.351714	–2.145146	1.977965
F	–1.899707	–2.570915	–0.110691
C	1.393074	0.565804	–2.180421
F	0.540527	0.149178	–3.146471
F	2.292510	–0.427345	–1.987978
F	2.069252	1.625835	–2.666265
C	–0.271915	2.144396	–1.021320
F	–1.009339	2.374218	0.084943
F	–1.141973	1.987721	–2.052471
F	0.440619	3.265135	–1.260843
H	0.298082	–1.241339	–0.943922
H	–1.132290	–0.263702	–1.071099
H	–0.116062	0.752616	2.143786
H	1.415006	1.520185	0.935560

Complex	**3**–Cl [Computational Model = B97D3/6–31+G(d); Solvent = CD_3CN]		
Atom	X	Y	Z
C	–0.932869	–1.604767	0.116403
C	–0.056142	–0.390175	–0.297045

C	0.179757	0.558350	0.888282
C	1.075715	1.795539	0.589729
O	1.253100	–0.848739	–0.714332
O	2.284517	1.473899	–0.055810
C	–2.289628	–1.751307	–0.631024
O	–2.230747	–1.510671	–2.012092
C	1.483360	2.448425	1.956570
F	2.101140	1.533102	2.752562
F	0.402230	2.916776	2.642997
F	2.350566	3.481453	1.806623
C	–3.340206	–0.726265	–0.090878
F	–3.609254	–0.919226	1.231082
F	–4.520469	–0.778559	–0.757306
F	–2.871550	0.546131	–0.222650
C	0.320808	2.844483	–0.308327
F	–0.911685	3.166478	0.177136
F	0.141069	2.343635	–1.562022
F	1.012619	4.006172	–0.450377
C	–2.803664	–3.224346	–0.412974
F	–4.038553	–3.436575	–0.936874
F	–2.854452	–3.581021	0.902489
F	–1.956985	–4.094714	–1.031367
Cl	0.438532	–2.202629	–3.352765
H	–0.344351	–2.503824	–0.099454
H	–1.117605	–1.608599	1.198220
H	–0.523112	0.135579	–1.135632
H	–0.782556	0.894582	1.287720
H	0.678050	–0.019836	1.676660
H	1.143498	–1.263529	–1.616632
H	2.138202	0.579382	–0.478021
H	–1.350246	–1.812347	–2.390834

Complex	**3**–Cl [Computational Model = B97D3/Def2–TZVP; Solvent = CD_3CN]		
Atom	X	Y	Z
C	–0.948332	–1.591405	0.134648
C	–0.038600	–0.408381	–0.278092
C	0.153614	0.576734	0.877936
C	1.029752	1.817552	0.555356
O	1.278671	–0.892712	–0.621819
O	2.141221	1.538001	–0.253705

C	–2.266451	–1.748948	–0.666273
O	–2.139093	–1.567211	–2.046285
C	1.592035	2.376166	1.908398
F	2.374951	1.442936	2.500300
F	0.608354	2.691343	2.786945
F	2.355688	3.477679	1.741444
C	–3.323433	–0.691514	–0.211852
F	–3.655762	–0.832853	1.094361
F	–4.464285	–0.750258	–0.929457
F	–2.830762	0.562431	–0.364739
C	0.188803	2.916608	–0.181957
F	–0.887490	3.321392	0.537119
F	–0.275095	2.438271	–1.361732
F	0.918195	4.016875	–0.469634
C	–2.809635	–3.204105	–0.410724
F	–4.016397	–3.418461	–0.979003
F	–2.923918	–3.503208	0.907213
F	–1.953716	–4.104630	–0.951798
Cl	0.569605	–2.335071	–3.203482
H	–0.365831	–2.501441	–0.022928
H	–1.181626	–1.553561	1.202004
H	–0.461842	0.092598	–1.149991
H	–0.818294	0.909407	1.244963
H	0.634968	0.027329	1.691898
H	1.188816	–1.358842	–1.498858
H	2.040751	0.590192	–0.542922
H	–1.245771	–1.886057	–2.367277

Complex	**4**–F [Computational Model = B97D3/6–31+G(d); Solvent = DMSO]		
Atom	X	Y	Z
C	–4.311926	1.418155	–1.985414
C	–3.395956	1.499755	–3.048923
C	–2.161188	0.840679	–2.940191
C	–1.852566	0.111448	–1.777001
C	–2.750969	0.007086	–0.692356
C	–3.986997	0.682052	–0.834209
B	–2.408671	–0.849397	0.662416
O	–1.097584	–1.541024	0.652852
O	–2.466828	0.035490	1.837870
H	–5.276796	1.926986	–2.056991

