In-silico COSMO-RS Predictive Screening of Ionic Liquids for the Dissolution of Plastic

Mood Mohan[1,2], Jay Keasling[1,3,4,5,6,7,8], Blake A. Simmons[1,3], Seema Singh[*,1,2]

[1] Deconstruction Division, Joint BioEnergy Institute, 5885 Hollis Street, Emeryville, California 94608, United States.

[2] Department of Biomass Science and Conversion Technology, Sandia National Laboratories, 7011 East Avenue, Livermore, California 94551, United States.

[3] Biological Systems and Engineering Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720, United States.

[4] QB3 Institute, University of California, Berkeley, California, 94720, United States

[5] Department of Bioengineering, University of California, Berkeley, California, 94720, United States

[6] Department of Chemical and Biomolecular Engineering, University of California, Berkeley, California, 94720, United States

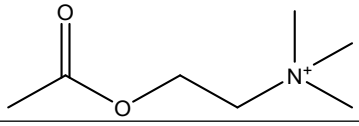
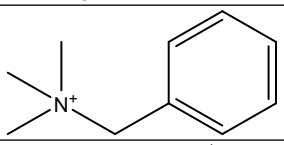
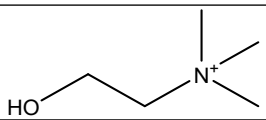
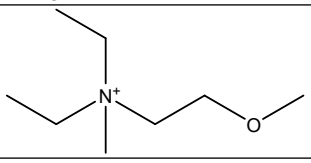
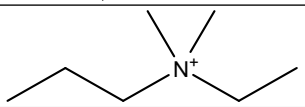
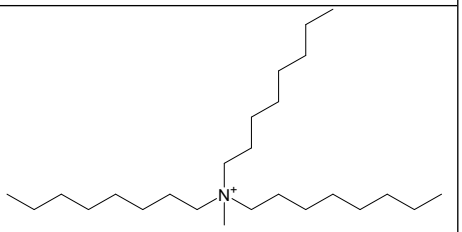
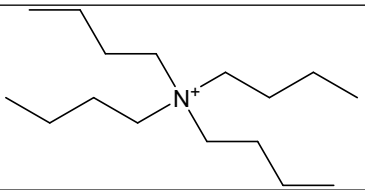
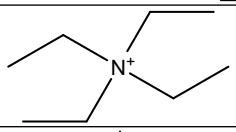
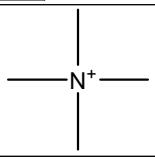
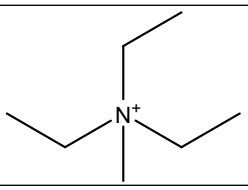
[7] Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark, Building 220, Kemitorvet, DK-2800, Kgs, Lyngby, Denmark

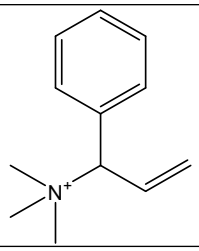
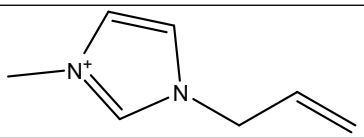
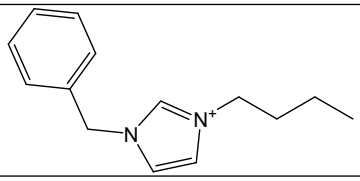
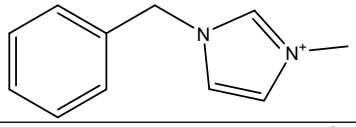
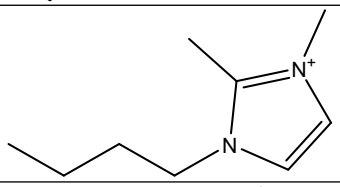
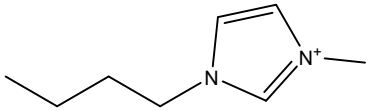
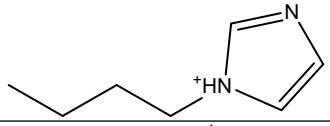
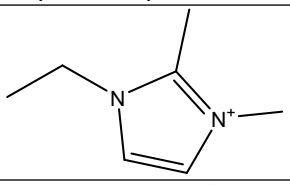
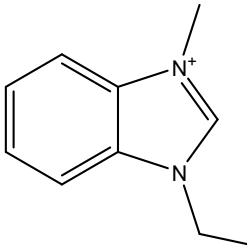
[8] Center for Synthetic Biochemistry, Shenzhen Institutes for Advanced Technologies, Shenzhen, Guangdong, 518055, China

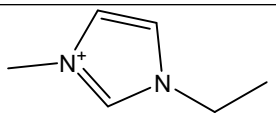
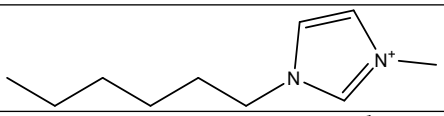
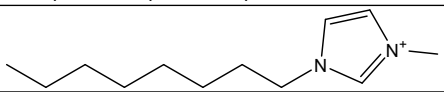
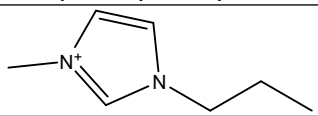
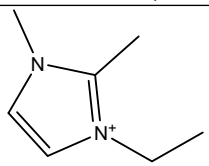
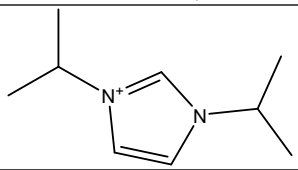
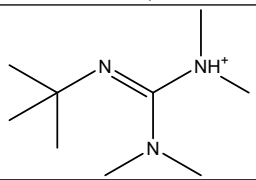
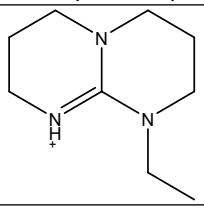
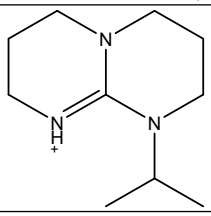
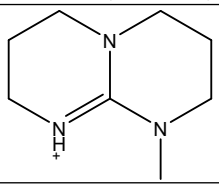
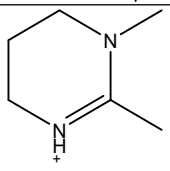
Corresponding Authors

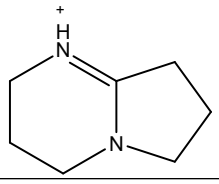
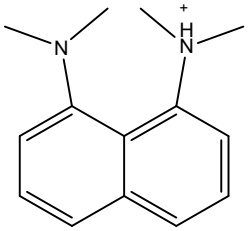
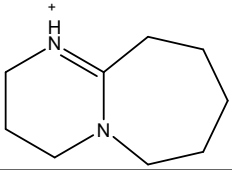
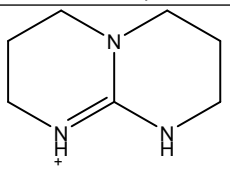
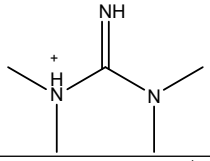
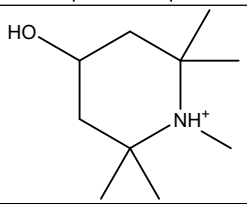
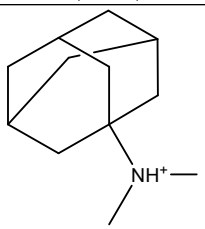
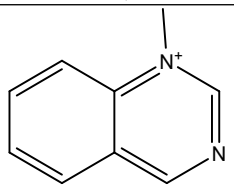
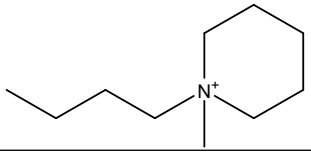
[*] E-mail: *ssingh@lbl.gov; seesing@sandia.gov* (Seema Singh)

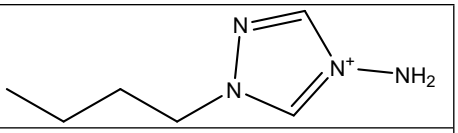
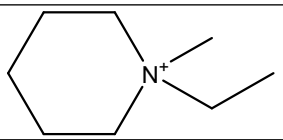
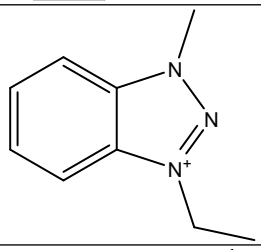
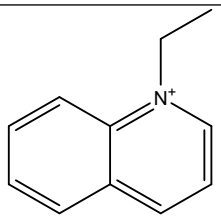
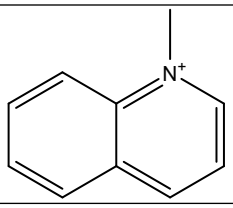
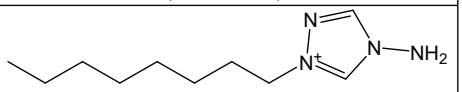
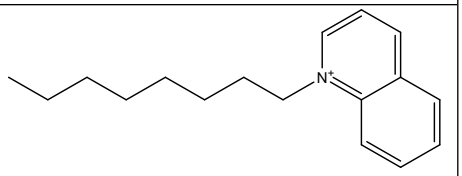
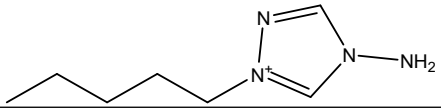
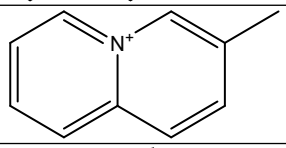
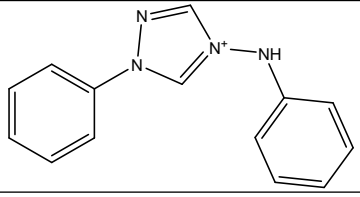
Table S1. List of cations used in this work

