Electronic Supplementary Material (ESI) for Green Chemistry.
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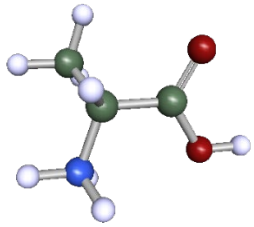
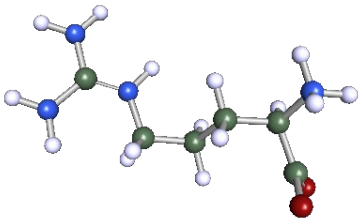
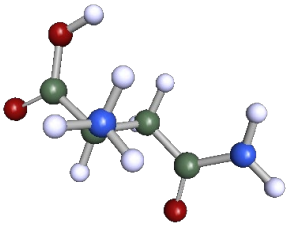
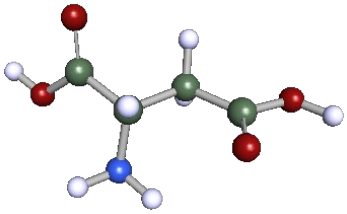
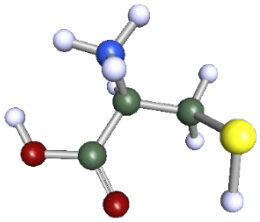
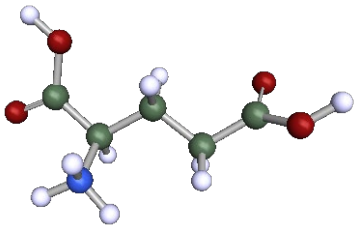
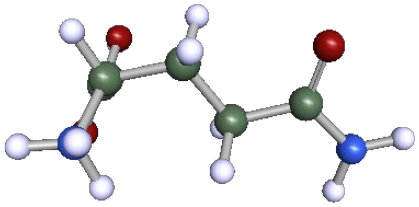
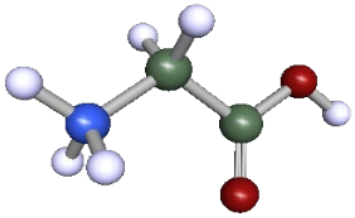
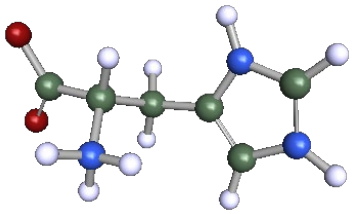
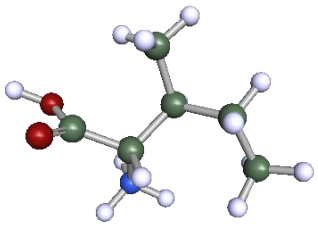
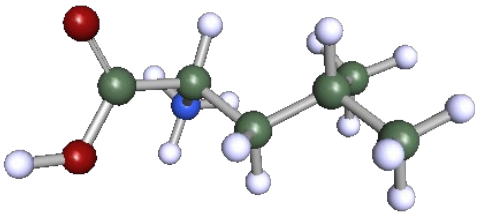
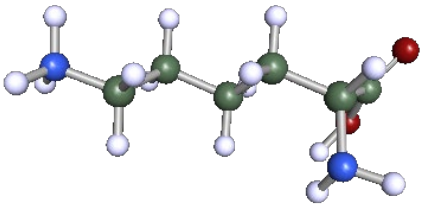
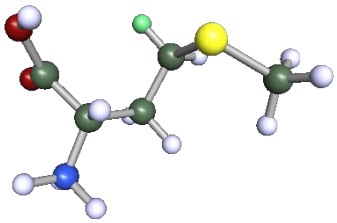
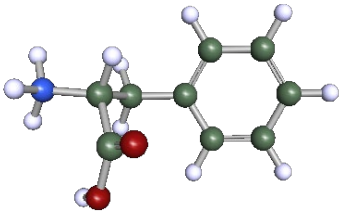
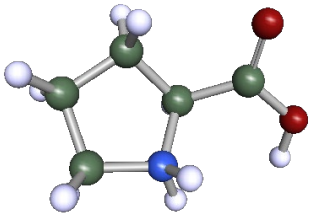
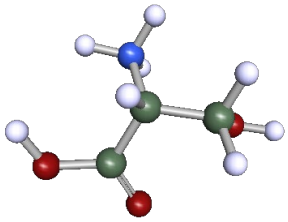
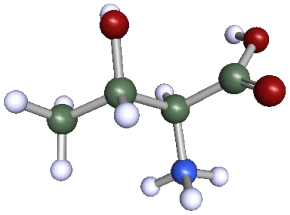
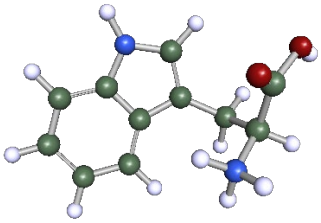
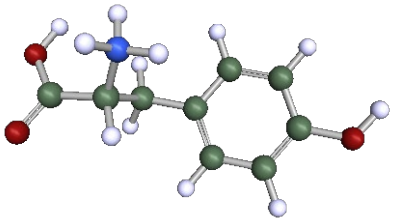
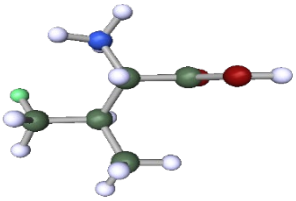
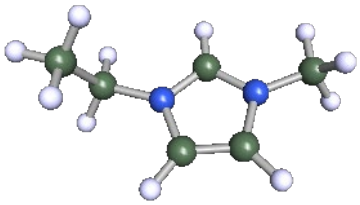
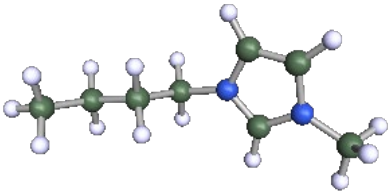
Supplementary Information

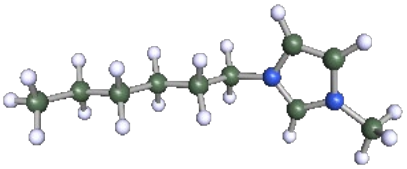
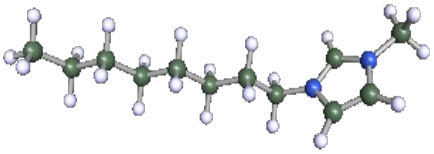
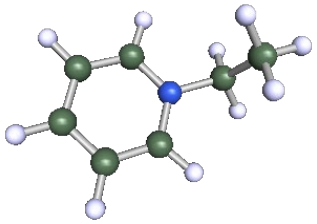
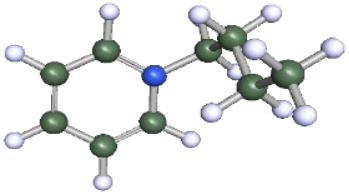
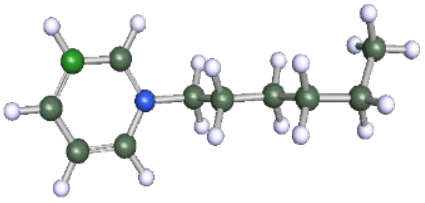
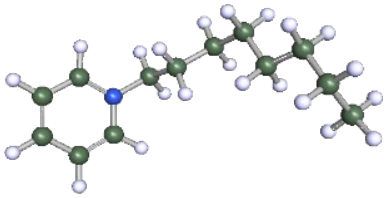
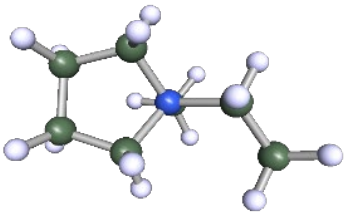
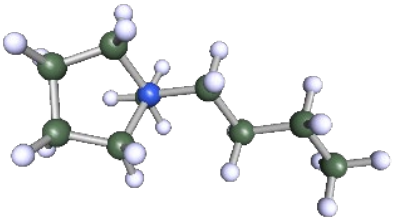
Table S1

Structure of cations (obtained from PubChem database) used in the screening of chitosan dissolution in ILs.

No.	List of Cations	Abbreviation	Structure
1	Alanine	[Ala]	
2	Arginine	[Arg]	
3	Asparagine	[Asn]	
4	Aspartic acid	[Asp]	
5	Cysteine	[Cys]	
6	Glutamic acid	[Glu]	

7	Glutamine	[Gln]	
8	Glycine	[Gly]	
9	Histidine	[His]	
10	Isoleucine	[Ile]	
11	Leucine	[Leu]	
12	Lysine	[Lys]	
13	Methionine	[Met]	
14	Phenylalanine	[Phe]	

15	Proline	[Pro]	
16	Serine	[Ser]	
17	Threonine	[Thr]	
18	Tryptophan	[Trp]	
19	Tyrosine	[Tyr]	
20	Valine	[Val]	
21	1-ethyl-3-methylimidazolium	[EMIM]	
22	1-butyl-3-methylimidazolium	[BMIM]	

23	1-hexyl-3-methylimidazolium	[HMIM]	
24	1-octyl-3-methylimidazolium	[OMIM]	
25	1-ethyl-pyridinium	[EPy]	
26	1-butyl-pyridinium	[BPy]	
27	1-hexyl-pyridinium	[HPy]	
28	1-octyl-pyridinium	[OPy]	
29	1-ethyl-1-methylpyrrolidinium	[EMPyrr]	
30	1-butyl-1-methylpyrrolidinium	[BMPyrr]	

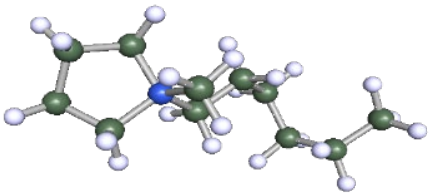
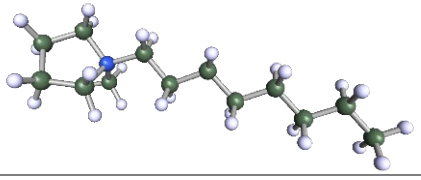
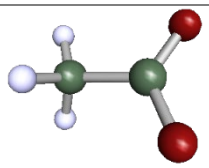
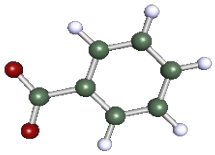
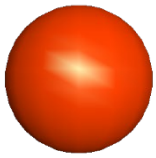
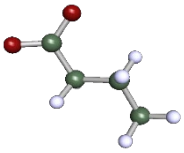
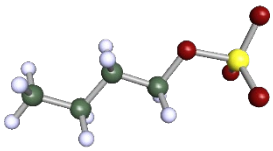
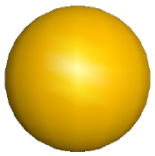
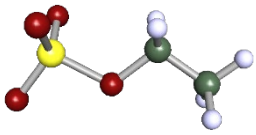
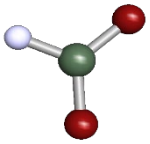
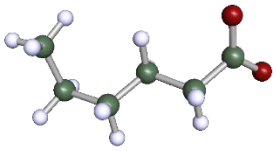
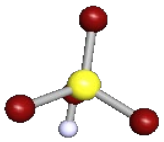
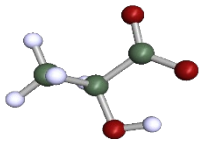
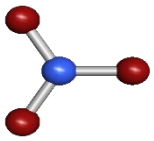
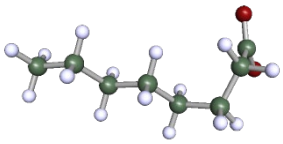
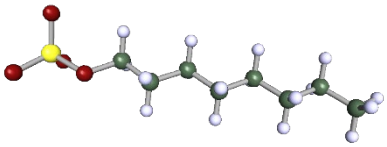
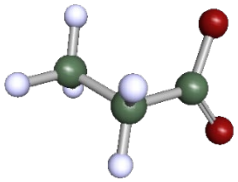
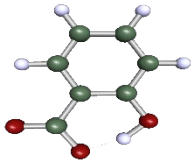
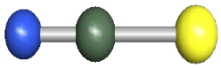
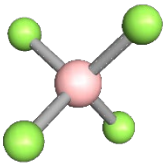
31	1-hexyl-1-methylpyrrolidinium	[HMPyrr]	
32	1-octyl-1-methylpyrrolidinium	[OMPyrr]	

Table S2

Structure of anions (obtained from PubChem database) used in the screening of chitosan dissolution in ILs.

No.	List of Anions	Abbreviation	Structure
1	Acetate	$[C_2H_3O_2]$	
2	Benzoate	$[C_7H_5O_2]$	
3	Bromide	[Br]	
4	Butanoate	$[C_4H_7O_2]$	
5	Butyl sulphate	$[C_4H_9SO_4]$	
6	Chloride	[Cl]	
7	Ethyl sulphate	$[C_2H_6SO_4]$	
8	Formate	$[CHO_2]$	
9	Hexanoate	$[C_6H_{11}O_2]$	

10	Hydrogen sulphate	$[HSO_4]$	
11	Iodide	$[I]$	
12	Lactate	$[C_3H_5O_3]$	
13	Nitrate	$[NO_3]$	
14	Octanoate	$[C_8H_{15}O_2]$	
15	Octyl sulphate	$[C_8H_{17}SO_4]$	
16	Propionate	$[C_3H_5O_2]$	
17	Salicylate	$[C_7H_5O_3]$	
18	Thiocyanate	$[SCN]$	
19	Tetrafluoroborate	$[BF_4]$	

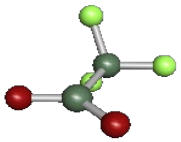
20	Trifluoroacetate	$[C_2F_3O_2]$	

Table S3

Logarithmic activity coefficients at infinite dilution (ln γ) of 640 ILs for the dissolution of chitosan.