H	–3.642337	2.068979	–3.947975
H	–1.439219	0.896406	–3.759085
H	–0.881614	–0.387222	–1.710646
H	–4.716654	0.627971	–0.021615
H	–1.096920	–2.231389	–0.030907
H	–2.135543	–0.461337	2.606911
F	–3.470304	–1.915476	0.787292

Complex	**5**–H_2PO_4 [Computational Model = B97D3/6–31+G(d); Solvent = DMSO]		
Atom	X	Y	Z
C	3.010616	0.688764	0.791558
C	3.542573	–0.608691	0.693670
C	2.736809	–1.646150	0.199069
C	1.412740	–1.382605	–0.193557
C	0.851904	–0.090687	–0.102885
C	1.685918	0.934324	0.398491
B	–0.680361	0.236855	–0.508458
O	–1.342797	–1.011472	–1.030445
O	–0.790179	1.376896	–1.402220
H	3.628570	1.504255	1.174970
H	4.572033	–0.807008	0.999420
H	3.139349	–2.658740	0.117986
H	0.801187	–2.201148	–0.577732
H	1.285115	1.947006	0.487992
H	–2.167010	–0.774866	–1.490502
H	–1.692114	1.741160	–1.372918
P	–1.783897	–0.312128	2.015524
O	–1.494654	0.656015	0.801023
O	–1.929674	–1.799241	1.378206
O	–3.295908	0.095844	2.527652
O	–0.885072	–0.265335	3.219222
H	–1.758664	–1.707747	0.374200
H	–3.923966	0.128227	1.780250

Complex	**6**–AcO [Computational Model = B97D3/6–31+G(d); Solvent = CD_3CN]		
Atom	X	Y	Z
C	–3.650001	2.328766	–4.449848
C	–2.572755	2.322699	–5.351507
C	–1.387412	1.648193	–5.014625
C	–1.284960	0.985462	–3.782172

C	–2.354798	0.977596	–2.857674
C	–3.537239	1.663283	–3.219774
B	–2.232932	0.232607	–1.469342
O	–3.307276	0.261431	–0.594588
O	–1.057678	–0.430514	–1.159632
O	–1.993445	–1.208686	1.242289
C	–1.522104	–0.755878	2.359770
C	–2.551206	–0.106489	3.298310
O	–0.311609	–0.809483	2.701710
H	–4.573762	2.851271	–4.706643
H	–2.656399	2.839562	–6.309483
H	–0.546946	1.640097	–5.711648
H	–0.359866	0.464292	–3.529529
H	–4.379610	1.674011	–2.525740
H	–3.065949	–0.246064	0.231567
H	–1.143026	–0.840657	–0.250822
H	–2.949429	0.806182	2.827219
H	–3.403039	–0.783976	3.458404
H	–2.108121	0.158831	4.266593

Complex	**6**–AcO [Computational Model = B97D3/6–31+G(d); Solvent = DMSO]		
Atom	X	Y	Z
C	–3.651622	2.319960	–4.456572
C	–2.573929	2.315241	–5.357718
C	–1.386175	1.646252	–5.018298
C	–1.281696	0.987763	–3.783736
C	–2.351986	0.978542	–2.859734
C	–3.536936	1.658520	–3.224496
B	–2.228009	0.238436	–1.469086
O	–3.304847	0.262251	–0.596964
O	–1.049022	–0.415474	–1.154233
O	–1.982650	–1.194092	1.247484
C	–1.517086	–0.731140	2.363221
C	–2.556765	–0.108225	3.307661
O	–0.303717	–0.754900	2.698748
H	–4.577191	2.838246	–4.715329
H	–2.659097	2.828875	–6.317277
H	–0.545434	1.639177	–5.714976
H	–0.354627	0.471062	–3.529145
H	–4.379718	1.668156	–2.530956

H	–3.062712	–0.241374	0.230923
H	–1.133895	–0.823206	–0.244048
H	–2.972314	0.800311	2.843521
H	–3.395752	–0.802279	3.464166
H	–2.117167	0.158842	4.277030

Complex	**7**–Cl [Computational Model = B97D3/6–31+G(d); Solvent = CD_3CN]		
Atom	X	Y	Z
C	–4.407674	0.834990	–2.332434
C	–3.459007	1.518905	–3.110604
C	–2.105403	1.497828	–2.735626
C	–1.707636	0.795410	–1.588287
C	–2.643806	0.099407	–0.789197
C	–4.000218	0.135189	–1.186890
B	–2.189751	–0.689756	0.499594
O	–3.145982	–1.363871	1.241080
O	–0.848951	–0.682816	0.847335
Cl	–1.145017	–2.513050	3.445520
H	–5.461048	0.848160	–2.619300
H	–3.772323	2.064412	–4.002769
H	–1.363982	2.027676	–3.336974
H	–0.653655	0.784545	–1.305278
H	–4.745079	–0.392928	–0.589163
H	–2.734083	–1.817662	2.018563
H	–0.694753	–1.213577	1.668631