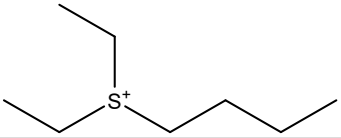
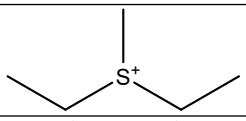
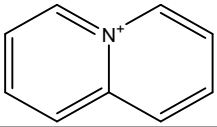
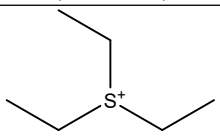
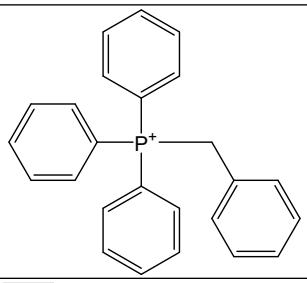
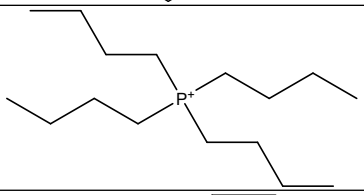
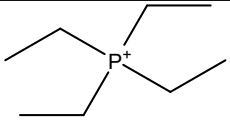
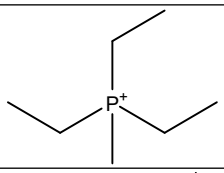
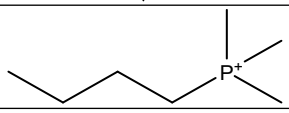
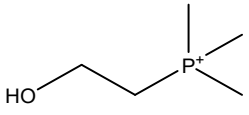
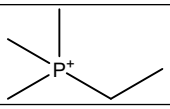
Sl. No.	Name of the cation and Acronym	Chem. Formula / mol. wt.	Chemical structure
1.	Acetylcholine $[ACh]^+$	$C_7H_{16}NO_2^+$ 146.21	
2.	Benzyltrimethylammonium $[BzTMA]^+$	$C_{10}H_{16}N^+$ 150.24	
3.	Cholinium $[Ch]^+$	$C_5H_{14}NO^+$ 104.17	
4.	Diethylmethyl(2-methoxyethyl)ammonium $[DEM\text{-}2\text{-}MeoEA]^+$	$C_8H_{20}NO^+$ 146.25	
5.	Ethyldimethylpropylammonium $[EDMPrA]^+$	$C_7H_{18}N^+$ 116.23	
6.	Methyltrioctylammonium $[MTOA]^+$	$C_{25}H_{54}N^+$ 368.71	
7.	Tetrabutylammonium $[TeBA]^+$	$C_{16}H_{36}N^+$ 242.47	
8.	Tetraethylammonium $[TeEA]^+$	$C_8H_{20}N^+$ 130.25	
9.	Tetramethylammonium $[TeMA]^+$	$C_4H_{12}N^+$ 74.15	
10.	Triethylmethylammonium $[TEMA]^+$	$C_7H_{18}N^+$ 116.23	

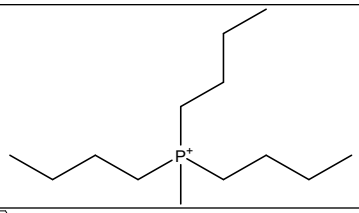
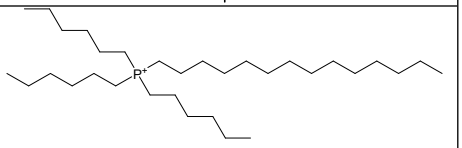
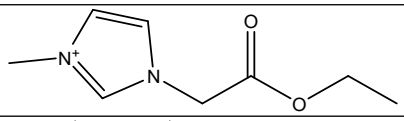
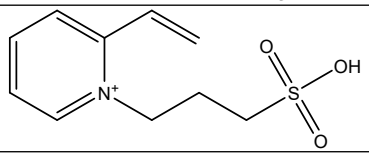
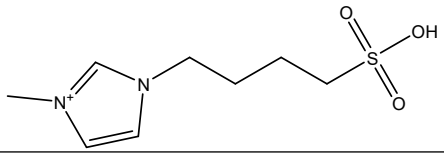
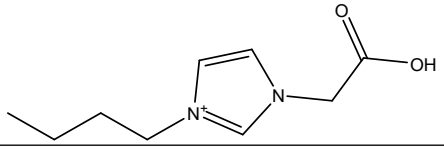
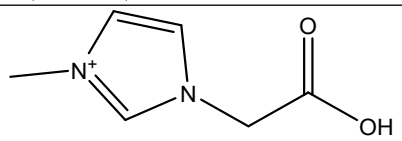
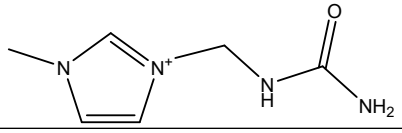
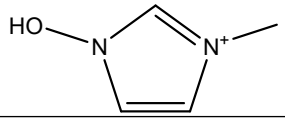
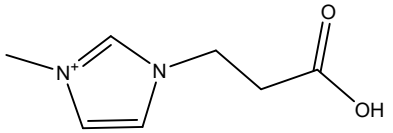
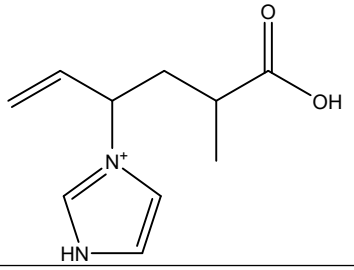
11.	Vinylbenzyltrimethylammonium $[VBeTMA]^+$	$C_{12}H_{18}N^+$ 176.28	
12.	1,3-dimethylimidazolium $[DMIM]^+$	$C_5H_9N_2^+$ 97.14	
13.	1-allyl-3-methylimidazolium $[AMIM]^+$	$C_7H_{11}N_2^+$ 123.18	
14.	1-benzyl-3-butylimidazolium $[BzBIM]^+$	$C_{14}H_{19}N_2^+$ 215.32	
15.	1-benzyl-3-methylimidazolium $[BzMIM]^+$	$C_{11}H_{13}N_2^+$ 173.24	
16.	1-butyl-2,3-dimethylimidazolium $[BDMIM]^+$	$C_9H_{17}N_2^+$ 153.25	
17.	1-butyl-3-methylimidazolium $[BMIM]^+$	$C_8H_{15}N_2^+$ 139.22	
18.	1-butylimidazolium $[1\text{-}BIM]^+$	$C_7H_{13}N_2^+$ 125.19	
19.	1-ethyl-2,3-dimethylimidazolium $[EDMIM]^+$	$C_7H_{13}N_2^+$ 125.19	
20.	1-ethyl-3-methylbenzoimidazolium $[EMBzIM]^+$	$C_{10}H_{13}N_2^+$ 161.23	