	$[C_2H_3O_2]$	$[C_7H_5O_2]$	[Br]	$[C_4H_7O_2]$	$[C_4H_9SO_4]$
[Ala]	14.9945	5.5007	32.5857	9.1590	-4.2662
[Arg]	4.8885	4.1684	15.2366	2.6791	6.3230
[Asn]	9.2902	0.2739	34.1557	1.2986	-3.9418
[Asp]	9.8447	0.6071	25.0717	4.0551	-6.1041
[Cys]	13.3162	2.8279	24.8710	7.6049	-11.2186
[Gln]	12.9301	4.9316	30.0680	7.0333	0.1183
[Glu]	9.5750	0.0170	21.4172	4.4208	-6.3733
[Gly]	15.4092	0.0555	49.9872	4.2574	-4.8089
[His]	11.3984	8.7467	23.4885	6.1287	10.5551
[Ile]	7.1171	5.5854	9.7719	6.7160	-5.3792
[Leu]	8.2396	5.1379	11.8488	7.2906	-4.8748
[Lys]	6.2437	2.5809	18.2482	3.0588	0.2450
[Met]	4.9250	3.0226	18.1464	2.6293	-0.0007
[Phe]	9.6676	7.6607	11.7385	7.1717	-10.6651
[Pro]	0.1600	1.3487	8.9265	-1.4976	-4.3143
[Ser]	15.7079	0.1568	32.7959	7.0785	-12.6536
[Thr]	10.6870	0.9439	29.6740	4.5328	-3.0046
[Trp]	3.3314	-1.0138	12.0590	0.5492	-6.1732
[Tyr]	7.4428	0.7153	13.0698	4.1049	-9.1613
[Val]	10.1949	5.6985	15.6317	8.4298	-4.6829

	[Cl]	[$C_2H_6SO_4$]	[CHO_2]	[$C_6H_{11}O_2$]	[HSO_4]
[Ala]	30.0205	-1.1757	21.5839	7.8716	5.1360
[Arg]	9.0501	10.1519	9.0855	0.6544	22.0472
[Asn]	31.1246	0.0040	18.2744	-1.2618	0.4822
[Asp]	24.1479	-3.7222	15.2614	3.2036	-4.1440
[Cys]	31.8008	-10.2385	19.3217	5.0957	-18.2958
[Gln]	28.0568	3.7114	13.3030	3.8508	10.0613
[Glu]	23.4736	-3.7222	23.9990	3.7338	-6.3444
[Gly]	50.6742	-3.0314	18.0446	2.0124	-22.5911
[His]	8.7278	17.7617	8.4539	6.3944	40.2089
[Ile]	10.5144	-4.8814	9.6426	7.1870	-1.9987
[Leu]	13.2039	-4.3824	10.6859	1.5030	-1.8769
[Lys]	15.2719	3.1997	9.0019	1.6890	10.8769
[Met]	14.9581	1.9922	10.3654	2.6822	5.6394
[Phe]	17.7402	-10.3406	4.6284	-3.3194	-13.0226
[Pro]	1.1913	-1.0232	19.6151	5.7618	9.4897
[Ser]	44.0592	-11.0961	16.8861	3.3778	-34.9979
[Thr]	28.2077	-0.1608	5.8083	0.4080	1.1257
[Trp]	14.0669	-5.0820	9.6359	4.1241	-5.6257
[Tyr]	16.9276	-7.8773	15.3599	7.8716	-8.2895
[Val]	16.9248	-3.7414	21.5839	8.3579	-0.4142

	[I]	[$C_3H_5O_3$]	[NO_3]	[$C_8H_{15}O_2$]	[$C_8H_{17}SO_4$]
[Ala]	22.5409	8.2618	9.9562	6.6845	-5.0401
[Arg]	19.4112	8.4376	18.8010	-0.3673	2.7601
[Asn]	19.5378	5.1634	7.8427	-3.1115	-6.3484
[Asp]	11.9306	3.9913	1.2171	1.5412	-7.0948
[Cys]	-3.8946	4.2074	-10.8223	5.8080	-10.8569
[Gln]	22.5898	8.6444	13.8686	3.6277	-2.0605
[Glu]	7.1295	3.0118	-1.7039	2.2936	-7.0450
[Gly]	10.2129	6.1073	-17.2411	1.2702	-5.0068
[His]	37.8077	15.3678	37.7594	-0.1076	4.4498
[Ile]	0.8327	4.6315	0.5370	7.2101	-4.4049
[Leu]	1.8199	4.9994	0.7513	7.5584	-3.9628
[Lys]	16.3376	5.3360	11.8896	0.9463	-1.3396
[Met]	15.4733	3.8078	7.7901	1.8515	-0.2505
[Phe]	-7.5286	2.8775	-7.1047	7.2159	-9.7048
[Pro]	9.8997	3.2593	12.2000	-3.0628	-5.8252
[Ser]	-14.1708	3.5597	-26.8943	3.3597	-12.6598
[Thr]	19.1186	5.1963	5.8197	1.8479	-3.9938
[Trp]	-0.2245	1.0710	-1.1678	-0.1590	-6.1534
[Tyr]	-2.8906	2.5118	-2.7374	3.2407	-9.3513
[Val]	5.0561	5.9667	2.5984	8.3164	-3.9984

	$[C_3H_5O_2]$	$[C_7H_5O_3]$	[SCN]	$[BF_4]$	$[C_2F_3O_2]$
[Ala]	10.9508	-5.5943	-10.0544	-41.8825	-4.7867
[Arg]	3.2065	5.2208	16.7564	15.2529	8.6784
[Asn]	3.5805	-7.6810	-16.0717	-49.1291	-8.9530
[Asp]	5.7361	-11.6078	-19.2305	-42.2363	-11.4978
[Cys]	9.4158	-11.8194	-33.3826	-76.4755	-13.1937
[Gln]	8.8598	-2.3950	-1.6384	-18.8498	-1.1834
[Glu]	6.0757	-11.9705	-20.1420	-40.0438	-11.9205
[Gly]	8.3674	-14.1094	-46.3696	-94.0122	-15.9594
[His]	7.9385	8.4335	35.4867	24.0258	12.6115
[Ile]	6.5710	-1.4108	-6.9788	-24.3324	-0.6378
[Leu]	7.3394	-2.2030	-7.2833	-24.5672	-1.5572
[Lys]	3.9191	-0.9426	4.6466	-4.3062	0.6539
[Met]	3.0783	-1.6005	0.0321	-10.9439	-0.4700
[Phe]	7.9689	-10.2811	-22.7146	-55.1759	-12.0961
[Pro]	-1.7450	-1.1201	6.4857	-15.9720	-0.5926
[Ser]	10.1022	-16.3379	-55.6218	-110.9657	-19.3503
[Thr]	6.3683	-9.1726	-14.5193	-37.4413	-9.0602
[Trp]	0.9734	-8.2223	-13.6586	-35.1296	-10.4862
[Tyr]	5.0367	-9.9299	-17.7341	-43.9722	-11.5175
[Val]	8.7749	-3.2197	-8.0454	-26.4786	-2.3705

	$[C_2H_3O_2]$	$[C_7H_5O_2]$	[Br]	$[C_4H_7O_2]$	$[C_4H_9SO_4]$
[EMIM]	-43.0966	-29.7175	-20.1992	-38.3110	-2.9698
[BMIM]	-38.9478	-28.3278	-12.4144	-34.9457	-1.7217
[HMIM]	-36.4855	-27.0365	-8.8177	-34.1656	-0.3414
[OMIM]	-34.4025	-25.4030	-6.5211	-32.1979	1.0778
[EPy]	-42.2562	-29.3666	-19.5752	-37.5867	-2.4004
[BPy]	-38.0756	-28.2658	-11.0774	-35.3299	-1.3535
[HPy]	-35.55401	-26.9873	-7.4832	-33.4839	-0.0566
[OPy]	-33.6113	-25.6751	-5.3205	-31.8332	-0.0793
[EMPyrr]	-58.446	-42.9481	-30.4786	-52.3524	-5.0000
[BMPyrr]	-52.7496	-40.7125	-20.3987	-49.1957	-3.1563
[HMPyrr]	-49.5021	-20.3020	-15.3515	-47.0009	-1.3944
[OMPyrr]	-46.9935	-37.2950	-12.1764	-45.0039	0.2555

	[Cl]	$[C_2H_6SO_4]$	$[CHO_2]$	$[C_6H_{11}O_2]$	$[HSO_4]$
[EMIM]	-33.6363	-4.7277	-37.7664	-37.5738	-7.6563
[BMIM]	-24.8133	-3.2066	-32.1679	-35.7784	-5.5252
[HMIM]	-20.5495	-1.7657	-29.2731	-34.2657	-4.5387
[OMIM]	-17.6851	-0.3401	-26.9285	-32.4666	-3.5725
[EPy]	-33.2840	-3.9280	-37.0260	-36.6017	-6.4530
[BPy]	-23.5743	-2.7030	-31.2315	-34.9152	-4.8970
[HPy]	-19.2011	-1.3920	-28.3147	-33.3214	-4.1352
[OPy]	-16.5350	1.2818	-26.2646	-16.9867	-3.3556
[EMPyrr]	-44.8648	-7.9701	-51.3823	-50.7290	-13.4010
[BMPyrr]	-33.7807	-5.2834	-43.6490	-48.5271	-8.9787
[HMPyrr]	-28.1112	-3.2033	-39.6338	-46.7541	-6.7953
[OMPyrr]	-24.5135	-1.4142	-36.8385	-45.0052	-5.2173

	[I]	[$C_3H_5O_3$]	[NO_3]	[$C_8H_{15}O_2$]	[$C_8H_{17}SO_4$]
[EMIM]	-7.3539	-24.7203	-12.8977	-35.7990	-0.1231
[BMIM]	-1.9139	-22.5249	-9.4331	-33.9449	1.2055
[HMIM]	0.5863	-20.8298	-7.5697	-32.6101	2.8591
[OMIM]	2.3084	-19.0499	-5.9697	-30.9170	3.9809
[EPy]	-6.2605	-24.1883	-12.0380	-34.6460	0.1747
[BPy]	-0.6378	-22.2360	-8.8698	-33.2533	1.4224
[HPy]	1.7032	-20.5854	-7.2055	-31.8216	2.7725
[OPy]	3.2432	-19.0586	-5.8135	-30.4288	4.1211
[EMPyrr]	-14.3851	-34.8252	-20.3491	-48.3361	-1.0491
[BMPyrr]	-6.3497	-31.5240	-14.2952	-46.6656	0.4641
[HMPyrr]	-2.3787	-29.2785	-11.1899	-45.1860	2.0217
[OMPyrr]	0.1722	-27.3288	-8.9920	-43.6150	3.5319

	[$C_3H_5O_2$]	[$C_7H_5O_3$]	[SCN]	[BF_4]	[$C_2F_3O_2$]
[EMIM]	-41.5885	-13.6179	-3.8829	3.4701	-12.5974
[BMIM]	-38.4852	-12.6266	-2.5217	4.0167	-11.6716
[HMIM]	-36.7147	-11.5289	-1.5316	4.9062	-10.1439
[OMIM]	-34.4821	-10.1874	-0.3981	6.0563	-8.4901
[EPy]	-40.6281	-13.3882	-2.6344	4.8547	-12.4019
[BPy]	-37.5759	-12.9485	-1.7440	4.8273	-11.6598
[HPy]	-35.4855	-11.9358	-1.0333	5.4732	-10.3778
[OPy]	-33.6312	-10.7136	-0.1215	6.5686	-8.8901
[EMPyrr]	-56.6471	-21.0828	-10.7897	2.8650	-18.7222
[BMPyrr]	-51.9589	-19.6433	-6.9065	6.0305	-16.6787
[HMPyrr]	-49.2874	-18.2003	-4.7726	7.9934	-14.7072
[OMPyrr]	-47.4521	-16.6672	-3.0649	9.7015	-7.7465

Table S4

Excess enthalpy (H^E) of 640 ILs for the dissolution of chitosan.

Cations	Anions	Hydrogen Bonding	Misfit Interactions	Van der Waals Forces	Excess Enthalpy (H^E)
[Ala]	$[C_2H_3O_2]$	-42.08613	3.40073	-9.39108	-48.0765
	$[C_7H_5O_2]$	-37.67600	4.36959	-12.57700	-45.8834
	[Br]	-23.58296	3.58253	-8.98951	-28.9899
	$[C_4H_7O_2]$	-42.01800	3.75622	-11.44600	-49.7078
	$[C_4H_9SO_4]$	-20.27200	6.10702	-13.37300	-27.5380
	[Cl]	-29.28726	3.51749	-8.70355	-34.4733
	$[C_2H_6SO_4]$	-20.26500	5.50839	-11.33800	-26.0946
	$[CHO_2]$	-37.72200	2.94629	-8.29220	-43.0679
	$[C_6H_{11}O_2]$	-43.24300	4.11137	-13.35900	-52.4906
	$[HSO_4]$	-24.50200	3.97210	-8.85610	-29.3860
	[I]	-16.71700	4.06029	-10.41000	-23.0667
	$[C_3H_5O_3]$	-33.86300	3.51414	-10.39500	-40.7439
	$[NO_3]$	-22.98300	3.61554	-7.85510	-27.2226
	$[C_8H_{15}O_2]$	-43.07000	4.39473	-15.27100	-53.9463
	$[C_8H_{17}SO_4]$	-20.09400	7.08679	-17.56600	-30.5732
	$[C_3H_5O_2]$	-43.02781	3.59367	-10.37014	-49.8043
	$[C_7H_5O_3]$	-28.04400	5.08677	-12.50800	-35.4652
	[SCN]	-19.35600	4.75921	-9.99250	-24.5893
	$[BF_4]$	-12.25654	6.49603	-7.87308	-13.6336
	$[C_2F_3O_2]$	-26.13200	4.38534	-9.07700	-30.8237
[Arg]	$[C_2H_3O_2]$	-34.89647	6.67687	-13.84860	-42.0682
	$[C_7H_5O_2]$	-32.00000	6.52099	-16.97300	-42.4520
	[Br]	-25.60498	6.82117	-13.32963	-32.1134
	$[C_4H_7O_2]$	-34.72200	6.57440	-15.79500	-43.9426
	$[C_4H_9SO_4]$	-23.50100	6.94645	-18.10300	-34.6576
	[Cl]	-28.70779	7.50232	-13.15280	-34.3583
	$[C_2H_6SO_4]$	-23.52700	6.53943	-16.14800	-33.1356
	$[CHO_2]$	-32.59400	6.29622	-12.79900	-39.0968