Complex	**7**–Cl [Computational Model = B97D3/6–31+G(d); Solvent = DMSO]		
Atom	X	Y	Z
C	–4.380822	0.757763	–2.396565
C	–3.433643	1.476252	–3.144840
C	–2.094156	1.510869	–2.723067
C	–1.708936	0.829451	–1.558916
C	–2.643905	0.099546	–0.789210
C	–3.985959	0.079247	–1.233955
B	–2.204390	–0.665323	0.518868
O	–3.158017	–1.376575	1.228546
O	–0.878589	–0.600898	0.915202
Cl	–1.191647	–2.432996	3.511063
H	–5.423206	0.727621	–2.719892
H	–3.737171	2.005344	–4.050149

H	–1.353972	2.067663	–3.301101
H	–0.665881	0.861992	–1.239454
H	–4.729444	–0.476023	–0.659581
H	–2.756287	–1.809466	2.022958
H	–0.732344	–1.121603	1.744295

Complex	**8**–Br [Computational Model = B97D3/6–31+G(d); Solvent = CD_3CN]		
Atom	X	Y	Z
C	–4.123126	1.707983	–1.921261
C	–3.418694	1.532386	–3.123838
C	–2.329745	0.646122	–3.169313
C	–1.951095	–0.058068	–2.016678
C	–2.645252	0.101772	–0.795274
C	–3.737781	0.999062	–0.773748
B	–2.215529	–0.694038	0.497536
O	–1.125312	–1.544609	0.420342
O	–2.944769	–0.513388	1.660987
Br	–1.192276	–2.578491	3.562340
H	–4.970066	2.395822	–1.880259
H	–3.716053	2.082146	–4.018837
H	–1.778795	0.505920	–4.101458
H	–1.103756	–0.744334	–2.061858
H	–4.291381	1.142525	0.155708
H	–0.952807	–1.987097	1.288578
H	–2.581930	–1.060848	2.401237

Complex	**8**–Br [Computational Model = B97D3/6–31+G(d); Solvent = DMSO]		
Atom	X	Y	Z
C	–4.123642	1.707233	–1.921773
C	–3.418308	1.532454	–3.123952
C	–2.328700	0.646965	–3.169009
C	–1.950263	–0.057270	–2.016330
C	–2.645331	0.101736	–0.795299
C	–3.738554	0.998243	–0.774213
B	–2.215810	–0.694002	0.497473
O	–1.124807	–1.543749	0.420933
O	–2.945790	–0.514300	1.660697
Br	–1.192764	–2.579041	3.562871
H	–4.971069	2.394469	–1.881127
H	–3.715488	2.082241	–4.018974

H	–1.777085	0.507411	–4.100840
H	–1.102370	–0.742875	–2.061285
H	–4.292941	1.141128	0.154872
H	–0.952325	–1.986018	1.289219
H	–2.583122	–1.061762	2.400939

Complex	**9**–HSO_4 [Computational Model = B97D3/6–31+G(d); Solvent = DMSO]		
Atom	X	Y	Z
C	3.228957	0.676506	0.726601
C	3.484459	–0.699561	0.846806
C	2.534702	–1.627025	0.387341
C	1.337802	–1.176181	–0.188908
C	1.058313	0.203664	–0.320978
C	2.029027	1.117984	0.149361
B	–0.287893	0.704829	–0.970737
O	–1.200103	–0.233291	–1.427121
O	–2.995766	1.740664	–2.364678
O	–0.518223	2.067380	–1.069503
S	–4.291031	2.032541	–1.649897
O	–4.473443	1.267227	–0.384586
O	–4.003541	3.638702	–1.194650
O	–5.479826	2.055951	–2.545795
H	3.963813	1.401364	1.082326
H	4.417109	–1.046708	1.295512
H	2.728315	–2.697593	0.478831
H	0.606321	–1.904647	–0.542801
H	1.840034	2.189151	0.060644
H	–1.995530	0.209848	–1.801943
H	–1.391526	2.240148	–1.492493
H	–4.775934	3.933770	–0.668427