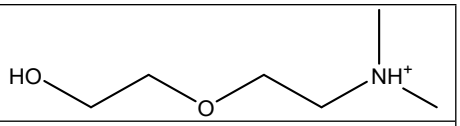
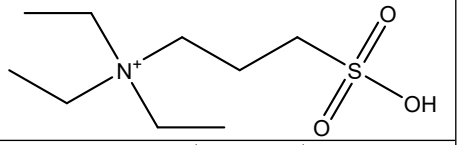
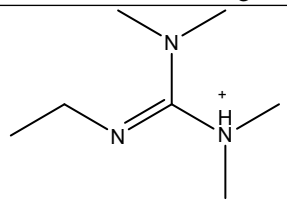
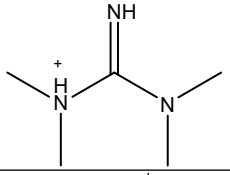
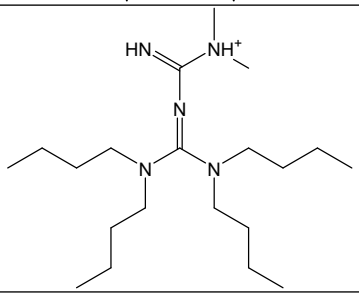
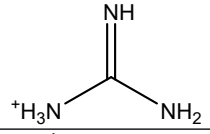
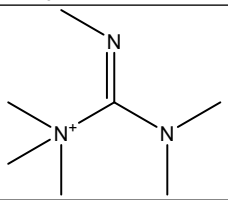
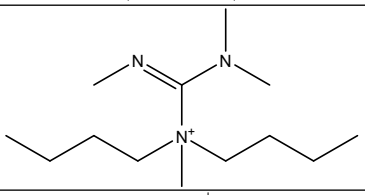
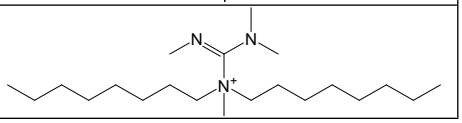
21.	1-ethyl-3-methylimidazolium $[EMIM]^+$	$C_6H_{11}N_2^+$ 111.17	
22.	1-hexyl-3-methylimidazolium $[HMIM]^+$	$C_{10}H_{19}N_2^+$ 167.28	
23.	1-octyl-3-methylimidazolium $[OMIM]^+$	$C_{12}H_{23}N_2^+$ 195.33	
24.	1-propyl-3-methylimidazolium $[PMIM]^+$	$C_7H_{13}N_2^+$ 125.19	
25.	1,2-dimethyl-3-ethylimidazolium $[DMEIM]^+$	$C_7H_{13}N_2^+$ 125.19	
26.	1,3-diisopropylimidazolium $[DIsoPIM]^+$	$C_9H_{17}N_2^+$ 153.25	
27.	2-tert-Butyl-1,1,3,3-tetramethylguanidinium $[tBTMGH]^+$	$C_9H_{22}N_3^+$ 172.30	
28.	7-ethyl-1,5,7-triazabicyclo(4.4.0)dec-5-ene $[ETBDH]^+$	$C_9H_{18}N_3^+$ 168.26	
29.	7-isopropyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene $[ITBDH]^+$	$C_{10}H_{20}N_3^+$ 182.29	
30.	7-methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene $[MTBDH]^+$	$C_8H_{16}N_3^+$ 154.24	
31.	1,2-dimethyl-1,4,5,6-tetrahydropyrimidine $[DMPH]^+$	$C_6H_{13}N_2^+$ 113.18	

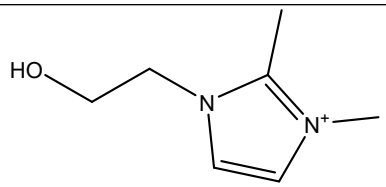
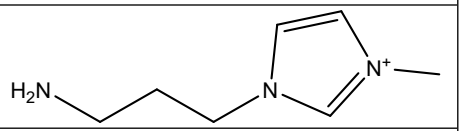
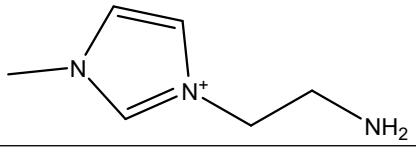
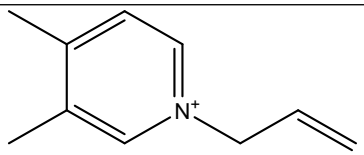
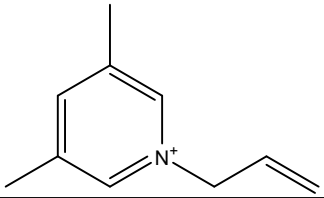
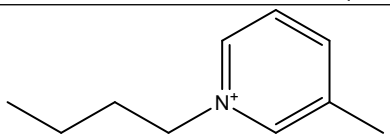
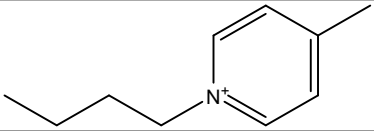
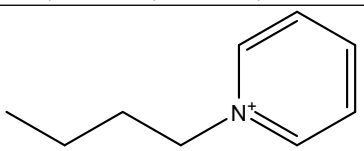
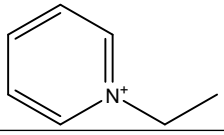
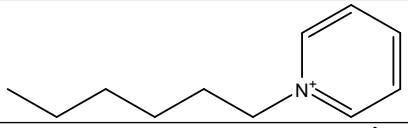
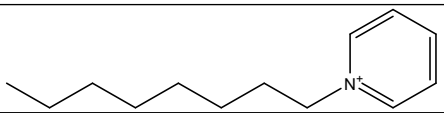
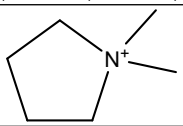
32.	1,5-diazabicyclo[4.3.0]non-5-ene $[DBNH]^+$	$C_7H_{13}N_2^+$ 125.19	
33.	1,8-bis(dimethylamino)naphthalene $[DMANH]^+$	$C_{14}H_{19}N_2^+$ 215.32	
34.	1,8-diazabicyclo[5.4.0]undec-7-ene $[DBUH]^+$	$C_9H_{17}N_2^+$ 153.25	
35.	1,5,7-triazabicyclo[4.4.0]dec-5-ene $[TBDH]^+$	$C_7H_{14}N_3^+$ 140.21	
36.	1,1,3,3-tetramethylguanidine $[TMGH]^+$	$C_5H_{14}N_3^+$ 116.19	
37.	1,2,2,6,6-pentamethyl-4-piperidinol $[PeMPipH]^+$	$C_{10}H_{22}NO^+$ 172.29	
38.	N,N-dimethyl-1-adamantylamine $[DMAAH]^+$	$C_{12}H_{22}N^+$ 180.31	
39.	1-alkyl quinazolinium $[AQunz]^+$	$C_9H_9N_2^+$ 145.18	
40.	1-butyl-1-methylpiperidinium $[BMPip]^+$	$C_{10}H_{22}N^+$ 156.29	

41.	4-amino-1-butyl-1,2,4-triazolium $[4AB124Tz]^+$	$C_6H_{13}N_4^+$ 141.20	
42.	1-ethyl-1-methylpiperidinium $[EMPip]^+$	$C_8H_{18}N^+$ 128.24	
43.	1-ethyl-3-methylbenzotriazolium $[EMBzTz]^+$	$C_9H_{12}N_3^+$ 162.22	
44.	1-ethylquinolinium $[1\text{-}EQ]^+$	$C_{11}H_{12}N^+$ 158.22	
45.	1-methylquinolinium $[1\text{-}MQ]^+$	$C_{10}H_{10}N^+$ 144.20	
46.	4-amino-1-octyl-1,2,4-triazolium $[4AO124Tz]^+$	$C_{10}H_{21}N_4^+$ 197.31	
47.	1-octylquinolinium $[1\text{-}OQ]^+$	$C_{17}H_{24}N^+$ 242.39	
48.	4-amino-1-pentyl-1,2,4-triazolium $[4AP124Tz]^+$	$C_7H_{15}N_4^+$ 155.22	
49.	3-methylquinolizinium $[3\text{-}MQunz]^+$	$C_{10}H_{10}N^+$ 144.20	
50.	1,2,4-Triazolium-4-anilino-1-phenyl $[4APh124Tz]^+$	$C_{14}H_{13}N_4^+$ 237.29	

51.	Diethylbutylsulfonium $[DEBS]^+$	$C_8H_{19}S^+$ 147.30	
52.	Diethylmethylsulfonium $[DEMS]^+$	$C_5H_{13}S^+$ 105.22	
53.	Quinolizinium $[Qunz]^+$	$C_9H_8N^+$ 130.17	
54.	Triethylsulfonium $[TES]^+$	$C_6H_{15}S^+$ 119.25	
55.	Benzyltriphenylphosphonium $[BzTPhP]^+$	$C_{25}H_{22}P^+$ 353.42	
56.	Tetrabutylphosphonium $[TeBP]^+$	$C_{16}H_{36}P^+$ 259.44	
57.	Tetraethylphosphonium $[TeEP]^+$	$C_8H_{20}P^+$ 147.22	
58.	Triethylmethylphosphonium $[TEMP]^+$	$C_7H_{18}P^+$ 133.19	
59.	Trimethylbutylphosphonium $[TMBP]^+$	$C_7H_{18}P^+$ 133.19	
60.	(2-hydroxyethyl)trimethylphosphonium $[TMEOHP]^+$	$C_5H_{14}OP^+$ 121.14	
61.	Trimethylethylphosphonium $[TMEP]^+$	$C_5H_{14}P^+$ 105.14	

62.	Tributylmethylphosphonium $[TBMP]^+$	$C_{13}H_{30}P^+$ 217.36	
63.	Trihexyltetradecylphosphoniu m $[THTeDP]^+$	$C_{32}H_{68}P^+$ 483.87	
64.	1-(2-ethoxy-2-oxoethyl)-3- methylimidazolium $[2EOMIM]^+$	$C_8H_{13}N_2O_2^+$ 169.20	
65.	1-(3-Sulfopropyl)-2- vinylpyridinium $[3SP2VPy]^+$	$C_{10}H_{14}NO_3S^+$ 228.29	
66.	1-(4-sulfobutyl)-3- methylimidazolium $[4SB3MIM]^+$	$C_8H_{15}N_2O_3S^+$ 219.28	
67.	1-carboxymethyl-3- butylimidazolium $[CMBIM]^+$	$C_9H_{15}N_2O_2^+$ 183.23	
68.	1-carboxymethyl-3- methylimidazolium $[CMMIM]^+$	$C_6H_9N_2O_2^+$ 141.15	
69.	1-ethylurea-3- methylimidazolium $[EUMIM]^+$	$C_6H_{11}N_4O^+$ 155.18	
70.	1-hydroxy-3- methylimidazolium $[(OH)MIM]^+$	$C_4H_7N_2O^+$ 99.11	
71.	1-methyl-3-(3- carboxyethyl)imidazolium $[M33CEIM]^+$	$C_7H_{11}N_2O_2^+$ 155.18	
72.	1-vinyl-3- carboxybutylimidazolium $[VCBIM]^+$	$C_{10}H_{15}N_2O_2^+$ 195.24	