	$[C_6H_{11}O_2]$	-31.90000	6.19391	-15.95500	-41.6611
	$[HSO_4]$	-30.57000	5.26215	-13.99900	-39.3069
	[I]	-22.24700	6.06225	-14.71000	-30.8948
	$[C_3H_5O_3]$	-30.18900	5.61354	-15.06200	-39.6375
	$[NO_3]$	-24.60900	5.24291	-12.76300	-32.1291
	$[C_8H_{15}O_2]$	-35.46400	7.15873	-19.60000	-47.9053
	$[C_8H_{17}SO_4]$	-23.38400	7.87425	-22.19400	-37.7038
	$[C_3H_5O_2]$	-35.52697	6.66886	-14.78078	-43.6389
	$[C_7H_5O_3]$	-26.89600	5.82300	-17.10100	-38.1740
	[SCN]	-22.79900	4.85967	-14.16500	-32.1043
	$[BF_4]$	-20.32719	4.99455	-12.15665	-27.4893
	$[C_2F_3O_2]$	-26.11200	5.03231	-13.36800	-34.4477
[Asn]	$[C_2H_3O_2]$	-44.95920	4.07395	-10.74914	-51.6344
	$[C_7H_5O_2]$	-40.22000	5.16439	-13.91200	-48.9676
	[Br]	-25.95266	2.92059	-10.31066	-33.3427
	$[C_4H_7O_2]$	-44.68900	4.71925	-12.70400	-52.6738
	$[C_4H_9SO_4]$	-22.58400	5.54044	-14.77600	-31.8196
	[Cl]	-31.61154	3.35726	-10.17565	-38.4299
	$[C_2H_6SO_4]$	-22.62500	4.84529	-12.78500	-30.5647
	$[CHO_2]$	-40.19900	3.30597	-9.68420	-46.5772
	$[C_6H_{11}O_2]$	-45.92200	5.27473	-14.62400	-55.2713
	$[HSO_4]$	-26.71400	3.68102	-10.32700	-33.3600
	[I]	-19.21200	3.16648	-11.67700	-27.7225
	$[C_3H_5O_3]$	-36.54700	3.88461	-11.79600	-44.4584
	$[NO_3]$	-25.54100	3.28038	-9.38150	-31.6421
	$[C_8H_{15}O_2]$	-45.67900	5.71487	-16.51100	-56.4751
	$[C_8H_{17}SO_4]$	-22.33900	6.63908	-18.91200	-34.6119
	$[C_3H_5O_2]$	-45.69286	4.50756	-11.69133	-52.8766
	$[C_7H_5O_3]$	-30.36700	5.67531	-13.90000	-38.5917
	[SCN]	-21.90100	4.90462	-11.21400	-28.2104

	$[BF_4]$	-15.00520	6.50566	-9.15675	-17.6563
	$[C_2F_3O_2]$	-28.02400	5.24981	-10.47200	-33.2462
[Asp]	$[C_2H_3O_2]$	-55.25812	3.83242	-9.88307	-61.3088
	$[C_7H_5O_2]$	-49.17200	4.91642	-13.21600	-57.4716
	[Br]	-31.78430	2.78763	-9.21291	-38.2096
	$[C_4H_7O_2]$	-44.68900	4.71925	-12.70400	-52.6738
	$[C_4H_9SO_4]$	-22.58400	5.54044	-14.77600	-31.8196
	[Cl]	-39.26796	3.02619	-9.04495	-45.2867
	$[C_2H_6SO_4]$	-22.62500	4.84529	-12.78500	-30.5647
	$[CHO_2]$	-40.19900	3.30597	-9.68420	-46.5772
	$[C_6H_{11}O_2]$	-56.71200	4.86889	-13.99600	-65.8391
	$[HSO_4]$	-31.16000	3.50473	-9.01030	-36.6656
	[I]	-22.69600	3.17942	-10.64500	-30.1616
	$[C_3H_5O_3]$	-44.79900	3.71227	-10.86400	-51.9507
	$[NO_3]$	-30.84600	3.15873	-8.09220	-35.7795
	$[C_8H_{15}O_2]$	-56.37500	5.27285	-15.94200	-67.0442
	$[C_8H_{17}SO_4]$	-27.26100	6.39931	-18.21100	-39.0727
	$[C_3H_5O_2]$	-56.42987	4.22672	-10.91403	-63.1172
	$[C_7H_5O_3]$	-36.78900	5.44971	-13.07800	-44.4173
	[SCN]	-25.63400	4.70713	-10.38700	-31.3139
	$[BF_4]$	-16.76837	6.15081	-8.36101	-18.9786
	$[C_2F_3O_2]$	-34.30700	4.78036	-9.70680	-39.2334
[Cys]	$[C_2H_3O_2]$	-49.23359	3.57403	-11.31037	-56.9699
	$[C_7H_5O_2]$	-44.40500	5.16925	-14.64200	-53.8778
	[Br]	-26.99751	3.86048	-10.85824	-33.9953
	$[C_4H_7O_2]$	-49.10800	4.10418	-13.29400	-58.2978
	$[C_4H_9SO_4]$	-23.70100	7.37223	-15.24700	-31.5758
	[Cl]	-33.34583	3.22317	-10.59518	-40.7178
	$[C_2H_6SO_4]$	-23.69500	6.80001	-13.24900	-30.1440
	$[CHO_2]$	-43.89400	3.36060	-10.23100	-50.7644
	$[C_6H_{11}O_2]$	-50.45300	4.37542	-15.22200	-61.2996
	$[HSO_4]$	-27.71500	6.07916	-10.75100	-32.3868
	[I]	-19.24500	5.40858	-12.27800	-26.1144
	$[C_3H_5O_3]$	-39.78800	4.41918	-12.29700	-47.6658
	$[NO_3]$	-27.27900	5.41625	-9.74120	-31.6040

	$[C_8H_{15}O_2]$	-50.29600	4.75166	-17.12000	-62.6643
	$[C_8H_{17}SO_4]$	-23.48300	8.30849	-19.39700	-34.5715
	$[C_3H_5O_2]$	-50.19286	3.83702	-12.27637	-58.6322
	$[C_7H_5O_3]$	-33.34600	6.77915	-14.57600	-41.1429
	[SCN]	-23.39800	7.52677	-11.88500	-27.7562
	$[BF_4]$	-14.25652	10.24587	-9.99910	-14.0098
	$[C_2F_3O_2]$	-30.74400	6.33422	-11.25500	-35.6648
[Gln]	$[C_2H_3O_2]$	-44.83159	4.33157	-11.69427	-52.1943
	$[C_7H_5O_2]$	-40.13400	5.29363	-14.83600	-49.6764
	[Br]	-27.16348	4.03769	-11.25353	-34.3793
	$[C_4H_7O_2]$	-44.57200	4.78590	-13.66400	-53.4501
	$[C_4H_9SO_4]$	-23.90500	6.47363	-15.71700	-33.1484
	[Cl]	-32.59954	4.11927	-11.08730	-39.5676
	$[C_2H_6SO_4]$	-23.94100	5.83809	-13.73000	-31.8329
	$[CHO_2]$	-40.48400	3.76118	-10.63200	-47.3548
	$[C_6H_{11}O_2]$	-45.88900	5.24577	-15.58800	-56.2312
	$[HSO_4]$	-28.46000	4.46173	-11.39100	-35.3893
	[I]	-21.18800	4.37787	-12.67300	-29.4831
	$[C_3H_5O_3]$	-36.65800	4.32614	-12.75000	-45.0819
	$[NO_3]$	-26.36000	4.08225	-10.36000	-32.6378
	$[C_8H_{15}O_2]$	-50.296	4.75166	-17.12000	-62.6643
	$[C_8H_{17}SO_4]$	-23.68500	7.53486	-19.85300	-36.0031
	$[C_3H_5O_2]$	-45.68967	4.59531	-12.64578	-53.7401
	$[C_7H_5O_3]$	-30.84000	5.78354	-14.82600	-39.8825
	[SCN]	-23.11700	5.10631	-12.18700	-30.1977
	$[BF_4]$	6.43648	-17.75792	-10.15328	-21.4747
	$[C_2F_3O_2]$	-28.94600	5.11738	-11.36400	-35.1926
[Glu]	$[C_2H_3O_2]$	-53.56757	4.37384	-11.02615	-60.2199
	$[C_7H_5O_2]$	-47.55400	5.62917	-14.28800	-56.2128
	[Br]	-31.27330	3.68263	-10.39065	-37.9813
	$[C_4H_7O_2]$	-53.21800	4.93597	-13.10200	-61.3840
	$[C_4H_9SO_4]$	-26.96100	6.57924	-15.07000	-35.4518
	[Cl]	-38.57703	3.55108	-10.25342	-45.2794
	$[C_2H_6SO_4]$	-27.53900	4.75259	-11.79400	-34.5804
	$[CHO_2]$	-48.38500	3.77277	-9.85910	-54.4713

	$[C_6H_{11}O_2]$	-54.9620	5.37180	-15.09000	-64.6802
	$[HSO_4]$	-30.65600	4.85343	-10.29500	-36.0976
	[I]	-22.49000	4.49846	-11.81300	-29.8045
	$[C_3H_5O_3]$	-43.44000	4.53953	-12.02400	-50.9245
	$[NO_3]$	-29.98700	4.43299	-9.35090	-34.9049
	$[C_8H_{15}O_2]$	-54.58600	5.78305	-17.02600	-65.8290
	$[C_8H_{17}SO_4]$	-26.70700	7.59674	-19.32600	-38.4363
	$[C_3H_5O_2]$	-54.70553	4.72566	-12.03823	-62.0181
	$[C_7H_5O_3]$	-35.56800	6.40582	-14.17800	-43.3402
	[SCN]	-25.02100	6.04048	-11.47100	-30.4515
	$[BF_4]$	-16.93930	7.66548	-9.41023	-18.6841
	$[C_2F_3O_2]$	-33.36600	5.72182	-10.76300	-38.4072
[Gly]	$[C_2H_3O_2]$	-42.56333	3.17867	-8.47101	-47.8557
	$[C_7H_5O_2]$	-37.94500	4.75791	-11.70500	-44.8921
	[Br]	-24.63771	2.28742	-7.89322	-30.2435
	$[C_4H_7O_2]$	-42.32100	3.75984	-10.50800	-49.0692
	$[C_4H_9SO_4]$	-21.13700	5.80397	-12.50300	-27.8360
	[Cl]	-30.28026	2.19287	-7.63240	-35.7198
	$[C_2H_6SO_4]$	-21.15400	5.24174	-10.43600	-26.3483
	$[CHO_2]$	-38.30800	2.65467	-7.31760	-42.9709
	$[C_6H_{11}O_2]$	-43.63600	4.06881	-12.46700	-52.0342
	$[HSO_4]$	-25.36500	4.62929	-7.65560	-28.3913
	[I]	-17.66400	3.62032	-9.29430	-23.3380
	$[C_3H_5O_3]$	-34.49800	3.52253	-9.47870	-40.4542
	$[NO_3]$	-23.70500	4.09293	-6.77360	-26.3857
	$[C_8H_{15}O_2]$	-43.39400	4.46302	-14.38100	-53.3120
	$[C_8H_{17}SO_4]$	-20.92100	6.67705	-16.71500	-30.9590
	$[C_3H_5O_2]$	-43.08466	3.61499	-9.40970	-48.8794
	$[C_7H_5O_3]$	-28.26500	5.97369	-11.63500	-33.9263
	[SCN]	-19.67200	6.73902	-9.03790	-21.9709
	$[BF_4]$	-12.91987	9.64623	-7.02079	-10.2944
	$[C_2F_3O_2]$	-26.36000	5.56005	-8.30560	-29.1056
[His]	$[C_2H_3O_2]$	-33.75818	5.77151	-12.56566	-40.5523
	$[C_7H_5O_2]$	-30.90700	5.81796	-15.73500	-40.8240

	[Br]	-24.27616	5.87507	-12.43921	-30.8403
	[$C_4H_7O_2$]	-33.57800	5.88933	-14.47900	-42.1677
	[$C_4H_9SO_4$]	-22.36900	6.13345	-16.70800	-32.9436
	[Cl]	-27.23006	6.86655	-11.91335	-32.2769
	[$C_2H_6SO_4$]	-22.41200	5.51115	-14.76000	-31.6609
	[CHO_2]	-31.36000	5.32884	-11.54600	-37.5772
	[$C_6H_{11}O_2$]	-34.49100	6.44856	-16.39000	-44.4324
	[HSO_4]	-29.03500	3.90146	-12.61000	-37.7435
	[I]	-21.19100	4.75362	-13.82400	-30.2614
	[$C_3H_5O_3$]	-28.99800	4.69734	-13.68900	-37.9897
	[NO_3]	-23.51600	3.88748	-11.41700	-31.0455
	[$C_8H_{15}O_2$]	-34.34200	6.70874	-18.26500	-45.8983
	[$C_8H_{17}SO_4$]	-22.22500	7.28051	-20.79700	-35.7415
	[$C_3H_5O_2$]	-34.40080	5.87546	-13.48216	-42.0075
	[$C_7H_5O_3$]	-25.82400	5.35223	-15.79200	-36.2638
	[SCN]	-21.86800	3.57773	-13.34300	-31.6333
	[BF_4]	-19.48146	3.82307	-10.69109	-26.3495
	[$C_2F_3O_2$]	-24.87600	4.69884	-11.99800	-32.1752
[Ile]	[$C_2H_3O_2$]	-40.05851	4.69433	-11.83371	-47.1979
	[$C_7H_5O_2$]	-36.11000	5.23529	-14.93100	-45.8057
	[Br]	-21.79447	5.68710	-11.43309	-27.5405
	[$C_4H_7O_2$]	-39.99200	4.71216	-13.84500	-49.1248
	[$C_4H_9SO_4$]	-18.86800	7.41951	-15.82200	-27.2705
	[Cl]	-27.12551	5.41957	-11.20352	-32.9095
	[$C_2H_6SO_4$]	-18.86200	7.03497	-13.80200	-25.6290
	[CHO_2]	-35.79100	4.49535	-10.75000	-42.0457
	[$C_6H_{11}O_2$]	-41.18200	5.00940	-15.79400	-51.9666
	[HSO_4]	-23.23800	5.71644	-11.48800	-29.0096
	[I]	-15.37600	6.22041	-12.82100	-21.9766
	[$C_3H_5O_3$]	-32.16200	4.71577	-12.86500	-40.3112
	[NO_3]	-21.79300	5.40089	-10.39200	-26.7841
	[$C_8H_{15}O_2$]	-41.10700	5.11512	-17.70700	-53.6989
	[$C_8H_{17}SO_4$]	-18.69900	8.21368	-20.00100	-30.4863
	[$C_3H_5O_2$]	-40.98688	4.66454	-12.80937	-49.1317
	[$C_7H_5O_3$]	-27.04100	5.62005	-14.87700	-36.2980
	[SCN]	-18.66100	5.85445	-12.30100	-25.1076