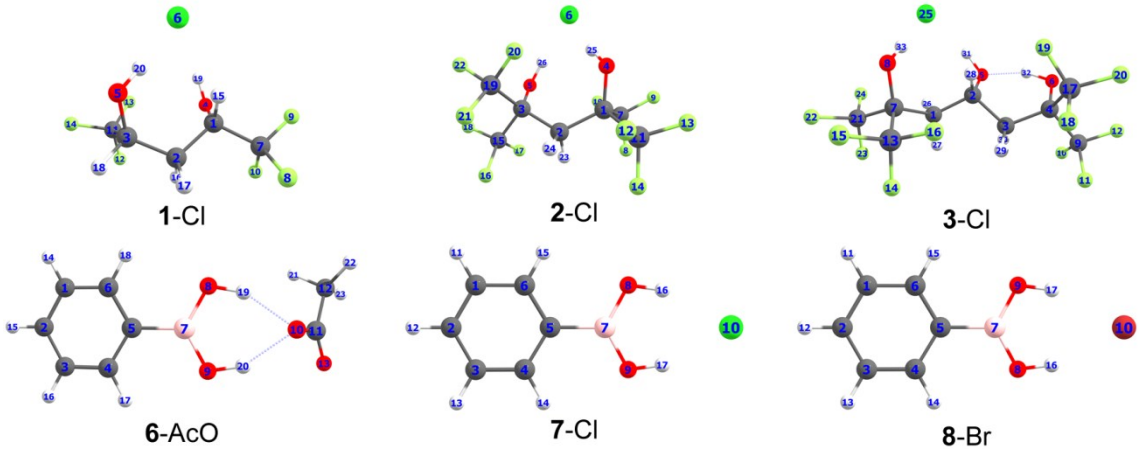

Figure S1. Atoms numeration to structures (**1**–**3**)–Cl, **6**–AcO, **7**–Cl and **8**–Br. Atoms color: H = white; C = gray; O = light red; Cl = green; F = light green; B = rose; Br = red.

Table S2. Bond lengths (r / Å) and angles (< / °) to structures **1**–Cl, **2**–Cl and **3**–Cl from the B97D3 computational method along with the 6–31+G(d) and Def2–TZVP basis sets.

	1–Cl	
Geometric Parameter	6–31+G(d)	Def2–TZVP
r[C(1)–C(2)]	1.537	1.532
r[C(1)–O(4)]	1.418	1.412
r[C(1)–C(7)]	1.539	1.536
r[C(1)–H(15)]	1.101	1.098
r[C(2)–C(3)]	1.552	1.549
r[C(2)–H(16)]	1.098	1.094
r[C(2)–H(17)]	1.098	1.094
r[C(3)–O(5)]	1.415	1.409
r[C(3)–C(11)]	1.549	1.545
r[C(3)–H(18)]	1.099	1.097
r[O(4)–H(19)]	0.993	0.991
r[O(5)–H(20)]	0.995	0.992
r[C(7)–F(8)]	1.371	1.363
r[C(7)–F(9)]	1.365	1.357
r[C(7)–F(10)]	1.368	1.361
r[C(11)–F(12)]	1.371	1.364
r[C(11)–F(13)]	1.359	1.351
r[C(11)–F(14)]	1.372	1.364
<[C(2)–C(1)–O(4)]	113.1	113.4
<[C(2)–C(1)–C(7)]	110.9	110.7
<[C(2)–C(1)–H(15)]	109.6	109.3
<[C(1)–C(2)–C(3)]	115.9	115.7
<[(C(1)–C(2)–H(16)]	109.8	109.6

<[C(1)–C(2)–H(17)]	108.1	108.1
<[O(4)–C(1)–C(7)]	107.5	107.6
<[O(4)–C(1)–H(15)]	110.3	110.4
<[C(1)–O(4)–H(19)]	106.0	105.7
<[C(7)–C(1)–H(15)]	105.2	105.1
<[C(1)–C(7)–F(8)]	111.8	111.8
<[C(1)–C(7)–F(9)]	111.7	111.5
<[C(1)–C(7)–F(10)]	112.7	112.6
<[C(3)–C(2)–H(16)]	109.6	109.7
<[C(3)–C(2)–H(17)]	106.0	106.3
<[C(2)–C(3)–O(5)]	115.1	115.2
<[C(2)–C(3)–C(11)]	115.5	115.0
<[C(2)–C(3)–H(18)]	106.2	106.2
<[H(16)–C(2)–H(17)]	107.1	107.1
<[O(5)–C(3)–C(11)]	110.4	110.8
<[O(5)–C(3)–H(18)]	105.4	105.7
<[C(3)–O(5)–H(20)]	111.0	111.1
<[C(11)–C(3)–H(18)]	102.9	102.5
<[C(3)–C(11)–F(12)]	111.6	111.3
<[C(3)–C(11)–F(13)]	114.8	114.9
<[C(3)–C(11)–F(14)]	110.1	110.0
<[F(8)–C(7)–F(9)]	106.7	106.8
<[F(8)–C(7)–F(10)]	106.8	106.9
<[F(9)–C(7)–F(10)]	106.8	106.9
<[F(12)–C(11)–F(13)]	107.2	107.2
<[F(12)–C(11)–C(14)]	106.4	106.5
<[F(13)–C(11)–C(14)]	106.3	106.4