73.	N,N-dimethyl-N-2-(2-hydroxyethoxy)ammonium $[DM(2OHE)A]^+$	$C_6H_{16}NO_2^+$ 134.20	
74.	Triethyl-(3-sulfopropyl)ammonium $[TE(3SP)A]^+$	$C_9H_{22}NO_3S^+$ 224.34	
75.	2-ethyl-1,1,3,3-tetramethylguanidinium $[2ETeG]^+$	$C_7H_{18}N_3^+$ 144.24	
76.	1,1,3,3-tetramethylguanidine $[TMGH]^+$	$C_5H_{14}N_3^+$ 116.19	
77.	Bis(bis(butyl(amino)methylene)dimethylguanidinium $[BAMDMG]^+$	$C_{20}H_{44}N_5^+$ 354.61	
78.	Guanidinium $[C(NH2)3]^+$	$CH_6N_3^+$ 60.08	
79.	Hexamethylguanidinium $[HMG]^+$	$C_7H_{18}N_3^+$ 144.24	
80.	N,N,N,N-tetramethyl-N,N-dibutylguanidinium $[TeMDBG]^+$	$C_{13}H_{30}N_3^+$ 228.40	
81.	N,N,N,N-tetramethyl-N,N-dioctylguanidinium $[TeMDOG]^+$	$C_{21}H_{46}N_3^+$ 340.62	

82.	1-(2-hydroxyethyl)-2,3-dimethylimidazolium $[C2(OH)DMIM]^+$	$C_7H_{13}N_2O^+$ 141.19	
83.	1,3-aminopropyl-3-methylimidazolium $[APrMIM]^+$	$C_7H_{14}N_3^+$ 140.21	
84.	1-methyl-3,2-aminoethylimidazolium $[MAEIM]^+$	$C_6H_{12}N_3^+$ 126.18	
85.	1-allyl-3,4-dimethylpyridinium $[A34DMPy]^+$	$C_{10}H_{14}N^+$ 148.23	
86.	1-allyl-3,5-dimethylpyridinium $[A35DMPy]^+$	$C_{10}H_{14}N^+$ 148.23	
87.	1-butyl-3-methylpyridinium $[B\text{-}3\text{-}MPy]^+$	$C_{10}H_{16}N^+$ 150.24	
88.	1-butyl-4-methylpyridinium $[B\text{-}4\text{-}MPy]^+$	$C_{10}H_{16}N^+$ 150.24	
89.	1-butylpyridinium $[BPy]^+$	$C_9H_{14}N^+$ 136.22	
90.	1-ethylpyridinium $[EPy]^+$	$C_7H_{10}N^+$ 108.16	
91.	1-hexylpyridinium $[HPy]^+$	$C_{11}H_{18}N^+$ 164.27	
92.	1-octylpyridinium $[OPy]^+$	$C_{13}H_{22}N^+$ 192.33	
93.	1,1-dimethylpyrrolidinium $[DMPyrr]^+$	$C_6H_{14}N^+$ 100.18	

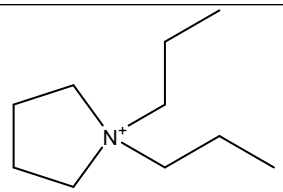
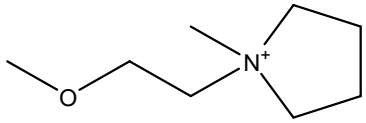
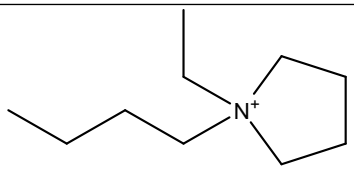
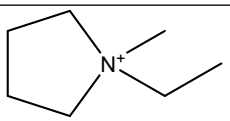
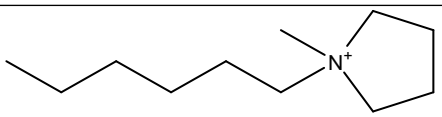
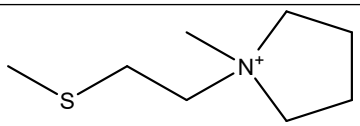
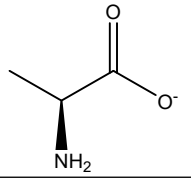
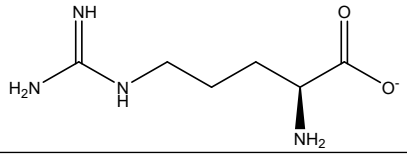
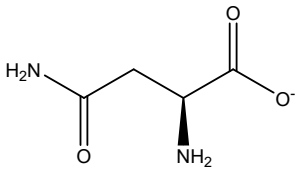
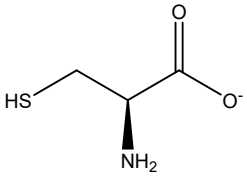
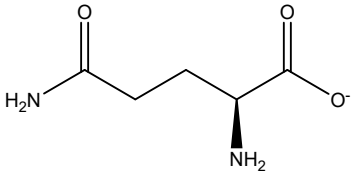
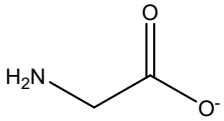
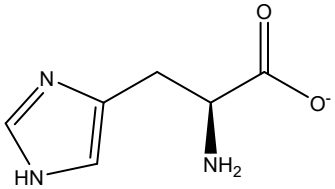
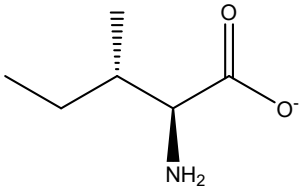
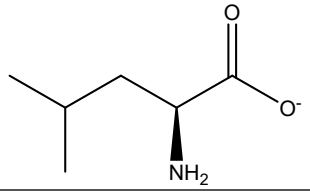
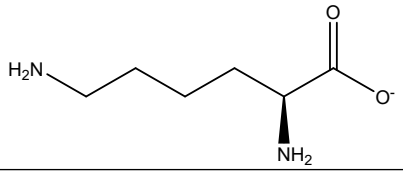
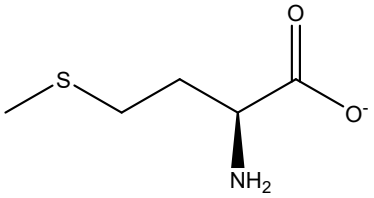
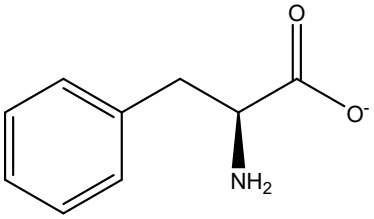
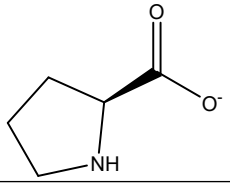
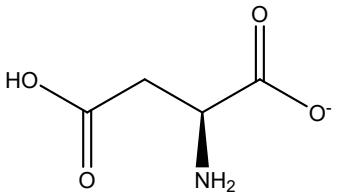
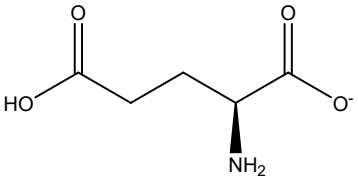
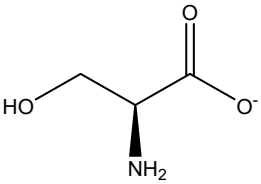
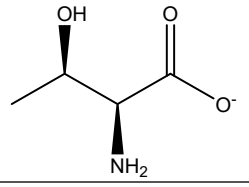
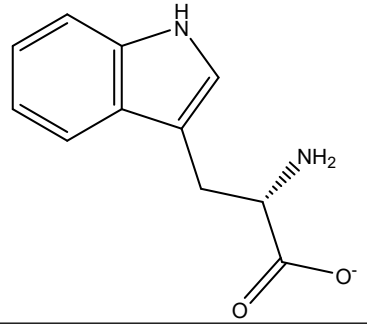
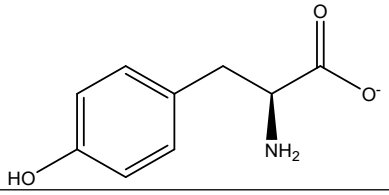
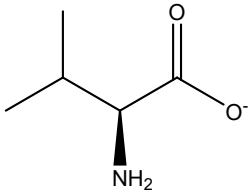
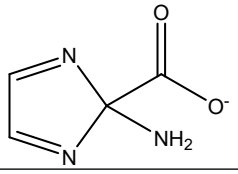
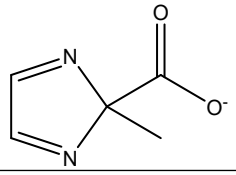
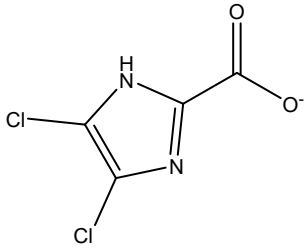
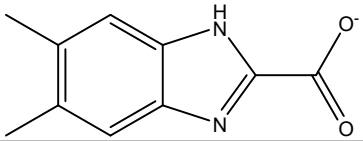
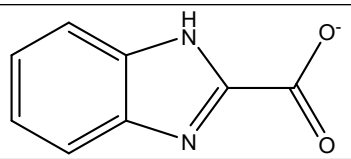
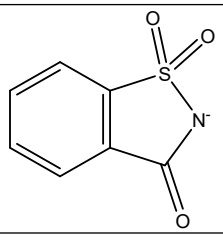
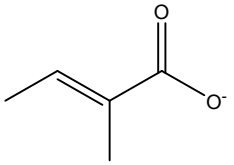
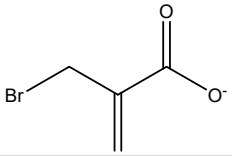
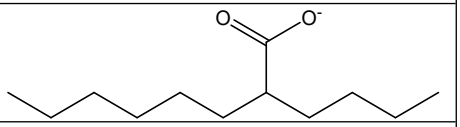
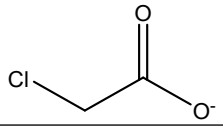
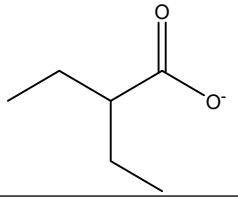
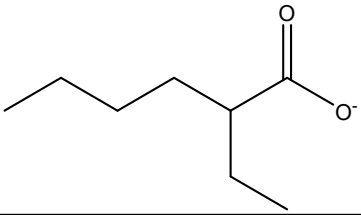
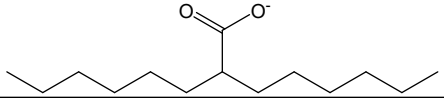
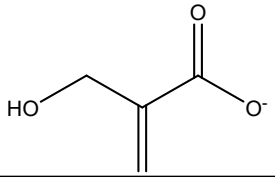
94.	1,1-dipropylpyrrolidinium $[DprPyrr]^+$	$C_{10}H_{22}N^+$ 156.29	
95.	1-(2-methoxyethyl)-1-methylpyrrolidinium $[12MeoEMPyrr]^+$	$C_8H_{18}NO^+$ 144.24	
96.	1-butyl-1-ethylpyrrolidinium $[BEPyrr]^+$	$C_{10}H_{22}N^+$ 156.29	
97.	1-ethyl-1-methylpyrrolidinium $[EMPyrr]^+$	$C_7H_{16}N^+$ 114.21	
98.	1-hexyl-1-methylpyrrolidinium $[HMPyrr]^+$	$C_{11}H_{24}N^+$ 170.32	
99.	1-methyl-1-(2-methylthioethyl)pyrrolidinium $[M12MThEPyrr]^+$	$C_8H_{18}NS^+$ 160.30	