	$[BF_4]$	-11.25588	7.26503	-10.28254	-14.2734
	$[C_2F_3O_2]$	-25.04500	4.76308	-11.35800	-31.6399
[Leu]	$[C_2H_3O_2]$	-40.56087	4.44311	-12.04984	-48.1676
	$[C_7H_5O_2]$	-36.45100	5.12069	-15.15500	-46.4853
	[Br]	5.11579	-22.25287	-11.66486	-28.8019
	$[C_4H_7O_2]$	-40.46810	4.51824	-14.05747	-50.0073
	$[C_4H_9SO_4]$	-19.18900	7.03702	-16.03500	-28.1870
	[Cl]	-27.69640	4.86124	-11.41236	-34.2475
	$[C_2H_6SO_4]$	-19.18500	6.65384	-14.01600	-26.5472
	$[CHO_2]$	-36.25000	4.19350	-10.96900	-43.0255
	$[C_6H_{11}O_2]$	-41.68400	4.81119	-16.00400	-52.8768
	$[HSO_4]$	-23.51200	5.38761	-11.70500	-29.8294
	[I]	-15.71000	5.72832	-13.06000	-23.0417
	$[C_3H_5O_3]$	-32.55200	4.47208	-13.07700	-41.1569
	$[NO_3]$	-22.04800	5.07487	-10.60400	-27.5771
	$[C_8H_{15}O_2]$	-41.56900	4.95449	-17.91500	-54.5295
	$[C_8H_{17}SO_4]$	-19.01700	7.81962	-20.21300	-31.4104
	$[C_3H_5O_2]$	-41.47798	4.46988	-13.02271	-50.0308
	$[C_7H_5O_3]$	-27.20300	5.53674	-15.09900	-36.7653
	[SCN]	-18.78900	5.66977	-12.54400	-25.6632
	$[BF_4]$	-11.49133	7.04661	-10.49220	-14.9369
	$[C_2F_3O_2]$	-25.23500	4.66170	-11.56700	-32.1403
[Lys]	$[C_2H_3O_2]$	-34.15288	5.43748	-12.65756	-41.3730
	$[C_7H_5O_2]$	-30.60200	6.05550	-15.70600	-40.2525
	[Br]	-20.36238	5.75590	-12.22720	-26.8337
	$[C_4H_7O_2]$	-34.02400	5.69834	-14.64400	-42.9697
	$[C_4H_9SO_4]$	-17.75800	7.56909	-16.71100	-26.8999
	[Cl]	-24.62229	5.83214	-12.02305	-30.8132
	$[C_2H_6SO_4]$	-17.77300	6.96596	-14.71800	-25.5250
	$[CHO_2]$	-30.78200	4.99416	-11.59000	-37.3778
	$[C_6H_{11}O_2]$	-31.14900	6.21867	-14.75500	-39.6853
	$[HSO_4]$	-22.59000	5.44823	-12.46800	-29.6098
	[I]	-15.65300	5.89391	-13.61800	-23.3771
	$[C_3H_5O_3]$	-27.67400	5.21002	-13.74300	-36.2070
	$[NO_3]$	-19.59700	5.17987	-11.33700	-25.7541

	$[C_8H_{15}O_2]$	-34.97000	6.47299	-18.48300	-46.9800
	$[C_8H_{17}SO_4]$	-17.61600	8.66416	-20.85600	-29.8078
	$[C_3H_5O_2]$	-34.94978	5.56517	-13.61557	-43.0002
	$[C_7H_5O_3]$	-23.32100	6.18961	-15.70800	-32.8394
	[SCN]	-17.20400	5.51797	-13.05600	-24.7420
	$[BF_4]$	-12.86858	6.47734	-11.01753	-17.4088
	$[C_2F_3O_2]$	-21.93500	5.37906	-12.16700	-28.7229
[Met]	$[C_2H_3O_2]$	-27.57208	4.89357	-12.57464	-35.2532
	$[C_7H_5O_2]$	-24.39400	5.51524	-15.77200	-34.6508
	[Br]	-15.91300	5.73584	-12.18457	-22.3617
	$[C_4H_7O_2]$	-27.40600	5.13161	-14.55800	-36.8324
	$[C_4H_9SO_4]$	-13.37600	7.74374	-16.57100	-22.2033
	[Cl]	-19.77290	5.64121	-11.90872	-26.0404
	$[C_2H_6SO_4]$	-13.40200	7.14233	-14.58400	-20.8437
	$[CHO_2]$	-24.90200	4.59441	-11.50400	-31.8116
	$[C_6H_{11}O_2]$	-28.37900	5.55924	-16.49000	-39.3098
	$[HSO_4]$	-17.95800	5.68115	-12.24600	-24.5229
	[I]	-11.29800	6.07352	-13.59100	-18.8155
	$[C_3H_5O_3]$	-27.67400	5.21002	-13.74300	-36.2070
	$[NO_3]$	-19.59700	5.17987	-11.33700	-25.7541
	$[C_8H_{15}O_2]$	-28.21700	5.78084	-18.38900	-40.8252
	$[C_8H_{17}SO_4]$	-17.61600	8.66416	-20.85600	-29.8078
	$[C_3H_5O_2]$	-28.26040	4.98002	-13.53901	-36.8194
	$[C_7H_5O_3]$	-23.32100	6.18961	-15.70800	-32.8394
	[SCN]	-17.20400	5.51797	-13.05600	-24.7420
	$[BF_4]$	-8.16247	7.44255	-11.05254	-11.7725
	$[C_2F_3O_2]$	-16.95500	5.40637	-12.25400	-23.8026
[Phe]	$[C_2H_3O_2]$	-46.24999	4.62551	-13.13025	-54.7547
	$[C_7H_5O_2]$	-41.76100	6.19112	-16.30000	-51.8699
	[Br]	-25.23251	5.52219	-12.71884	-32.4292
	$[C_4H_7O_2]$	-46.20200	5.06998	-15.10200	-56.2340
	$[C_4H_9SO_4]$	-22.02800	8.95331	-17.13100	-30.2057
	[Cl]	-31.33279	4.55193	-12.49273	-39.2736
	$[C_2H_6SO_4]$	-22.00300	8.43096	-15.16700	-28.739

	$[CHO_2]$	-41.23800	4.53514	-12.07700	-48.7799
	$[C_6H_{11}O_2]$	-47.50200	5.30066	-17.01800	-59.2193
	$[HSO_4]$	-25.99800	7.57230	-12.91400	-31.3397
	[I]	-17.82200	7.22355	-14.15900	-24.7575
	$[C_3H_5O_3]$	-37.22100	5.63775	-14.17500	-45.7583
	$[NO_3]$	-25.24600	6.89000	-11.81900	-30.1750
	$[C_8H_{15}O_2]$	-47.39000	5.64987	-18.91000	-60.6501
	$[C_8H_{17}SO_4]$	-21.85900	9.86518	-21.24500	-33.2388
	$[C_3H_5O_2]$	-47.26604	4.79467	-14.08536	-56.5567
	$[C_7H_5O_3]$	-31.15600	7.84827	-16.28800	-39.5957
	[SCN]	-21.59300	8.62388	-13.76700	-26.7361
	$[BF_4]$	-13.10358	11.02352	-11.56775	-13.6478
	$[C_2F_3O_2]$	-28.86700	7.21699	-12.66400	-34.3140
[Pro]	$[C_2H_3O_2]$	-38.46692	5.39592	-10.46227	-43.5333
	$[C_7H_5O_2]$	-34.86000	5.35415	-13.58500	-43.0909
	[Br]	-20.47735	5.71367	-10.25360	-25.0173
	$[C_4H_7O_2]$	-38.41700	5.52259	-12.46300	-45.3574
	$[C_4H_9SO_4]$	-17.89000	6.32179	-14.46800	-26.0362
	[Cl]	-25.42798	6.49073	-9.93012	-28.8674
	$[C_2H_6SO_4]$	-17.89700	5.67537	-12.45500	-24.6766
	$[CHO_2]$	-34.09800	4.88064	-9.38520	-38.6026
	$[C_6H_{11}O_2]$	-39.46500	6.10888	-14.40900	-47.7651
	$[HSO_4]$	-22.28700	3.92500	-10.11800	-28.4800
	[I]	-14.54800	4.89698	-11.65000	-21.3010
	$[C_3H_5O_3]$	-30.87600	4.46643	-11.49600	-37.9056
	$[NO_3]$	-20.96800	3.84833	-9.03940	-26.1591
	$[C_8H_{15}O_2]$	-39.44400	6.32698	-16.31800	-49.4350
	$[C_8H_{17}SO_4]$	-17.71600	7.47979	-18.63800	-28.8742
	$[C_3H_5O_2]$	-39.26226	5.48702	-11.43252	-45.2078
	$[C_7H_5O_3]$	-26.24600	4.96843	-13.53600	-34.8136
	[SCN]	-18.28300	3.68323	-11.14100	-25.7408
	$[BF_4]$	-10.79239	4.42292	-8.90804	-15.2775
	$[C_2F_3O_2]$	-23.91600	4.31197	-10.00900	-29.6130
[Ser]	$[C_2H_3O_2]$	-56.47820	3.57022	-9.46461	-62.3726
	$[C_7H_5O_2]$	-50.59900	5.24733	-12.70500	-58.0567

	[Br]	-31.70515	3.15868	-8.88104	-37.4275
	$[C_4H_7O_2]$	-56.25500	4.25626	-11.50900	-63.5077
	$[C_4H_9SO_4]$	-27.74600	7.01456	-13.47700	-34.2084
	[Cl]	-39.19332	2.64031	-8.68290	-45.2359
	$[C_2H_6SO_4]$	-27.73000	6.33220	-11.41800	-32.8158
	$[CHO_2]$	-50.60200	3.17036	-8.32040	-55.7520
	$[C_6H_{11}O_2]$	-57.91700	4.64750	-13.47000	-66.7395
	$[HSO_4]$	-31.56200	5.84877	-8.68500	-34.3982
	[I]	-22.79100	4.86797	-10.28400	-28.2070
	$[C_3H_5O_3]$	-45.69400	4.28506	-10.46700	-51.8759
	$[NO_3]$	-31.47600	5.20373	-7.79370	-34.0660
	$[C_8H_{15}O_2]$	-57.62000	5.09269	-15.38900	-67.9163
	$[C_8H_{17}SO_4]$	-27.70500	7.98150	-17.65500	-37.3785
	$[C_3H_5O_2]$	-57.62143	3.96889	-10.45916	-64.1117
	$[C_7H_5O_3]$	-37.98200	6.72419	-12.62800	-43.8858
	[SCN]	-26.91400	7.83843	-10.02000	-29.0956
	$[BF_4]$	-17.41247	11.02110	-8.02326	-14.4146
	$[C_2F_3O_2]$	-35.31500	6.40415	-9.29970	-38.2106
[Thr]	$[C_2H_3O_2]$	-41.45596	3.96986	-10.20940	-47.6955
	$[C_7H_5O_2]$	-36.56900	5.07554	-13.39700	-44.8905
	[Br]	-24.53538	3.58745	-9.68298	-30.6309
	$[C_4H_7O_2]$	-56.25500	4.25626	-11.50900	-63.5077
	$[C_4H_9SO_4]$	-27.74600	7.01456	-13.47700	-34.2084
	[Cl]	-30.26478	3.57587	-9.52380	-36.2127
	$[C_2H_6SO_4]$	-27.73000	6.33220	-11.41800	-32.8158
	$[CHO_2]$	-50.60200	3.17036	-8.32040	-55.752
	$[C_6H_{11}O_2]$	-42.52900	4.90354	-14.19900	-51.8245
	$[HSO_4]$	-24.89200	4.39265	-9.62310	-30.1225
	[I]	-17.56800	4.19459	-11.10300	-24.4764
	$[C_3H_5O_3]$	-33.55600	4.04026	-11.22200	-40.7377
	$[NO_3]$	-22.99800	3.98103	-8.65960	-27.6766
	$[C_8H_{15}O_2]$	-42.18700	5.26784	-16.11800	-53.0372
	$[C_8H_{17}SO_4]$	-20.61400	7.36424	-18.41600	-31.6658
	$[C_3H_5O_2]$	-42.32452	4.27528	-11.19596	-49.2452
	$[C_7H_5O_3]$	-27.09100	5.79903	-13.32300	-34.6150