	2–Cl	
Geometric Parameter	6–31+G(d)	Def2–TZVP
r[C(1)–C(2)]	1.572	1.568
r[C(1)–O(4)]	1.393	1.388
r[C(1)–(7)]	1.579	1.578
r[C(1)–C(11)]	1.578	1.576
r[C(2)–C(3)]	1.573	1.568
r[C(2)–H(23)]	1.094	1.090
r[C(2)–H(24)]	1.094	1.090
r[C(3)–O(5)]	1.393	1.388
r[C(3)–C(15)]	1.578	1.576
r[C(3)–C(19)]	1.579	1.577

r[O(4)–H(25)]	1.004	1.001
r[O(5)–H(26)]	1.004	1.001
r[C(7)–F(8)]	1.366	1.358
r[C(7)–F(9)]	1.356	1.349
r[C(7)–F(10)]	1.357	1.349
r[C(11)–F(12)]	1.360	1.354
r[C(11)–F(13)]	1.355	1.348
r[C(11)–F(14)]	1.361	1.354
r[C(15)–F(16)]	1.361	1.354
r[C(15)–F(17)]	1.360	1.354
r[C(15)–F(18)]	1.355	1.348
r[C(19)–F(20)]	1.356	1.349
r[C(19)–F(21)]	1.366	1.358
r[C(19)–F(22)]	1.356	1.349
<[C(2)–C(1)–O(4)]	118.3	118.4
<[C(2)–C(1)–C(7)]	110.2	110.1
<[C(2)–C(1)–C(11)]	105.7	105.5
<[C(1)–C(2)–C(3)]	122.6	122.9
<[C(1)–C(2)–H(23)]	106.2	106.1
<[C(1)–C(2)–H(24)]	107.6	107.5
<[O(4)–C(1)–C(7)]	110.1	110.0
<[O(4)–C(1)–C(11)]	102.9	103.0
<[C(1)–O(4)–H(25)]	114.0	114.1
<[C(7)–C(1)–C(11)]	109.2	109.2
<[C(1)–C(7)–F(8)]	112.4	112.5
<[C(1)–C(7)–F(9)]	112.0	111.9
<[C(1)–C(7)–F(10)]	110.8	110.8
<[C(1)–C(11)–F(12)]	109.7	109.7
<[C(1)–C(11)–F(13)]	112.7	112.5
<[C(1)–C(11)–F(14)]	112.5	112.6
<[C(3)–C(2)–H(23)]	107.6	107.5
<[C(3)–C(2)–H(24)]	106.2	106.1
<[C(2)–C(3)–O(5)]	118.3	118.4
<[C(2)–C(3)–C(15)]	105.6	105.5
<[C(2)–C(3)–C(19)]	110.2	110.1
<[H(23)–C(2)–H(24)]	105.6	105.6
<[O(5)–C(3)–C(15)]	102.9	103.1
<[O(5)–C(3)–C(19)]	110.1	110.0
<[C(3)–O(5)–H(26)]	113.9	114.1

<[C(15)–C(3)–C(19)]	109.2	109.2
<[C(3)–C(15)–F(16)]	112.4	112.6
<[C(3)–C(15)–F(17)]	109.7	109.6
<[C(3)–C(15)–F(18)]	112.7	112.6
<[C(3)–C(19)–F(20)]	110.8	110.8
<[C(3)–C(19)–F(21)]	112.4	112.5
<[C(3)–C(19)–F(22)]	112.0	111.9
<[F(8)–C(7)–F(9)]	107.4	107.4
<[F(8)–C(7)–F(10)]	107.0	107.0
<[F(9)–C(7)–F(10)]	107.0	107.0
<[F(12)–C(11)–F(13)]	107.2	107.2
<[F(12)–C(11)–F(14)]	107.1	107.1
<[F(13)–C(11)–F(14)]	107.5	107.5
<[F(16)–C(15)–F(17)]	107.1	107.1
<[F(16)–C(15)–F(18)]	107.5	107.5
<[F(17)–C(15)–F(18)]	107.1	107.2
<[F(20)–C(19)–F(21)]	107.0	107.0
<[F(20)–C(19)–F(22)]	107.0	107.0
<[F(21)–C(19)–F(22)]	107.4	107.4

	3–Cl	
Geometric Parameter	6–31+G(d)	Def2–TZVP
r[C(1)–C(2)]	1.554	1.548
r[C(1)–C(7)]	1.556	1.550
r[C(1)–H(26)]	1.096	1.092
r[C(1)–H(27)]	1.097	1.093
r[C(2)–C(3)]	1.536	1.531
r[C(2)–O(5)]	1.449	1.445
r[C(2)–H(28)]	1.094	1.091
r[C(3)–C(4)]	1.556	1.553
r[C(3)–H(29)]	1.095	1.091
r[C(3)–H(30)]	1.097	1.094
r[C(4)–O(6)]	1.408	1.403
r[C(4)–C(9)]	1.569	1.568
r[C(4)–C(17)]	1.574	1.568
r[O(5)–H(31)]	0.999	0.997
r[O(5)–H(32)]	1.697	1.669
r[O(6)–H(32)]	1.000	0.996
r[C(7)–O(8)]	1.403	1.398
r[C(7)–C(13)]	1.564	1.563