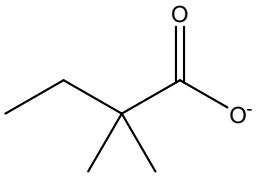
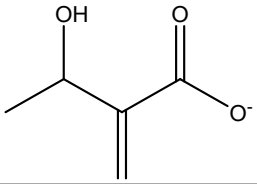
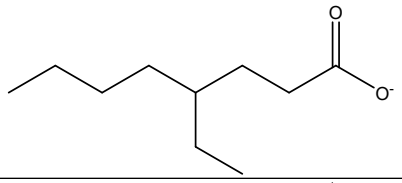
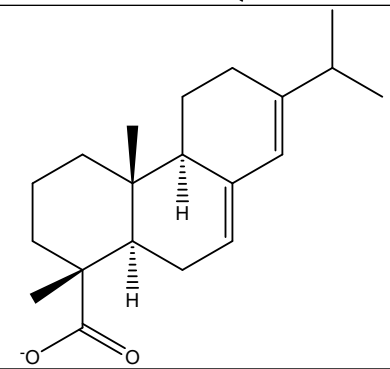
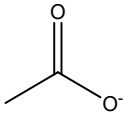
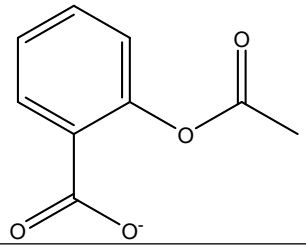
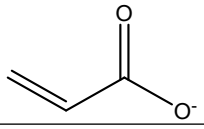
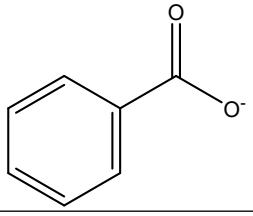
Table S2. List of anions used in this work

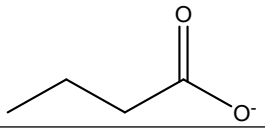
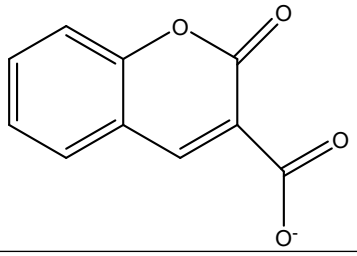
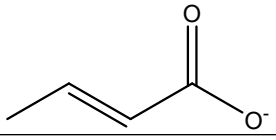
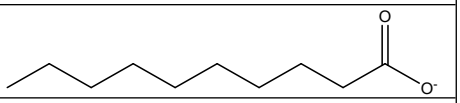
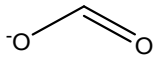
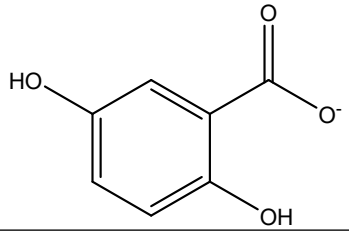
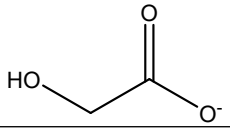
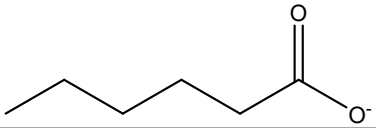
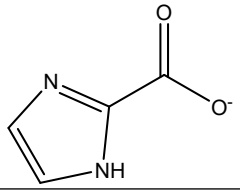
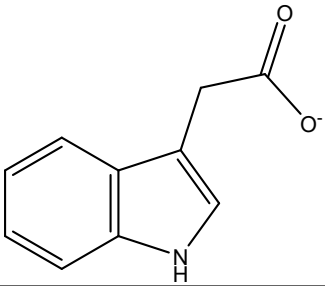
Sl. No.	Name of the anion and Acronym	Chem. formula & mol. wt.	Chemical structure
1.	Alaninate $[Ala]^-$	$C_3H_6NO_2^-$ 88.09	
2.	Argininate $[Arg]^-$	$C_6H_{13}N_4O_2^-$ 173.20	
3.	Asparaginate $[Aspg]^-$	$C_4H_7N_2O_3^-$ 131.11	
4.	Cysteinate $[Cyst]^-$	$C_3H_6NO_2S^-$ 120.15	
5.	Glutaminate $[Glumn]^-$	$C_5H_9N_2O_3^-$ 145.14	
6.	Glycinate $[Gly]^-$	$C_2H_4NO_2^-$ 74.06	
7.	Histidinate $[His]^-$	$C_6H_8N_3O_2^-$ 154.15	
8.	Isoleucinate $[Isole]^-$	$C_6H_{12}NO_2^-$ 130.17	