	[SCN]	-18.81200	5.45129	-10.70300	-24.0637
	[BF_4]	-12.91444	7.16339	-8.67112	-14.4222
	[$C_2F_3O_2$]	-25.53200	5.19444	-9.91540	-30.2530
[Trp]	[$C_2H_3O_2$]	-43.83079	5.28686	-14.47811	-53.0220
	[$C_7H_5O_2$]	-39.16500	6.43087	-17.63100	-50.3651
	[Br]	-24.74475	4.85275	-14.08616	-33.9782
	[$C_4H_7O_2$]	-41.13500	4.46740	-12.24100	-48.9086
	[$C_4H_9SO_4$]	-20.82200	6.33781	-14.21300	-28.6972
	[Cl]	-30.55178	4.69438	-13.90261	-39.7600
	[$C_2H_6SO_4$]	-20.84700	5.69786	-12.16700	-27.3161
	[CHO_2]	-37.48500	3.40367	-9.09260	-43.1739
	[$C_6H_{11}O_2$]	-44.88900	6.14935	-18.32700	-57.0667
	[HSO_4]	-25.23200	5.98247	-14.36500	-33.6145
	[I]	-17.61300	5.65875	-15.53700	-27.4913
	[$C_3H_5O_3$]	-35.39000	5.41627	-15.54700	-45.5207
	[NO_3]	-24.22400	5.54611	-13.24100	-31.9189
	[$C_8H_{15}O_2$]	-44.66600	6.52048	-20.20600	-58.3515
	[$C_8H_{17}SO_4$]	-21.14700	8.37825	-22.57600	-35.3448
	[$C_3H_5O_2$]	-44.63145	5.57886	-15.42013	-54.4727
	[$C_7H_5O_3$]	-29.24600	7.18684	-17.64600	-39.7052
	[SCN]	-20.45600	6.89751	-15.11400	-28.6725
	[BF_4]	-12.89370	8.27485	-12.95530	-17.5742
	[$C_2F_3O_2$]	-26.98700	6.57773	-13.98300	-34.3923
[Tyr]	[$C_2H_3O_2$]	-54.67455	4.85890	-13.27924	-63.0949
	[$C_7H_5O_2$]	-48.97800	6.01617	-16.46200	-59.4238
	[Br]	-30.62599	4.55778	-12.79580	-38.8640
	[$C_4H_7O_2$]	-54.46300	5.33918	-15.26400	-64.3878
	[$C_4H_9SO_4$]	-26.65300	7.23264	-17.27400	-36.6944
	[Cl]	-37.89254	4.31263	-12.65482	-46.2347
	[$C_2H_6SO_4$]	-26.65200	6.66812	-15.28700	-35.2709
	[CHO_2]	-48.97700	4.40854	-12.20900	-56.7775
	[$C_6H_{11}O_2$]	-56.10400	5.74951	-17.19100	-67.5455
	[HSO_4]	-30.33200	5.63759	-12.96900	-37.6634
	[I]	-21.81800	5.41332	-14.25300	-30.6577
	[$C_3H_5O_3$]	-44.15500	5.05979	-14.31000	-53.4052

	$[NO_3]$	-30.29300	5.19017	-11.91200	-37.0148
	$[C_8H_{15}O_2]$	-55.85300	6.12483	-19.09000	-68.8182
	$[C_8H_{17}SO_4]$	-26.41800	8.20604	-21.41200	-39.6240
	$[C_3H_5O_2]$	-55.81062	5.16040	-14.24117	-64.8914
	$[C_7H_5O_3]$	-36.65700	6.80035	-16.42600	-46.2827
	[SCN]	-25.72200	6.54765	-13.88400	-33.0584
	$[BF_4]$	-16.33559	8.04946	-11.73973	-20.0259
	$[C_2F_3O_2]$	-33.99900	6.14297	-12.83800	-40.6940
[Val]	$[C_2H_3O_2]$	-40.13443	4.08852	-11.08384	-47.1298
	$[C_7H_5O_2]$	-36.13700	4.88181	-14.19000	-45.4452
	[Br]	-22.05235	4.78468	-10.66426	-27.9319
	$[C_4H_7O_2]$	-40.05500	4.22246	-13.09100	-48.9235
	$[C_4H_9SO_4]$	-19.05500	6.88903	-15.09100	-27.257
	[Cl]	-27.40863	4.49827	-10.40733	-33.3177
	$[C_2H_6SO_4]$	-19.04900	6.45334	-13.07200	-25.6677
	$[CHO_2]$	-35.90400	3.82431	-9.99830	-42.078
	$[C_6H_{11}O_2]$	-40.85200	4.44680	-15.04300	-51.4482
	$[HSO_4]$	-23.40100	5.14097	-10.72200	-28.9820
	[I]	-15.57500	5.44112	-12.04200	-22.1759
	$[C_3H_5O_3]$	-32.26100	4.22451	-12.12000	-40.1565
	$[NO_3]$	-21.86700	4.78161	-9.65370	-26.7391
	$[C_8H_{15}O_2]$	-41.15600	4.68350	-16.95000	-53.4225
	$[C_8H_{17}SO_4]$	-18.88500	7.71668	-19.26900	-30.4373
	$[C_3H_5O_2]$	-41.06014	4.13854	-12.05579	-48.9774
	$[C_7H_5O_3]$	-26.99700	5.47657	-14.14100	-35.6614
	[SCN]	-18.58300	5.54977	-11.52100	-24.5542
	$[BF_4]$	-11.35901	7.05172	-9.46724	-13.7745
	$[C_2F_3O_2]$	-25.05300	4.62902	-10.63000	-31.0540

Cations	Anions	Hydrogen Bonding	Misfit Interactions	Van der Waals Forces	Excess Enthalpy (H^E)
[EMIM]	$[C_2H_3O_2]$	-9.9070	12.7391	-12.0300	-9.1979
	$[C_7H_5O_2]$	-8.4906	10.9237	-15.1960	-12.7629
	[Br]	-5.7722	12.3369	-12.1680	-5.6033
	$[C_4H_7O_2]$	-9.7674	11.9781	-13.9750	-11.7643
	$[C_4H_9SO_4]$	-4.5239	9.3428	-16.1000	-11.2811
	[Cl]	-7.2558	14.0077	-11.5370	-4.7851
	$[C_2H_6SO_4]$	-4.6058	9.2741	-14.1320	-9.4637
	$[CHO_2]$	-8.8553	12.1156	-10.9850	-7.7247
	$[C_6H_{11}O_2]$	-10.1070	12.4505	-15.8900	-13.5465
	$[HSO_4]$	-10.1020	8.2082	-11.9480	-13.8418
	[I]	-4.1327	10.1126	-13.5680	-7.5881
	$[C_3H_5O_3]$	-7.7036	9.8502	-13.1070	-10.9604
	$[NO_3]$	-5.1500	8.7786	-10.7370	-7.1084
	$[C_8H_{15}O_2]$	-6.8351	13.9156	-17.1580	-10.0775
	$[C_8H_{17}SO_4]$	-4.3708	9.9542	-20.1970	-14.6136
	$[C_3H_5O_2]$	-10.1270	12.5181	-12.9740	-10.5829
	$[C_7H_5O_3]$	-5.8865	8.2842	-15.1970	-12.7993
	[SCN]	-4.0110	7.4504	-13.0830	-9.6436
	$[BF_4]$	-2.9910	6.2971	-10.3410	-7.0349
	$[C_2F_3O_2]$	-5.5832	7.5951	-11.3050	-9.2931
[BMIM]	$[C_2H_3O_2]$	-9.8292	12.5244	-14.0360	-11.3408
	$[C_7H_5O_2]$	-8.4488	11.1651	-17.1740	-14.4577
	[Br]	-5.6316	11.7974	-14.1680	-8.0022
	$[C_4H_7O_2]$	-9.7162	12.0062	-15.9980	-13.708
	$[C_4H_9SO_4]$	-4.4394	9.7671	-18.1220	-12.7943
	[Cl]	-7.1156	13.3089	-13.5340	-7.3407
	$[C_2H_6SO_4]$	-4.5064	9.5991	-16.1400	-11.0473
	$[CHO_2]$	-8.7552	11.7758	-12.9820	-9.9614
	$[C_6H_{11}O_2]$	-10.0610	12.5216	-17.9220	-15.4614
	$[HSO_4]$	-9.8998	8.30448	-13.9550	-15.5503
	[I]	-2.9755	11.0046	-15.0710	-7.0419
	$[C_3H_5O_3]$	-7.6334	9.9979	-15.1230	-12.7585
	$[NO_3]$	-5.0364	8.8132	-12.7270	-8.9502

	$[C_8H_{15}O_2]$	-9.9894	12.3518	-19.8130	-17.4506
	$[C_8H_{17}SO_4]$	-4.3006	10.3870	-22.2340	-16.1476
	$[C_3H_5O_2]$	-10.0660	12.4312	-14.9860	-12.6208
	$[C_7H_5O_3]$	-5.9458	8.7440	-17.1800	-14.3818
	[SCN]	-3.9393	7.7895	-15.0290	-11.1788
	$[BF_4]$	-2.8611	6.8790	-12.3559	-8.338
	$[C_2F_3O_2]$	-5.4812	8.0975	-13.2440	-10.6277
[HMIM]	$[C_2H_3O_2]$	-9.7048	12.4848	-16.0690	-13.289
	$[C_7H_5O_2]$	-5.6648	13.0529	-18.5370	-11.1489
	[Br]	-5.4948	11.6236	-16.2060	-10.0772
	$[C_4H_7O_2]$	-9.6059	12.0918	-18.0380	-15.5521
	$[C_4H_9SO_4]$	-4.3465	10.0832	-20.1620	-14.4253
	[Cl]	-6.9735	13.0155	-15.5650	-9.523
	$[C_2H_6SO_4]$	-4.4041	9.8739	-18.1720	-12.7022
	$[CHO_2]$	-8.6252	11.6973	-15.0110	-11.9389
	$[C_6H_{11}O_2]$	-9.9524	12.6258	-19.9670	-17.2936
	$[HSO_4]$	-9.7706	8.5580	-15.9810	-17.1936
	[I]	-2.8490	11.2562	-17.0240	-8.6168
	$[C_3H_5O_3]$	-7.5258	10.1718	-17.1600	-14.514
	$[NO_3]$	-4.9238	8.9938	-14.7520	-10.682
	$[C_8H_{15}O_2]$	-9.8860	12.4917	-21.8620	-19.2563
	$[C_8H_{17}SO_4]$	-4.2194	10.7092	-24.2830	-17.7932
	$[C_3H_5O_2]$	-6.8681	14.0647	-16.3480	-9.1514
	$[C_7H_5O_3]$	-5.8734	9.1408	-19.1930	-15.9256
	[SCN]	-3.8588	8.1605	-17.0370	-12.7353
	$[BF_4]$	-2.7522	7.3994	-14.3940	-9.7468
	$[C_2F_3O_2]$	-5.4723	8.4645	-15.3520	-12.3598
[OMIM]	$[C_2H_3O_2]$	-9.6920	12.4953	-18.0940	-15.2907
	$[C_7H_5O_2]$	-8.4289	11.5544	-21.2080	-18.0825
	[Br]	-5.4373	11.6020	-18.2320	-12.0673
	$[C_4H_7O_2]$	-9.6059	12.0918	-18.0380	-15.5521
	$[C_4H_9SO_4]$	-4.3465	10.0832	-20.1620	-14.4253
	[Cl]	-6.9857	12.8575	-17.6010	-11.7292
	$[C_2H_6SO_4]$	-4.4041	9.8739	-18.1720	-12.7022
	$[CHO_2]$	-8.6252	11.6973	-15.0110	-11.9389
	$[C_6H_{11}O_2]$	-10.0430	12.6728	-22.0100	-19.3802

	$[HSO_4]$	-9.7332	8.8541	-18.0110	-18.8901
	[I]	-3.8505	10.0825	-19.6120	-13.38
	$[C_3H_5O_3]$	-9.6883	12.1403	-20.0770	-17.625
	$[NO_3]$	-4.9179	9.2287	-16.7820	-12.4712
	$[C_8H_{15}O_2]$	-9.9809	12.5600	-23.9070	-21.3279
	$[C_8H_{17}SO_4]$	-4.2234	10.9795	-26.3270	-19.5709
	$[C_3H_5O_2]$	-9.9412	12.4938	-19.0480	-16.4954
	$[C_7H_5O_3]$	-5.8631	9.4836	-21.2020	-17.5815
	[SCN]	-3.8586	8.5381	-19.0500	-14.3705
	$[BF_4]$	-2.7067	7.9059	-16.4340	-11.2348
	$[C_2F_3O_2]$	-5.5068	8.7820	-17.3840	-14.1088
[EPy]	$[C_2H_3O_2]$	-9.3672	12.5114	-11.7830	-8.6388
	$[C_7H_5O_2]$	-5.3667	12.1915	-14.4560	-7.6312
	[Br]	-5.6464	11.9755	-12.0150	-5.6859
	$[C_4H_7O_2]$	-9.1795	11.7813	-13.7110	-11.1092
	$[C_4H_9SO_4]$	-4.3845	9.0396	-15.8280	-11.1729
	[Cl]	-3.5527	10.3949	-8.3160	-1.4738
	$[C_2H_6SO_4]$	-4.4809	8.9385	-13.8700	-9.4124
	$[CHO_2]$	-8.4283	11.8616	-10.7480	-7.3147
	$[C_6H_{11}O_2]$	-9.5156	12.2472	-15.6180	-12.8864
	$[HSO_4]$	-9.9115	7.8223	-11.7140	-13.8032
	[I]	-3.0561	10.6526	-13.0240	-5.4275
	$[C_3H_5O_3]$	-7.2763	9.6106	-12.8400	-10.5057
	$[NO_3]$	-4.9473	8.4541	-10.4880	-6.9812
	$[C_8H_{15}O_2]$	-9.3985	12.0584	-17.4950	-14.8351
	$[C_8H_{17}SO_4]$	-4.2137	9.6815	-19.9150	-14.4472
	$[C_3H_5O_2]$	-9.5511	12.3125	-12.7190	-9.9576
	$[C_7H_5O_3]$	-5.4842	8.0922	-14.9730	-12.365
	[SCN]	-3.7274	7.1983	-12.9530	-9.4821
	$[BF_4]$	-2.9679	5.9829	-10.0560	-7.041
	$[C_2F_3O_2]$	-5.1795	7.4278	-11.0250	-8.7767
[BPy]	$[C_2H_3O_2]$	-9.1540	12.2964	-13.7790	-10.6366
	$[C_7H_5O_2]$	-7.7234	11.0317	-16.9420	-13.6337
	[Br]	-5.3947	11.4358	-14.0140	-7.9729
	$[C_4H_7O_2]$	-9.0037	11.8140	-15.7310	-12.9207
	$[C_4H_9SO_4]$	-4.2155	9.5187	-17.8490	-12.5458