r[C(7)–C(21)]	1.575	1.574
r[O(8)–H(33)]	1.005	1.001
r[C(9)–F(10)]	1.361	1.354
r[C(9)–F(11)]	1.364	1.356
r[C(9)–F(12)]	1.357	1.351
r[C(13)–F(14)]	1.363	1.355
r[C(13)–F(15)]	1.356	1.349
r[C(13)–F(16)]	1.362	1.356
r[C(17)–F(18)]	1.363	1.356
r[C(17)–F(19)]	1.362	1.355
r[C(17)–F(20)]	1.360	1.351
r[C(21)–F(22)]	1.358	1.351
r[C(21)–F(23)]	1.364	1.356
r[C(21)–F(24)]	1.363	1.355
<[C(2)–C(1)–C(7)]	116.0	116.1
<[C(2)–C(1)–H(26)]	106.6	106.6
<[C(2)–C(1)–H(27)]	111.1	111.1
<[C(1)–C(2)–C(3)]	111.3	111.4
<[C(1)–C(2)–O(5)]	109.8	110.1
<[C(1)–C(2)–H(28)]	109.8	109.6
<[C(7)–C(1)–H(26)]	107.2	107.1
<[C(7)–C(1)–H(27)]	109.1	109.1
<[C(1)–C(7)–O(8)]	114.8	114.8
<[C(1)–C(7)–C(13)]	111.0	110.9
<[C(1)–C(7)–C(21)]	107.8	107.7
<[H(26)–C(1)–H(27)]	106.4	106.5
<[C(3)–C(2)–O(5)]	106.2	106.3
<[C(3)–C(2)–H(28)]	111.1	110.9
<[C(2)–C(3)–C(4)]	115.5	115.4
<[C(2)–C(3)–H(29)]	109.6	109.8
<[C(2)–C(3)–H(30)]	107.4	107.1
<[O(5)–C(2)–H(28)]	108.5	108.5
<[C(2)–O(5)–H(31)]	107.0	106.5
<[C(2)–O(5)–H(32)]	99.5	96.2
<[C(4)–C(3)–H(29)]	109.4	109.2
<[C(4)–C(3)–H(30)]	107.2	107.9
<[C(3)–C(4)–O(6)]	113.6	114.1
<[C(3)–C(4)–C(9)]	108.3	107.9
<[C(3)–C(4)–C(17)]	111.3	110.8

<[H(29)–C(3)–H(30)]	107.4	107.2
<[O(6)–C(4)–C(9)]	105.8	106.5
<[O(6)–C(4)–C(17)]	107.6	107.1
<[C(4)–O(6)–H(32)]	105.8	106.1
<[C(9)–C(4)–C(17)]	110.1	110.4
<[C(4)–C(9)–F(10)]	110.3	109.8
<[C(4)–C(9)–F(11)]	112.1	112.4
<[C(4)–C(9)–F(12)]	112.7	112.7
<[C(4)–C(17)–F(18)]	112.8	112.7
<[C(4)–C(17)–F(19)]	110.1	110.2
<[C(4)–C(17)–F(20)]	112.6	112.4
<[H(31)–O(5)–C(32)]	122.2	119.9
<[O(5)–H(32)–O(6)]	152.6	154.8
<[O(8)–C(7)–C(13)]	104.8	105.1
<[O(8)–C(7)–C(21)]	108.1	108.2
<[C(7)–O(8)–H(33)]	110.9	110.9
<[C(13)–C(7)–C(21)]	110.2	110.2
<[C(7)–C(13)–F(14)]	112.0	112.1
<[C(7)–C(13)–F(15)]	112.9	112.8
<[C(7)–C(13)–F(16)]	110.3	110.3
<[C(7)–C(21)–F(22)]	112.9	112.7
<[C(7)–C(21)–F(23)]	113.0	113.0
<[C(7)–C(21)–F(24)]	109.4	109.4
<[F(10)–C(9)–F(11)]	107.2	107.2
<[F(10)–C(9)–F(12)]	106.6	106.8
<[F(11)–C(9)–F(12)]	107.5	107.5
<[F(14)–C(13)–F(15)]	107.4	107.5
<[F(14)–C(13)–F(16)]	107.1	107.1
<[F(15)–C(13)–F(16)]	106.7	106.7
<[F(18)–C(17)–F(19)]	107.2	107.2
<[F(18)–C(17)–F(20)]	107.2	107.4
<[F(19)–C(17)–F(20)]	106.6	106.7
<[F(22)–C(21)–F(23)]	107.3	107.4
<[F(22)–C(21)–F(24)]	106.9	106.9
<[F(23)–C(21)–F(24)]	107.1	107.1

Table S3. Bond lengths (r / Å) and angles (< / °) to structures **6**–AcO, **7**–Cl and **8**–Br from the B97D3/6–31+G(d) computational model along with the acetonitrile and DMSO solvents.