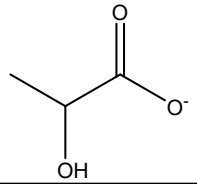
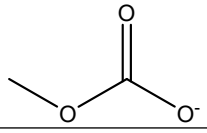
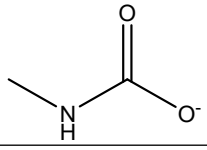
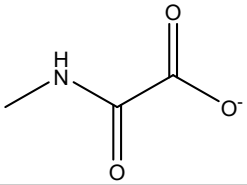
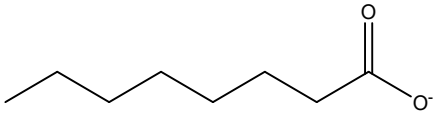
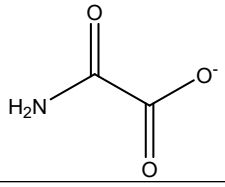
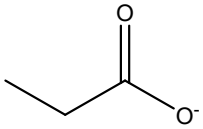
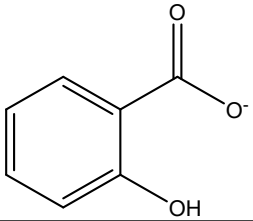
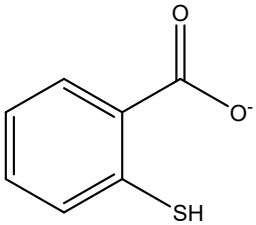
9.	Leucinate $[Leu]^-$	$C_6H_{12}NO_2^-$ 130.17	
10.	Lysinate $[Lys]^-$	$C_6H_{13}N_2O_2^-$ 145.18	
11.	Methioninate $[Met]^-$	$C_5H_{10}NO_2S^-$ 148.20	
12.	Phenylalaninate $[Phe]^-$	$C_9H_{10}NO_2^-$ 164.18	
13.	Prolinate $[Pro]^-$	$C_5H_8NO_2^-$ 114.12	
14.	Asparate monoanion $[AspMA]^-$	$C_4H_6NO_4^-$ 132.10	
15.	Glutamate monoanion $[GluMA]^-$	$C_5H_8NO_4^-$ 146.12	
16.	Serinate $[Ser]^-$	$C_3H_6NO_3^-$ 104.09	

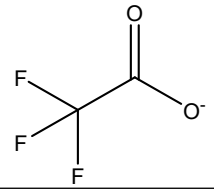
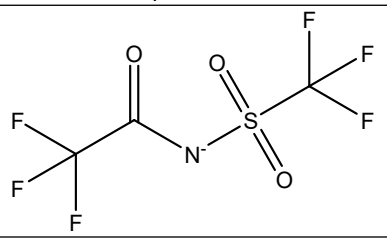
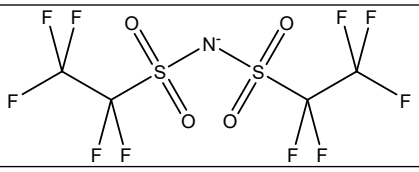
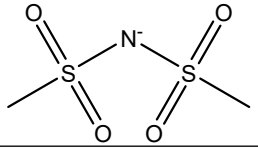
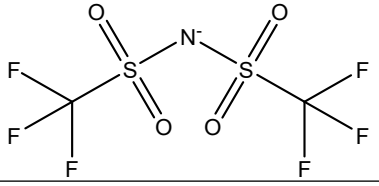
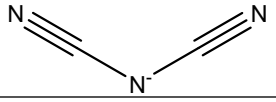
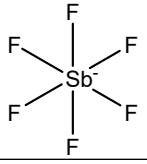
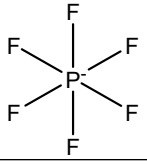
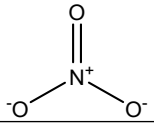
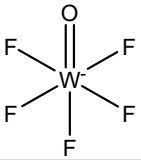
17.	Threoninate $[Thr]^-$	$C_4H_8NO_3^-$ 118.11	
18.	Tryptophanate $[Try]^-$	$C_{11}H_{11}N_2O_2^-$ 203.22	
19.	Tyrosinate $[Tyro]^-$	$C_9H_{10}NO_3^-$ 180.18	
20.	Valinate $[Val]^-$	$C_5H_{10}NO_2^-$ 116.14	
21.	2-Aminoimidazolate $[2AIm]^-$	$C_4H_4N_3O_2^-$ 126.10	
22.	2-methylimidazolate $[2MIm]^-$	$C_5H_5N_2O_2^-$ 125.11	
23.	4,5-Dichloroimidazolate $[45DCIm]^-$	$C_4HCl_2N_2O_2^-$ 179.96	
24.	5,6-Dimethylbenzimidazolate $[56DMBeIm]^-$	$C_{10}H_9N_2O_2^-$ 189.19	

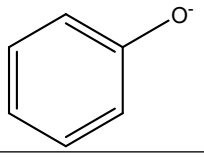
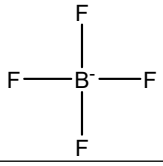
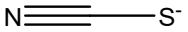
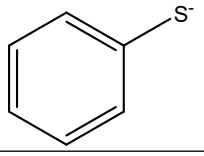
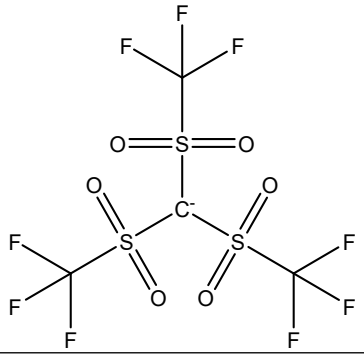
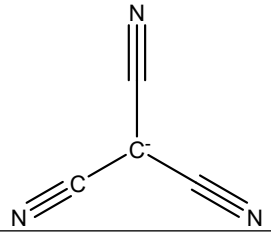
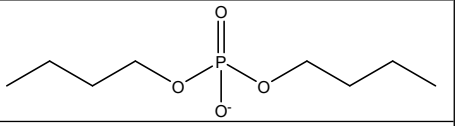
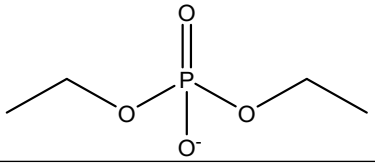
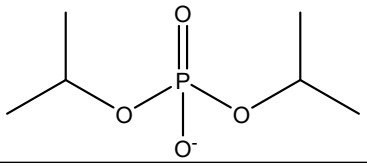
25.	Benzimidazolate $[BeIm]^-$	$C_8H_5N_2O_2^-$ 161.14	
26.	Saccharinate $[Sac]^-$	$C_7H_4NO_3S^-$ 182.17	
27.	(E)-2-Methylbut-2-enoate $[2\text{-Mbut}]^-$	$C_5H_7O_2^-$ 99.11	
28.	2-(Bromomethyl)acrylate $[2\text{-BrMAcr}]^-$	$C_4H_4BrO_2^-$ 163.98	
29.	2-butyl octanoate $[2\text{-BOA}]^-$	$C_{12}H_{23}O_2^-$ 199.31	
30.	Chloroacetate $[2\text{-ClAce}]^-$	$C_2H_2ClO_2^-$ 93.49	
31.	2-ethyl butyrate $[2\text{-EBA}]^-$	$C_6H_{11}O_2^-$ 115.15	
32.	2-ethyl hexanoate $[2\text{-EHA}]^-$	$C_8H_{15}O_2^-$ 143.21	
33.	2-hexyl octanoate $[2\text{-HOA}]^-$	$C_{14}H_{27}O_2^-$ 227.37	
34.	2-(hydroxymethyl)acrylate $[2\text{-(OH)MAcr}]^-$	$C_4H_5O_3^-$ 101.08	

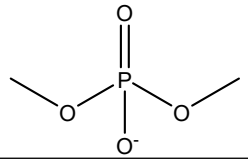
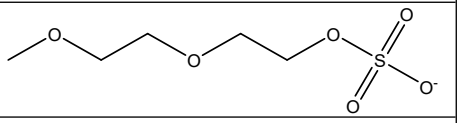
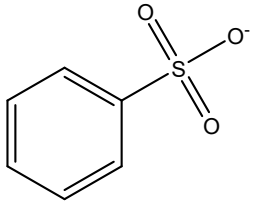
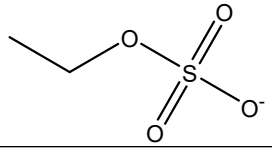
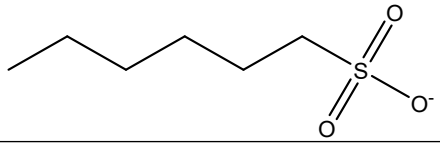
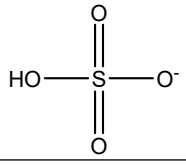
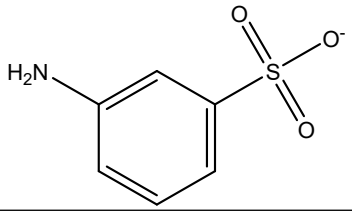
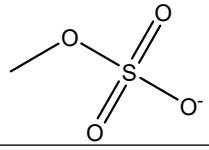
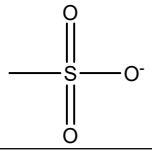
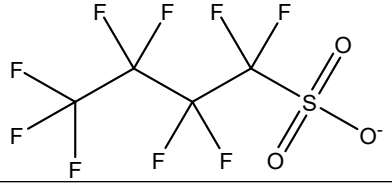
35.	2,2-dimethylbutyrate [22-DMB]$^-$	$C_6H_{11}O_2^-$ 115.15	
36.	3-hydroxy-2-methylenebutyrate [3-(OH)2-MBut]$^-$	$C_5H_7O_3^-$ 115.11	
37.	4-ethyl octanoate [4-EOA]$^-$	$C_{10}H_{19}O_2^-$ 171.26	
38.	Abietate [Abt]$^-$	$C_{20}H_{29}O_2^-$ 301.45	
39.	Acetate [Ace]$^-$	$C_2H_3O_2^-$ 59.04	
40.	Acetylsalicylate [AceSal]$^-$	$C_9H_7O_4^-$ 179.15	
41.	Acrylate [Acryl]$^-$	$C_3H_3O_2^-$ 71.06	
42.	Benzoate [Benzoate]$^-$	$C_7H_5O_2^-$ 121.12	