	[Cl]	-6.8334	12.9489	-13.2760	-7.1605
	$[C_2H_6SO_4]$	-4.2924	9.3340	-15.8730	-10.8314
	$[CHO_2]$	-8.1967	11.5236	-12.7300	-9.4031
	$[C_6H_{11}O_2]$	-9.3426	12.3170	-17.6500	-14.6756
	$[HSO_4]$	-9.6961	8.0491	-13.6920	-15.339
	[I]	-3.8507	9.5723	-15.3950	-9.6734
	$[C_3H_5O_3]$	-7.0925	9.7937	-14.8510	-12.1498
	$[NO_3]$	-4.7360	8.5527	-12.4620	-8.6453
	$[C_8H_{15}O_2]$	-6.3360	13.9351	-18.8710	-11.2719
	$[C_8H_{17}SO_4]$	-4.0645	10.1631	-21.9530	-15.8544
	$[C_3H_5O_2]$	-9.3583	12.2267	-14.7250	-11.8566
	$[C_7H_5O_3]$	-5.3686	8.6548	-16.9390	-13.6528
	[SCN]	-3.5852	7.6111	-14.8860	-10.8601
	$[BF_4]$	-2.7664	6.6615	-12.0620	-8.1669
	$[C_2F_3O_2]$	-5.0681	7.9611	-13.0370	-10.144
[HPy]	$[C_2H_3O_2]$	-9.0707	12.2491	-15.7910	-12.6126
	$[C_7H_5O_2]$	-5.1485	12.9675	-18.2870	-10.468
	[Br]	-5.2730	11.2655	-16.0300	-10.0375
	$[C_4H_7O_2]$	-8.9374	11.8910	-12.2620	-9.3084
	$[C_4H_9SO_4]$	-4.1382	9.8502	-16.7850	-11.073
	[Cl]	-6.7145	12.6470	-15.2850	-9.3525
	$[C_2H_6SO_4]$	-4.2042	9.6284	-12.8450	-7.4208
	$[CHO_2]$	-8.1010	11.4419	-6.2779	-2.937
	$[C_6H_{11}O_2]$	-9.2812	12.4095	-19.6800	-16.5517
	$[HSO_4]$	-9.5776	8.3265	-15.6970	-16.9481
	[I]	-3.7392	9.6296	-17.4020	-11.5116
	$[C_3H_5O_3]$	-7.0147	9.9737	-10.7620	-7.803
	$[NO_3]$	-4.6364	8.7552	-6.3372	-2.2184
	$[C_8H_{15}O_2]$	-9.1828	12.3026	-21.5720	-18.4522
	$[C_8H_{17}SO_4]$	-4.0000	10.4955	-24.9770	-18.4815
	$[C_3H_5O_2]$	-9.2653	12.2465	-16.7210	-13.7398
	$[C_7H_5O_3]$	-5.3184	9.0644	-14.7950	-11.049
	[SCN]	-3.5132	8.00334	-9.2801	-4.78996
	$[BF_4]$	-2.6628	7.21512	-14.0830	-9.53068
	$[C_2F_3O_2]$	-5.0157	8.3608	-15.0530	-11.7079

[OPy]	**[$C_2H_3O_2$]**	**-9.0176**	**12.2785**	**-17.8110**	**-14.5501**
	[$C_7H_5O_2$]	-7.6310	11.4692	-20.9390	-17.1008
	[Br]	-5.1882	11.2637	-18.0490	-11.9735
	[$C_4H_7O_2$]	-8.8949	11.9883	-12.269	-9.1756
	[$C_4H_9SO_4$]	-4.0766	10.1633	-16.7930	-10.7063
	[Cl]	-6.6342	12.5359	-17.3050	-11.4033
	[$C_2H_6SO_4$]	-4.1354	9.9318	-12.8460	-7.0496
	[CHO_2]	-8.0392	11.4742	-6.2747	-2.8397
	[$C_6H_{11}O_2$]	-9.2425	12.5064	-21.7110	-18.4471
	[HSO_4]	-9.4849	8.6564	-17.7130	-18.5415
	[I]	-3.6571	9.8117	-19.4140	-13.2594
	[$C_3H_5O_3$]	-6.9593	10.1716	-10.7670	-7.5547
	[NO_3]	-4.5632	9.0278	-6.3305	-1.8659
	[$C_8H_{15}O_2$]	-9.1490	12.4205	-23.6060	-20.3345
	[$C_8H_{17}SO_4$]	-3.9483	10.7955	-24.9920	-18.1448
	[$C_3H_5O_2$]	-9.2387	12.2985	-18.7640	-15.7042
	[$C_7H_5O_3$]	-5.2821	9.4275	-14.7830	-10.6376
	[SCN]	-3.4595	8.41156	-9.2490	-4.29694
	[BF_4]	-2.5812	7.7466	-16.1120	-10.9466
	[$C_2F_3O_2$]	-4.9766	8.71466	-17.074	-13.3359
[EMPyrr]	[$C_2H_3O_2$]	-4.4588	15.3480	-12.1060	-1.2168
	[$C_7H_5O_2$]	-3.5879	13.0985	-15.1510	-5.6404
	[Br]	-2.8233	14.7372	-12.0390	-0.1251
	[$C_4H_7O_2$]	-4.3141	14.3865	-12.2470	-2.1746
	[$C_4H_9SO_4$]	-2.1408	10.7378	-16.7470	-8.15
	[Cl]	-3.5295	16.7004	-11.6390	1.5319
	[$C_2H_6SO_4$]	-2.2089	10.7908	-12.7910	-4.2091
	[CHO_2]	-4.0323	14.6582	-6.2228	4.4031
	[$C_6H_{11}O_2$]	-4.4656	14.8623	-16.0340	-5.6373
	[HSO_4]	-7.8192	9.78924	-11.9870	-10.017
	[I]	-2.0660	12.0864	-13.4360	-3.4156
	[$C_3H_5O_3$]	-3.4467	11.8853	-10.7440	-2.3054
	[NO_3]	-2.4125	10.6223	-6.2936	1.9162
	[$C_8H_{15}O_2$]	-4.3751	14.5703	-17.9380	-7.7428
	[$C_8H_{17}SO_4$]	-2.0238	11.2445	-24.9590	-15.7383
	[$C_3H_5O_2$]	-4.3931	15.1318	-13.0680	-2.3293

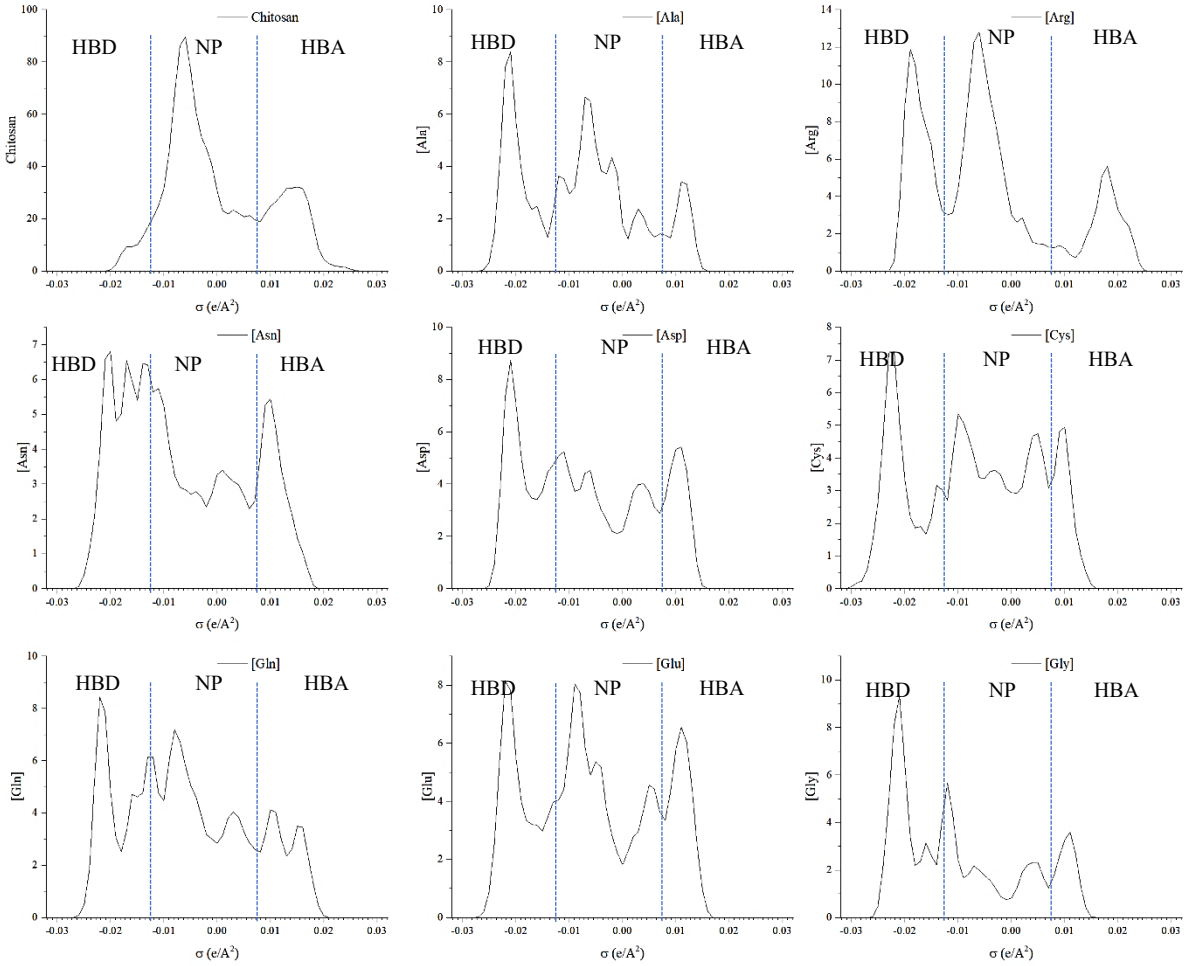
	$[C_7H_5O_3]$	-2.4663	9.7770	-14.6510	-7.3403
	[SCN]	-1.7645	9.0117	-8.9235	-1.6763
	$[BF_4]$	-1.5454	7.4309	-10.5030	-4.6175
	$[C_2F_3O_2]$	-2.3846	9.1261	-11.4120	-4.6705
[BMPyrr]	$[C_2H_3O_2]$	-4.4133	14.9694	-14.1440	-3.5879
	$[C_7H_5O_2]$	-3.5678	13.2508	-17.1680	-7.485
	[Br]	-2.7252	13.9801	-14.0730	-2.8181
	$[C_4H_7O_2]$	-4.2925	14.3232	-12.2470	-2.2163
	$[C_4H_9SO_4]$	-2.0697	11.1077	-16.7430	-7.705
	[Cl]	-3.4310	15.7857	-13.6830	-1.3283
	$[C_2H_6SO_4]$	-2.1261	11.0060	-12.7830	-3.9031
	$[CHO_2]$	-3.9638	14.1104	-6.2194	3.9272
	$[C_6H_{11}O_2]$	-4.4529	14.8801	-18.0740	-7.6468
	$[HSO_4]$	-7.7171	9.7171	-14.0200	-12.02
	[I]	-1.9694	11.6344	-15.4620	-5.797
	$[C_3H_5O_3]$	-3.3932	11.9203	-10.7410	-2.2139
	$[NO_3]$	-2.3207	10.4200	-6.2888	1.8105
	$[C_8H_{15}O_2]$	-4.3705	14.6645	-19.9800	-9.686
	$[C_8H_{17}SO_4]$	-1.9654	11.6773	-24.9580	-15.2461
	$[C_3H_5O_2]$	-4.4887	14.8492	-15.1060	-4.7455
	$[C_7H_5O_3]$	-2.4369	10.2303	-14.6350	-6.8416
	[SCN]	-1.7027	9.1303	-8.8875	-1.4599
	$[BF_4]$	-1.4418	7.7527	-12.5490	-6.2381
	$[C_2F_3O_2]$	-2.2747	9.5374	-13.4510	-6.1883
[HMPyrr]	$[C_2H_3O_2]$	-4.2967	14.8767	-16.1960	-5.616
	$[C_7H_5O_2]$	-3.4758	13.4511	-19.2100	-9.2347
	[Br]	-2.6179	13.7042	-16.1360	-5.0497
	$[C_4H_7O_2]$	-4.2925	14.3232	-12.2470	-2.2163
	$[C_4H_9SO_4]$	-2.0697	11.1077	-16.7430	-7.705
	[Cl]	-3.3147	15.3903	-15.7380	-3.6624
	$[C_2H_6SO_4]$	-2.1261	11.0060	-12.7830	-3.9031
	$[CHO_2]$	-3.9638	14.1104	-6.2194	3.9272
	$[C_6H_{11}O_2]$	-4.3518	14.9875	-20.1270	-9.4913
	$[HSO_4]$	-7.6140	9.8714	-16.0700	-13.8126
	[I]	-1.3596	12.6741	-16.9680	-5.6535
	$[C_3H_5O_3]$	-3.2932	12.0637	-10.7440	-1.9735