6–AcO

Geometric Parameter	Acetonitrile	DMSO
r[C(1)–C(2)]	1.405	1.405
r[C(1)–C(6)]	1.403	1.403
r[C(1)–H(14)]	1.092	1.092
r[C(2)–C(3)]	1.405	1.405
r[C(2)–H(15)]	1.092	1.092
r[C(3)–C(4)]	1.403	1.403
r[C(3)–H(16)]	1.092	1.092
r[C(4)–C(5)]	1.414	1.414
r[C(4)–H(17)]	1.091	1.091
r[C(5)–C(6)]	1.414	1.414
r[C(5)–B(7)]	1.580	1.580
r[C(6)–H(18)]	1.092	1.091
r[B(7)–O(8)]	1.386	1.386
r[C(7)–O(9)]	1.385	1.384
r[O(8)–H(19)]	0.999	0.999
r[O(9)–H(20)]	1.001	1.001
r[O(10)–C(11)]	1.295	1.295
r[O(10)–H(19)]	1.760	1.763
r[O(10)–C(20)]	1.757	1.756
r[C(11)–C(12)]	1.537	1.537
r[C(11)–O(13)]	1.259	1.259
r[C(12)–H(21)]	1.102	1.102
r[C(12)–H(22)]	1.100	1.100
r[C(12)–C(23)]	1.097	1.097
<[C(2)–C(1)–C(6)]	119.9	119.9
<[C(2)–C(1)–H(14)]	120.0	120.0
<[C(1)–C(2)–C(3)]	119.7	119.7
<[C(1)–C(2)–H(15)]	120.2	120.2
<[C(6)–C(1)–H(14)]	120.1	120.1
<[C(1)–C(6)–C(5)]	121.4	121.4
<[C(1)–C(6)–H(18)]	119.4	119.4
<[C(3)–C(2)–H(15)]	120.2	120.2
<[C(2)–C(3)–C(4)]	119.9	119.9
<[C(2)–C(3)–H(16)]	120.0	120.0
<[C(4)–C(3)–H(16)]	120.1	120.1
<[C(3)–C(4)–C(5)]	121.4	121.4
<[C(3)–C(4)–H(17)]	119.4	119.4
<[C(5)–C(4)–H(17)]	119.2	119.2

<[C(4)–C(5)–C(6)]	117.6	117.6
<[C(4)–C(5)–B(7)]	121.2	121.2
<[C(6)–C(5)–B(7)]	121.2	121.2
<[C(5)–C(6)–H(18)]	119.2	119.2
<[C(5)–B(7)–O(8)]	119.0	119.0
<[C(5)–B(7)–O(9)]	119.2	119.2
<[O(8)–B(7)–O(9)]	121.8	121.8
<[B(7)–O(8)–H(19)]	108.9	108.9
<[B(7)–O(9)–H(20)]	109.1	109.1
<[O(8)–H(19)–H(10)]	154.1	154.0
<[O(9)–H(20)–O(10)]	154.0	154.1
<[O(10)–C(11)–C(12)]	115.5	121.6
<[O(10)–C(11)–O(13)]	124.7	118.9
<[C(11)–O(10)–H(19)]	121.7	115.6
<[C(11)–O(10)–H(20)]	118.9	124.7
<[C(12)–C(11)–O(13)]	119.7	107.9
<[C(11)–C(12)–H(21)]	109.3	119.7
<[C(11)–C(12)–H(22)	110.3	109.3
<[C(11)–C(12)–H(23)	111.8	110.3
<[H(21)–C(12)–H(22)	107.0	111.8
<[H(21)–C(12)–H(23)	108.8	107.0
<[H(22)–C(12)–H(23)	109.5	108.8
<[H(19)–O(10)–H(20)	107.9	109.5