43.	Butyrate $[But]^-$	$C_4H_7O_2^-$ 87.10	
44.	Coumarine-3-carboxylate $[C3C]^-$	$C_{10}H_5O_4^-$ 189.15	
45.	Crotonate $[Crotonate]^-$	$C_4H_5O_2^-$ 85.08	
46.	Decanoate $[Dec]^-$	$C_{10}H_{19}O_2^-$ 171.26	
47.	Formate $[For]^-$	CHO_2^- 45.02	
48.	Gentisate $[Gen]^-$	$C_7H_5O_4^-$ 153.11	
49.	Glycolate $[Glyco]^-$	$C_2H_3O_3^-$ 75.04	
50.	Hexanoate $[Hex]^-$	$C_6H_{11}O_2^-$ 115.15	
51.	Imidazole-2-carboxylate $[Im2C]^-$	$C_4H_3N_2O_2^-$ 111.08	
52.	Indole-3-acetate $[I3A]^-$	$C_{10}H_8NO_2^-$ 174.18	

53.	Lactate $[Lac]^-$	$C_3H_5O_3^-$ 89.07	
54.	Methyl carbonate $[MCb]^-$	$C_2H_3O_3^-$ 75.04	
55.	N-methylcarbamate $[N\text{-}MCb]^-$	$C_2H_4NO_2^-$ 74.06	
56.	N-methyloxamate $[NMeO]^-$	$C_3H_4NO_3^-$ 102.07	
57.	Octanoate $[Oct]^-$	$C_8H_{15}O_2^-$ 143.21	
58.	Oxamate $[Oxa]^-$	$C_2H_2NO_3^-$ 88.04	
59.	Propionate $[Prop]^-$	$C_3H_5O_2^-$ 73.07	
60.	Salicylate $[Sal]^-$	$C_7H_5O_3^-$ 137.11	
61.	Thiosalicylate $[ThioSal]^-$	$C_7H_5O_2S^-$ 153.18	

62.	Trifluoroacetate $[TFA]^-$	$C_2F_3O_2^-$ 113.02	
63.	2,2,2-trifluoro-N-(trifluoromethylsulfonyl)acetamide $[TSAC]^-$	$C_3F_6NO_3S^-$ 244.09	
64.	Bis(pentafluoroethylsulfonyl)imide $[B(F_5)SI]^-$	$C_4F_{10}NO_4S_2^-$ 380.15	
65.	Bis(methanesulfonyl)amide $[MSA]^-$	$C_2H_6NO_4S_2^-$ 172.19	
66.	Bis(trifluoromethylsulfonyl)imide $[TFMI]^-$	$C_2F_6NO_4S_2^-$ 280.14	
67.	Dicyanamide $[DCN]^-$	$C_2N_3^-$ 66.04	
68.	Hexafluoroantimonate $[SbF_6]^-$	F_6Sb^- 235.75	
69.	Hexafluorophosphate $[PF_6]^-$	F_6P^- 144.96	
70.	Nitrate $[NO_3]^-$	NO_3^- 62.00	
71.	Oxypentafluorotungstate $[WOF_5]^-$	F_5OW^- 294.83	

72.	Phenolate $[Phenolate]^-$	$C_6H_5O^-$ 93.11	
73.	Tetrafluoroborate $[BF_4]^-$	BF_4^- 86.80	
74.	Thiocyanate $[SCN]^-$	CNS- 58.08	
75.	Thiophenolate $[PhS]^-$	$C_6H_5S^-$ 109.17	
76.	tri(trifluoromethylsulfonyl)methide $[TFMSM]^-$	$C_4F_9O_6S_3^-$ 411.20	
77.	Tricynamide $[TCN]^-$	$C_4N_3^-$ 90.07	
78.	Dibutyl phosphate $[DBPO_4]^-$	$C_8H_{18}O_4P^-$ 209.20	
79.	Diethylphosphate $[DEPO_4]^-$	$C_4H_{10}O_4P^-$ 153.09	
80.	Diisopropyl phosphate $[DIsoPrPO_4]^-$	$C_6H_{14}O_4P^-$ 181.15	

81.	Dimethylphosphate $[DMPO_4]^-$	$C_2H_6O_4P^-$ 125.04	
82.	2-(2-methoxyethoxy) ethyl sulfate [22-(ME)OHES]$^-$	$C_5H_{11}O_6S^-$ 199.20	
83.	Benzenesulfonate $[BenS]^-$	$C_6H_5O_3S^-$ 157.16	
84.	Ethyl sulfate $[EtSO_4]^-$	$C_2H_5O_4S^-$ 125.12	
85.	Hexane-1-sulfonate $[HSO_3]^-$	$C_6H_{13}O_3S^-$ 165.23	
86.	Hydrogen sulfate $[HSO_4]^-$	HSO_4^- 97.06	
87.	Metanilate [MetA]$^-$	$C_6H_6NO_3S^-$ 172.18	
88.	Methyl sulfate $[MeSO_4]^-$	$CH_3O_4S^-$ 111.09	
89.	Methylsulfonate $[MeSO_3]^-$	$CH_3O_3S^-$ 95.09	
90.	Nonafluorobutanesulfonate $[F_9BSO_3]^-$	$C_4F_9O_3S^-$ 299.09	

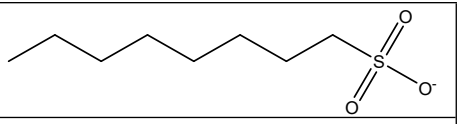
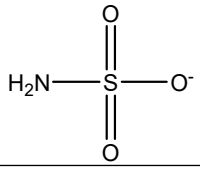
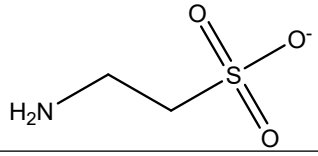
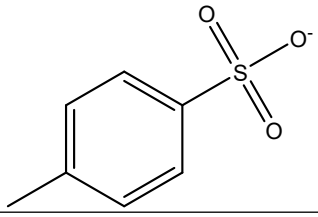
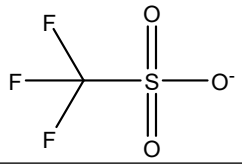
91.	Octane-1-sulfonate $[OctSO_3]^-$	$C_8H_{17}O_3S^-$ 193.28	
92.	Sulfamate $[NH_2SO_3]^-$	$H_2NO_3S^-$ 96.08	
93.	Taurinate $[Tau]^-$	$C_2H_6NO_3S^-$ 124.13	
94.	Tosylate $[Tosy]^-$	$C_7H_7O_3S^-$ 171.19	
95.	Triflate $[CF_3SO_3]^-$	$CF_3O_3S^-$ 149.06	

Table S3: COSMO-RS predicted logarithmic activity coefficients of PET in different ILs at 363.15 K

	[ACh]+	[BzTMA]+	[Ch]+	[DEM-2-MeoEA]+	[EDMPrA]+	[MTOA]+	[TeBA]+	[TeEA]+	[TeMA]+	[TEMA]+	[VBeTMA]+
[Ala]-	2.19	1.35	2.16	0.88	0.84	0.15	0.15	0.37	1.07	0.59	1.09
[Arg]-	2.31	1.49	2.37	1.16	1.17	0.25	0.38	0.81	1.74	1.02	1.23
[Aspg]-	2.57	1.74	2.55	1.26	1.25	0.29	0.45	0.81	1.52	1.02	1.45
[Cyst]-	2.41	1.40	2.45	0.96	0.95	0.06	0.10	0.50	1.58	0.75	1.10
[Glumn]-	2.44	1.58	2.49	1.18	1.18	0.26	0.38	0.77	1.68	1.00	1.30
[Gly]-	1.85	1.27	1.60	0.71	0.61	0.16	0.14	0.13	0.16	0.29	1.05
[His]-	2.72	1.71	2.82	1.35	1.37	0.26	0.42	0.97	2.14	1.22	1.40
[Isole]-	2.11	1.20	2.20	0.91	0.92	0.12	0.12	0.53	1.61	0.78	0.94
[Leu]-	2.11	1.17	2.20	0.91	0.92	0.11	0.11	0.54	1.64	0.79	0.92
[Lys]-	2.07	1.22	2.14	0.90	0.91	0.12	0.14	0.52	1.52	0.76	0.97
[Met]-	2.10	1.18	2.16	0.84	0.84	0.03	0.04	0.45	1.55	0.69	0.91
[Phe]-	2.05	1.11	2.13	0.84	0.85	0.01	0.04	0.49	1.62	0.74	0.86
[Pro]-	2.10	1.25	2.14	0.85	0.85	0.12	0.10	0.40	1.34	0.65	0.99
[AspMA]-	2.97	1.93	3.11	1.50	1.55	0.38	0.54	1.09	2.27	1.36	1.59
[GluMA]-	2.80	1.81	2.95	1.45	1.49	0.38	0.53	1.08	2.29	1.34	1.49
[Ser]-	2.57	1.76	2.56	1.26	1.24	0.35	0.47	0.78	1.42	1.00	1.47
[Thr]-	2.44	1.44	2.51	1.02	1.02	0.12	0.17	0.56	1.65	0.82	1.13
[Try]-	2.19	1.25	2.26	1.05	1.07	0.12	0.22	0.77	1.86	1.00	1.01
[Tyro]-	2.57	1.58	2.70	1.33	1.38	0.29	0.43	1.04	2.25	1.29	1.30
[Val]-	2.28	1.30	2.38	0.97	0.98	0.13	0.14	0.56	1.69	0.82	1.02
[2AIm]-	2.32	1.47	2.19	0.91	0.85	0.06	0.10	0.35	0.85	0.56	1.17
[2MIm]-	2.59	1.43	2.65	1.00	0.99	0.04	0.05	0.51	1.72	0.79	1.10
[45DCIm]-	2.85	1.28	2.99	1.10	1.12	-0.09	-0.02	0.76	2.61	1.08	0.92
[56DMBeIm]-	2.10	1.03	2.16	0.81	0.81	-0.07	-0.06	0.46	1.69	0.72	0.77
[BeIm]-	2.62	1.32	2.74	1.00	1.01	-0.06	-0.02	0.60	2.12	0.89	0.98
[Sac]-	2.61	1.44	2.73	1.08	1.11	-0.03	0.08	0.70	2.15	0.99	1.11
[2-Mbut]-	2.11	1.22	2.14	0.83	0.81	0.10	0.07	0.38	1.34	0.62	0.96