	$[NO_3]$	-2.2256	10.4983	-6.2867	1.986
	$[C_8H_{15}O_2]$	-4.2740	14.8211	-22.0340	-11.4869
	$[C_8H_{17}SO_4]$	-1.9000	12.0136	-24.9680	-14.8544
	$[C_3H_5O_2]$	-4.3780	14.8391	-17.1570	-6.6959
	$[C_7H_5O_3]$	-2.3636	10.6183	-14.6330	-6.3783
	[SCN]	-1.6303	9.4125	-8.8816	-1.0994
	$[BF_4]$	-1.3611	8.164-	-14.6020	-15.9631
	$[C_2F_3O_2]$	-2.2786	9.8722	-15.5030	-7.9094
[OMPyrr]	$[C_2H_3O_2]$	-4.2830	14.8623	-18.2430	-7.6637
	$[C_7H_5O_2]$	-3.4717	13.6429	-21.2490	-11.0778
	[Br]	-2.5744	13.6270	-18.1910	-7.1384
	$[C_4H_7O_2]$	-4.1828	14.4708	-12.2530	-1.965
	$[C_4H_9SO_4]$	-1.9632	11.7024	-16.7540	-7.0148
	[Cl]	-3.2768	15.2005	-17.7880	-5.8643
	$[C_2H_6SO_4]$	-2.0071	11.4986	-12.7870	-3.2955
	$[CHO_2]$	-3.8220	13.9221	-6.2183	3.8818
	$[C_6H_{11}O_2]$	-4.3508	15.0760	-22.1750	-11.4498
	$[HSO_4]$	-5.3363	11.5196	-17.5070	-11.3237
	[I]	-1.8347	11.6637	-19.5700	-9.741
	$[C_3H_5O_3]$	-3.27100	12.2319	-10.7460	-1.7851
	$[NO_3]$	-2.1858	10.6961	-6.2851	2.2252
	$[C_8H_{15}O_2]$	-4.2768	14.9395	-24.0820	-13.4193
	$[C_8H_{17}SO_4]$	-1.8753	12.3090	-24.9790	-14.5453
	$[C_3H_5O_2]$	-4.2332	14.9327	-19.2030	-8.5035
	$[C_7H_5O_3]$	-2.3512	10.9652	-14.6330	-6.019
	[SCN]	-1.6014	9.7612	-8.8770	-0.7172
	$[BF_4]$	-1.3134	8.6205	-16.6500	-9.3429
	$[C_2F_3O_2]$	-2.2620	10.2101	-17.5460	-9.5979

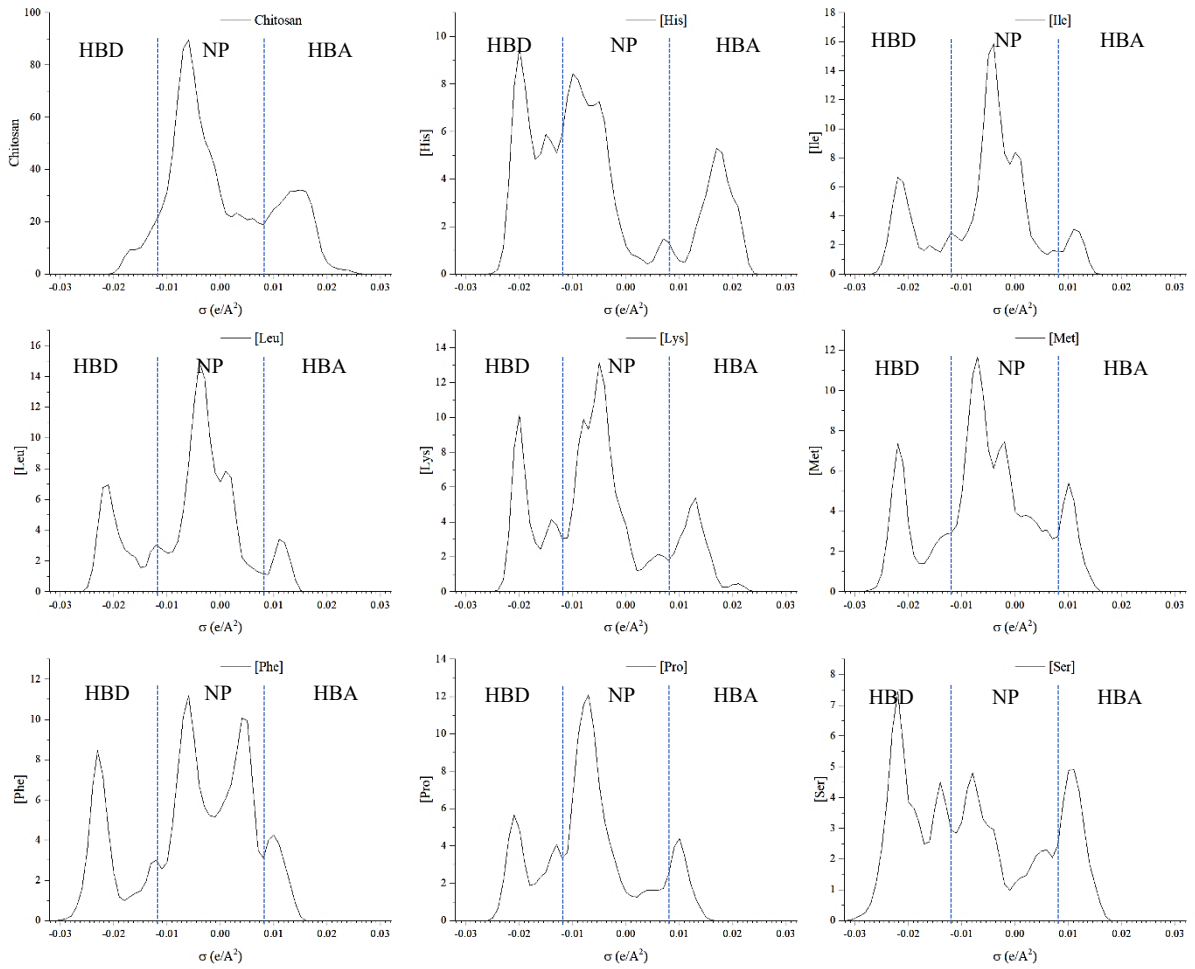
Figure S1

Sigma profile of individual amino acid cations (a, b, c) and imidazolium, pyridinium, and pyrrolidinium cations (d, e).

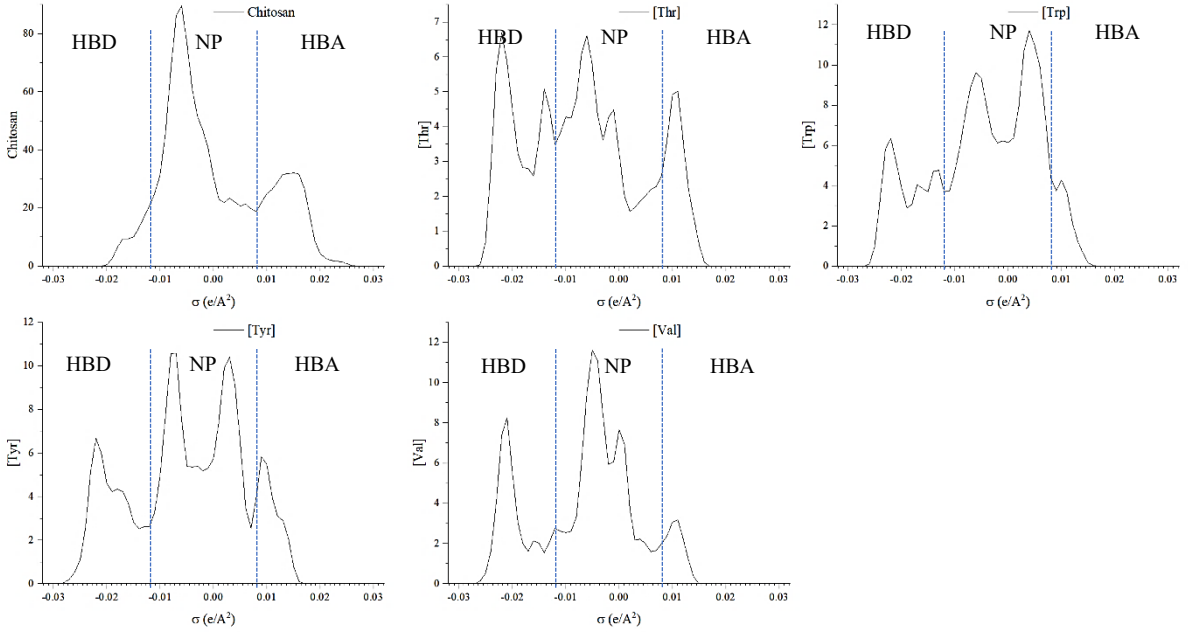
a)



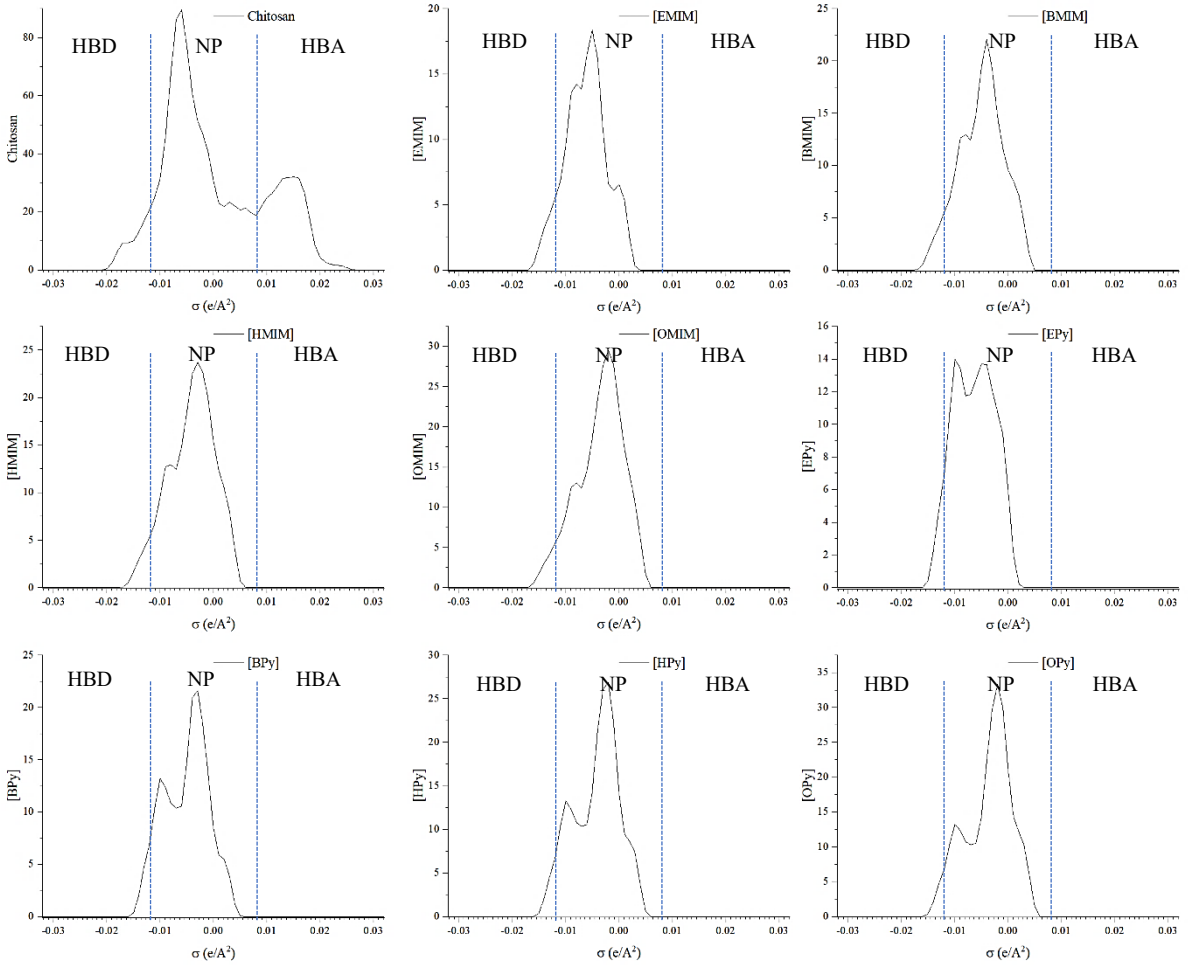
b)


Chitosan
HBD
NP
HBA
Chitosan
σ (e/A²)
[His]
[His]
[Ile]
[Ile]
[Leu]
[Leu]
[Lys]
[Lys]
[Met]
[Met]
[Phe]
[Phe]
[Pro]
[Pro]
[Ser]
[Ser]

c)


Chitosan
HBD
NP
HBA
Chitosan
σ (e/A²)
[Thr]
HBD
NP
HBA
[Thr]
σ (e/A²)
[Trp]
HBD
NP
HBA
[Trp]
σ (e/A²)
[Tyr]
HBD
NP
HBA
[Tyr]
σ (e/A²)
[Val]
HBD
NP
HBA
[Val]
σ (e/A²)

d)


Chitosan
HBD
NP
HBA
Chitosan
σ (e/A²)
[EMIM]
[EMIM]
[BMIM]
[BMIM]
[HMIM]
[HMIM]
[OMIM]
[OMIM]
[EPy]
[EPy]
[BPy]
[BPy]
[HPy]
[HPy]
[OPy]
[OPy]

e)