7–Cl

Geometric Parameter	Acetonitrile	DMSO
r[C(1)–C(2)]	1.405	1.405
r[C(1)–C(6)]	1.403	1.403
r[C(1)–H(11)]	1.092	1.092
r[C(2)–C(3)]	1.405	1.405
r[C(2)–H(12)]	1.092	1.092
r[C(3)–C(4)]	1.403	1.403
r[C(3)–H(13)]	1.092	1.092
r[C(4)–C(5)]	1.414	1.414
r[C(4)–H(14)]	1.091	1.091
r[C(5)–C(6)]	1.414	1.414
r[C(5)–B(7)]	1.578	1.578
r[C(6)–H(15)]	1.091	1.091
r[B(7)–(8)]	1.385	1.385
r[B(7)–O(9)]	1.385	1.385

r[O(8)–H(16)]	0.990	0.990
r[O(9)–H(17)]	0.990	0.990
<[C(2)–C(1)–C(6)]	119.9	119.9
<[C(2)–C(1)–H(11)]	120.0	120.0
<[C(1)–C(2)–C(3)]	119.7	119.7
<[C(1)–C(2)–H(12)]	120.1	120.1
<[C(6)–C(1)–H(11)]	120.1	120.1
<[C(1)–C(6)–C(5)]	121.4	121.4
<[C(1)–C(6)–H(15)]	119.4	119.4
<[C(3)–C(2)–H(12)]	120.1	120.1
<[C(2)–C(3)–C(4)]	119.9	119.9
<[C(2)–C(3)–H(13)]	120.0	120.0
<[C(4)–C(3)–H(13)]	120.1	120.1
<[C(3)–C(4)–C(5)]	121.4	121.4
<[C(3)–C(4)–H(14)]	119.4	119.4
<[C(5)–C(4)–H(14)]	119.2	119.2
<[C(4)–C(5)–C(6)]	117.6	117.6
<[C(4)–C(5)–B(7)]	121.1	121.2
<[C(6)–C(5)–B(7)]	121.2	121.2
<[C(5)–C(6)–H(15)]	119.2	119.2
<[C(5)–B(7)–O(8)]	118.8	118.8
<[C(5)–B(7)–O(9)]	118.8	118.8
<[O(8)–B(7)–O(9)]	122.4	122.4
<[B(7)–O(8)–H(16)]	110.9	110.9
<[B(7)–O(9)–H(17)]	110.9	110.9

8–Br

Geometric Parameter	Acetonitrile	DMSO
r[C(1)–C(2)]	1.405	1.405
r[C(1)–C(6)]	1.403	1.403
r[C(1)–H(11)]	1.092	1.092
r[C(2)–C(3)]	1.405	1.405
r[C(2)–H(12)]	1.092	1.092
r[C(3)–C(4)]	1.403	1.403
r[C(3)–H(13)]	1.092	1.092
r[C(4)–C(5)]	1.414	1.414
r[C(4)–H(14)]	1.091	1.091
r[C(5)–C(6)]	1.414	1.414
r[C(5)–B(7)]	1.578	1.578
r[C(6)–H(15)]	1.091	1.091

r[B(7)–O(8)]	1.385	1.385
r[B(7)–O(9)]	1.385	1.385
r[O(8)–H(16)]	0.990	0.990
r[O(9)–H(17)]	0.990	0.990
<[C(2)–C(1)–C(6)]	120.0	120.0
<[C(2)–C(1)–H(11)]	120.0	120.0
<[C(1)–C(2)–C(3)]	119.7	119.7
<[C(1)–C(2)–H(12)]	120.2	120.2
<[C(6)–C(1)–H(11)]	120.0	120.0
<[C(1)–C(6)–H(5)]	121.4	121.4
<[C(1)–C(6)–H(15)]	119.4	119.4
<[C(3)–C(2)–H(12)]	120.2	120.2
<[C(2)–C(3)–C(4)]	120.0	120.0
<[C(2)–C(3)–H(13)]	120.0	120.0
<[C(4)–C(3)–H(13)]	120.1	120.1
<[C(3)–C(4)–C(5)]	121.4	121.4
<[C(3)–C(4)–H(14)]	119.4	119.4
<[C(5)–C(4)–H(14)]	119.2	119.2
<[C(4)–C(5)–C(6)]	117.7	117.7
<[C(4)–C(5)–B(7)]	121.1	121.1
<[C(6)–C(5)–B(7)]	121.2	121.2
<[C(5)–C(6)–H(15)]	119.2	119.2
<[C(5)–B(7)–O(8)]	118.6	118.6
<[C(5)–B(7)–O(9)]	118.6	118.6
<[O(8)–B(7)–O(9)]	122.8	122.8
<[B(7)–O(8)–H(16)]	111.3	111.3
<[B(7)–O(9)–H(17)]	111.3	111.3

Table S4. Average bond length (r / Å) between the anions and the main atoms of the receptors related the anion recognition from the B97D3 computational method along with the 6–31+G(d) basis set.

Complex	Interaction	r
1–Cl	O–H···Cl^-	2.175
2–Cl	O–H···Cl^-	2.038
3–Cl	O–H···Cl^-	2.082
4–F	B···F^-	1.510
5–H_2PO_4	B···O^-–P	1.598
	P–OH···O–B	1.622
6–AcO	B–OH···O^-–C	1.760
7–Cl	O–H···Cl^-	2.248

8–Br	O–H···Br^-	2.363
9–HSO_4	B–OH···O^-–S	1.903