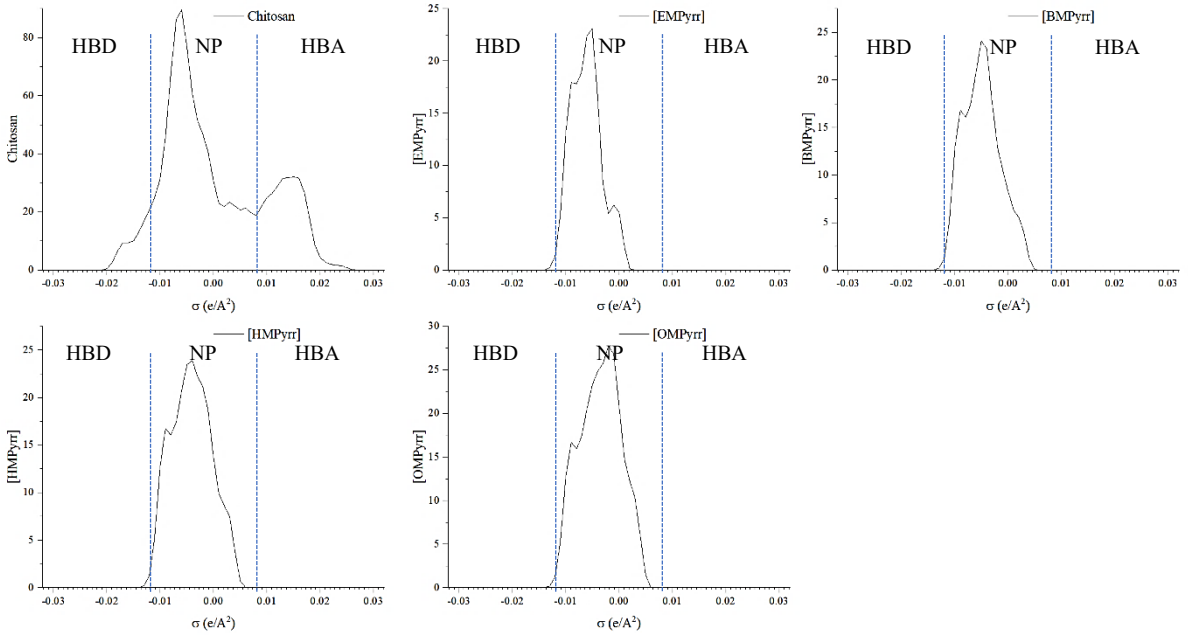
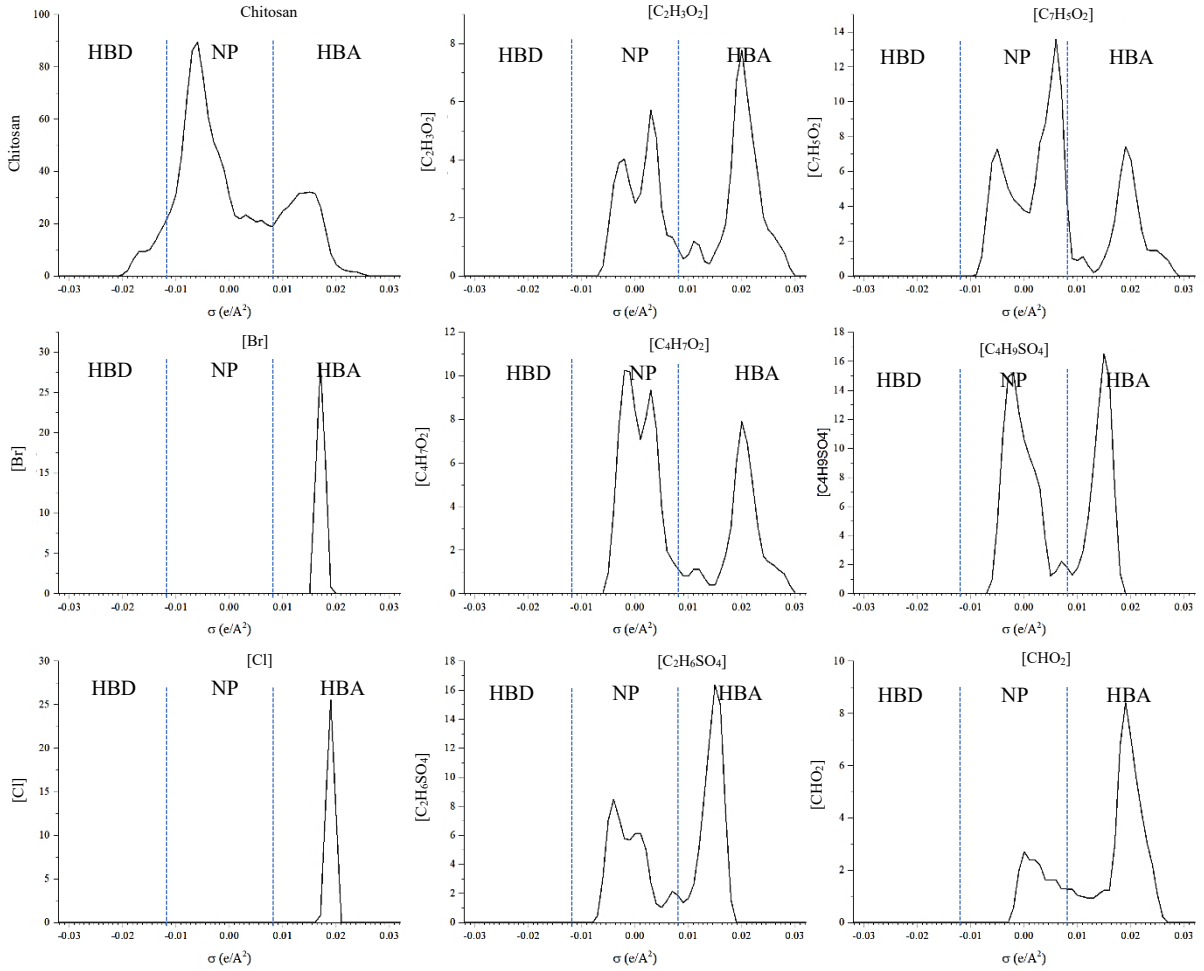

Chitosan
HBD
NP
HBA
Chitosan
σ (e/A²)
[EMPyrr]
[EMPyrr]
[BMPyrr]
[BMPyrr]
[HMPyrr]
[HMPyrr]
[OMPyrr]
[OMPyrr]

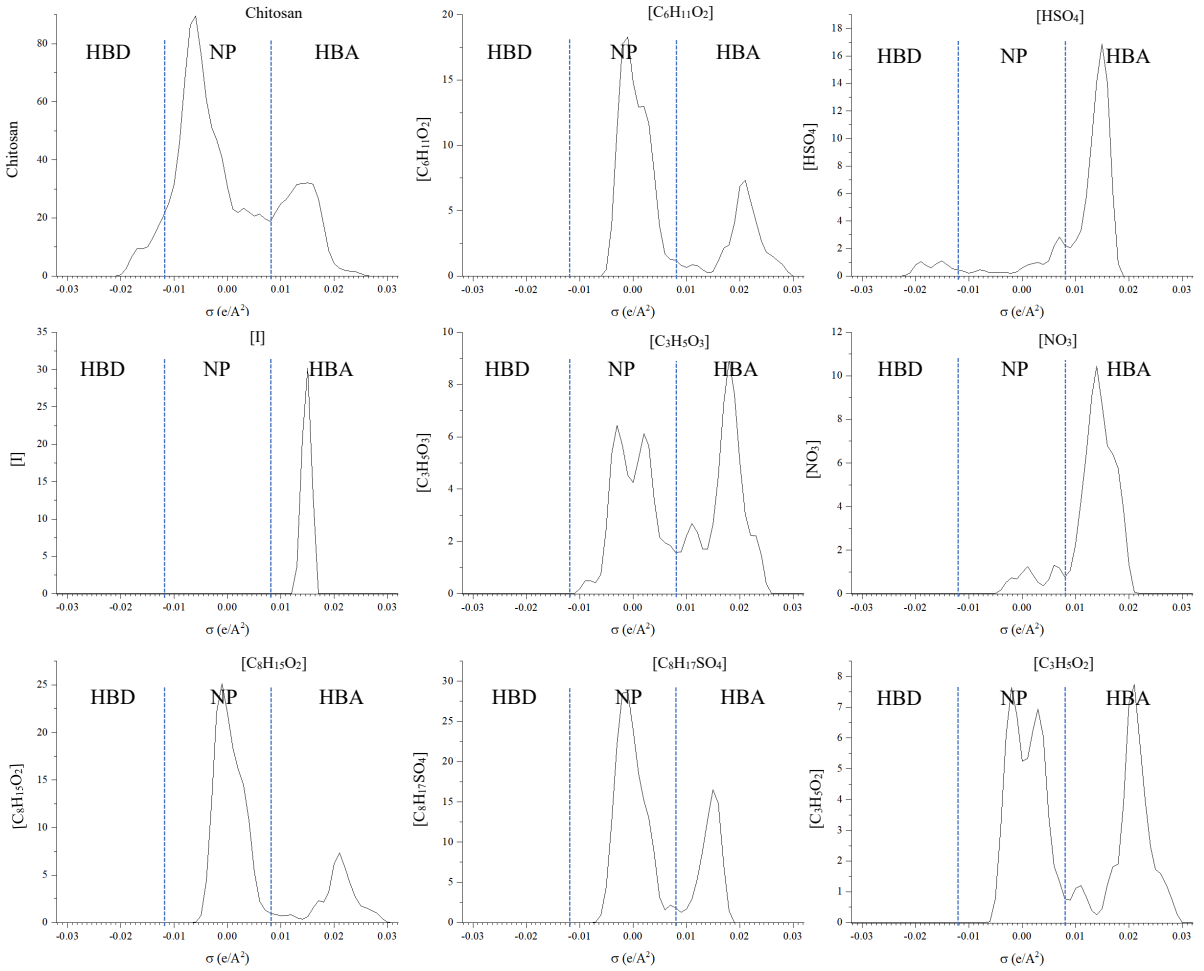
Figure S2

Sigma profile of individual anions (a, b, c)

a)



b)


Chitosan
HBD
NP
HBA
Chitosan
σ (e/A²)
[C6H11O2]
[C6H11O2]
[HSO4]
[HSO4]
[I]
[I]
[C3H5O3]
[C3H5O3]
[NO3]
[NO3]
[C8H15O2]
[C8H15O2]
[C8H17SO4]
[C8H17SO4]
[C3H5O2]
[C3H5O2]

c)

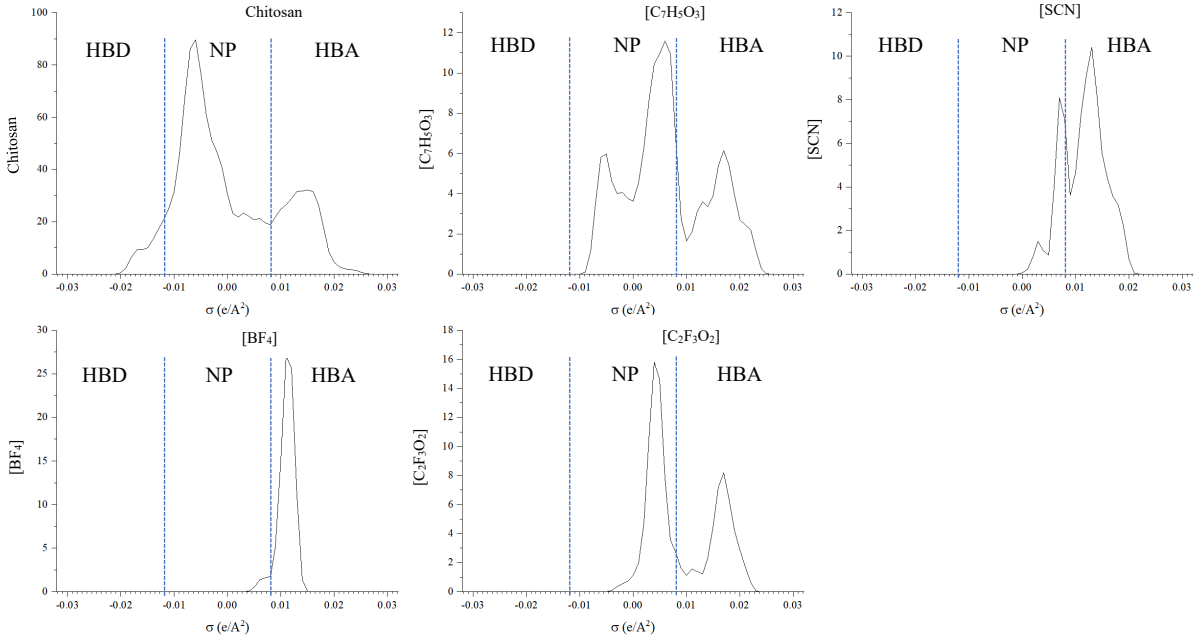

Chitosan
HBD
NP
HBA
Chitosan
σ (e/A²)
[C7H5O3]
HBD
NP
HBA
[C7H5O3]
σ (e/A²)
[SCN]
HBD
NP
HBA
[SCN]
σ (e/A²)
[BF4]
HBD
NP
HBA
[BF4]
σ (e/A²)
[C2F3O2]
HBD
NP
HBA
[C2F3O2]
σ (e/A²)

Figure S3

Suggested formation of hydrogen bonds between [Ser]$^+$ and chitosan.

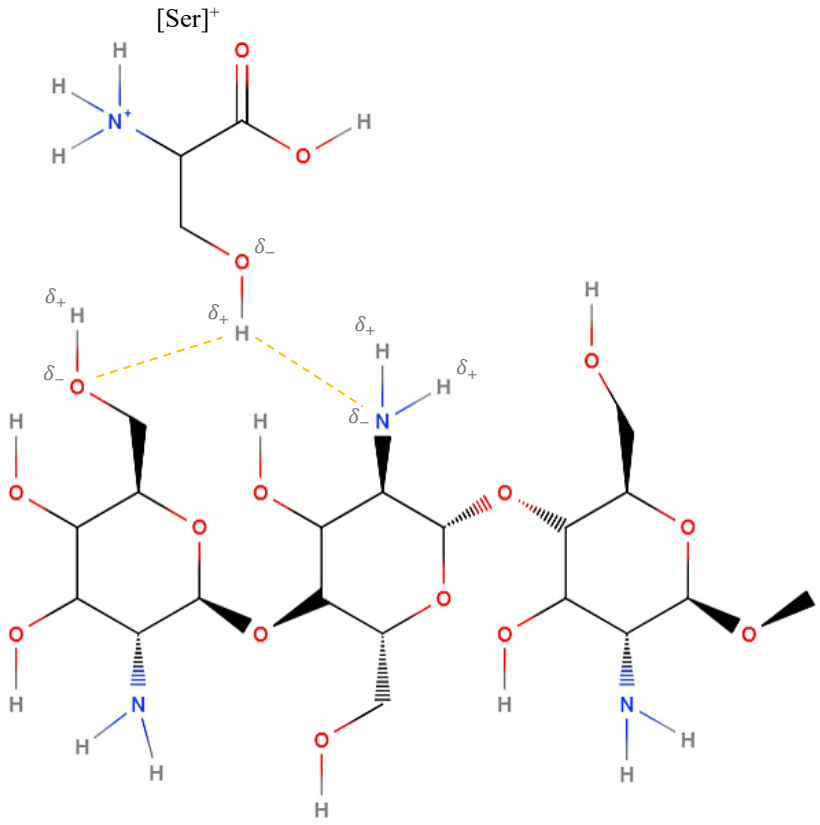


Figure S4

Suggested formation of hydrogen bonds between $[BF_4]^-$ and chitosan.