[2-BrMAcr]-	2.42	1.26	2.49	0.90	0.89	-0.04	-0.03	0.48	1.85	0.76	0.96
[2-BOA]-	1.33	0.78	1.42	0.63	0.65	0.10	0.05	0.37	1.07	0.55	0.63
[2-ClAce]-	2.57	1.55	2.56	1.03	1.00	0.12	0.17	0.50	1.34	0.75	1.22
[2-EBA]-	1.99	1.14	2.07	0.85	0.86	0.14	0.11	0.47	1.45	0.71	0.91
[2-EHA]-	1.73	0.99	1.81	0.78	0.79	0.12	0.09	0.45	1.34	0.68	0.79
[2-HOA]-	1.12	0.65	1.20	0.53	0.55	0.08	0.03	0.30	0.90	0.47	0.52
[2-(OH)MAcr]-	2.60	1.49	2.68	1.04	1.04	0.09	0.14	0.57	1.75	0.84	1.16
[22-DMB]-	2.07	1.17	2.15	0.89	0.90	0.15	0.13	0.51	1.52	0.75	0.93
[3-$(OH)_2$-MBut]-	2.71	1.66	2.83	1.29	1.31	0.29	0.39	0.88	2.04	1.14	1.35
[4-EOA]-	1.53	0.89	1.62	0.69	0.71	0.09	0.05	0.40	1.21	0.60	0.70
[Abt]-	1.06	0.57	1.12	0.47	0.48	0.04	0.00	0.26	0.84	0.41	0.45
[Ace]-	1.65	1.16	1.33	0.61	0.48	0.17	0.12	0.02	-0.21	0.15	0.98
[AceSal]-	2.20	1.22	2.27	0.90	0.91	0.01	0.06	0.54	1.73	0.79	0.94
[Acryl]-	2.12	1.33	1.99	0.80	0.73	0.12	0.10	0.25	0.70	0.45	1.07
[Benzoate]-	2.30	1.27	2.36	0.89	0.89	0.03	0.05	0.47	1.64	0.72	0.99
[But]-	2.08	1.24	2.10	0.84	0.82	0.15	0.12	0.38	1.20	0.61	1.00
[C3C]-	2.18	1.25	2.24	0.90	0.91	0.01	0.08	0.54	1.68	0.78	0.99
[Crotonate]-	2.03	1.22	1.99	0.77	0.72	0.10	0.07	0.27	0.98	0.49	0.98
[Dec]-	1.49	0.87	1.58	0.68	0.70	0.09	0.05	0.39	1.18	0.59	0.69
[For]-	1.18	1.10	0.44	0.43	0.21	0.17	0.13	-0.24	-1.63	-0.21	0.99
[Gen]-	3.24	2.26	3.39	1.84	1.90	0.58	0.84	1.48	2.62	1.74	1.91
[Glyco]-	1.53	1.35	1.09	0.78	0.64	0.41	0.45	0.23	-0.51	0.29	1.23
[Hex]-	1.93	1.12	2.01	0.83	0.84	0.13	0.10	0.44	1.40	0.68	0.89
[Im2C]-	2.18	1.41	2.08	0.89	0.84	0.13	0.18	0.39	0.95	0.59	1.15
[I3A]-	2.32	1.35	2.40	1.09	1.11	0.15	0.24	0.77	1.91	1.01	1.09
[Lac]-	1.94	1.43	1.77	0.92	0.85	0.36	0.39	0.42	0.51	0.57	1.23
[MCb]-	2.15	1.40	2.00	0.82	0.75	0.12	0.13	0.25	0.61	0.45	1.14
[N-MCb]-	1.74	1.19	1.50	0.64	0.54	0.15	0.11	0.08	0.13	0.23	0.99
[NMeO]-	2.13	1.32	2.07	0.80	0.75	0.08	0.09	0.28	0.98	0.50	1.06

[Oct]-	1.71	0.99	1.79	0.76	0.78	0.11	0.07	0.43	1.32	0.66	0.79
[Oxa]-	2.28	1.63	2.01	1.02	0.93	0.21	0.31	0.46	0.47	0.62	1.36
[Prop]-	2.04	1.27	1.96	0.80	0.74	0.17	0.13	0.28	0.81	0.48	1.03
[Sal]-	2.65	1.76	2.73	1.33	1.35	0.33	0.47	0.92	1.91	1.16	1.46
[ThioSal]-	2.33	1.26	2.39	0.91	0.91	-0.03	0.02	0.52	1.77	0.78	0.97
[TFA]-	3.28	1.69	3.55	1.32	1.35	0.07	0.16	0.86	2.73	1.21	1.26
[TSAC]-	1.71	0.62	1.64	0.70	0.68	-0.04	0.04	0.54	1.43	0.71	0.42
[B(F_5)SI]-	1.00	0.24	0.93	0.37	0.33	-0.08	-0.05	0.26	0.71	0.35	0.14
[MSA]-	2.77	1.61	2.90	1.17	1.20	0.04	0.17	0.75	2.12	1.03	1.25
[TFMI]	1.73	0.66	1.65	0.73	0.72	-0.03	0.06	0.58	1.48	0.75	0.45
[DCN]-	3.40	1.74	3.64	1.21	1.22	-0.15	-0.08	0.66	2.52	1.03	1.26
[SbF_6]-	3.27	1.34	3.38	1.35	1.39	-0.07	0.07	1.06	3.27	1.43	0.92
[PF_6]-	4.14	1.87	4.60	1.66	1.76	-0.06	0.13	1.27	4.32	1.74	1.31
[NO_3]-	2.57	1.83	2.17	1.07	0.97	0.11	0.21	0.41	0.14	0.59	1.47
[WOF_5]-	3.62	1.58	3.86	1.50	1.57	-0.04	0.12	1.17	3.72	1.58	1.11
[Phenolate]-	2.60	1.39	2.69	1.02	1.02	0.05	0.08	0.57	1.91	0.86	1.06
[BF_4]-	4.12	2.36	4.42	1.67	1.74	0.03	0.22	1.09	2.85	1.50	1.74
[SCN]-	3.30	1.90	3.29	1.22	1.21	-0.13	-0.03	0.61	1.58	0.92	1.41
[PhS]-	2.59	1.34	2.71	0.98	0.98	-0.08	-0.04	0.54	1.99	0.84	1.00
[TFMSM]-	1.19	0.41	1.06	0.52	0.51	0.00	0.08	0.44	0.97	0.54	0.27
[TCN]-	2.91	1.24	3.06	0.97	0.98	-0.27	-0.23	0.58	2.62	0.92	0.86
[$DBPO_4$]-	1.60	0.88	1.69	0.68	0.70	0.04	0.03	0.40	1.28	0.60	0.68
[$DEPO_4$]-	2.11	1.21	2.21	0.87	0.88	0.07	0.08	0.48	1.59	0.73	0.94
[$DIsoPrPO_4$]-	1.91	1.07	2.01	0.81	0.83	0.06	0.07	0.48	1.52	0.71	0.83
[$DMPO_4$]-	2.33	1.39	2.38	0.93	0.92	0.09	0.12	0.45	1.48	0.70	1.10
[22-(ME)OHES]-	2.19	1.20	2.28	0.93	0.96	0.02	0.11	0.62	1.80	0.86	0.92
[BzS]-	2.52	1.41	2.63	1.01	1.03	0.00	0.07	0.60	1.94	0.88	1.09
[$EtSO_4$]-	2.80	1.59	2.94	1.13	1.15	0.05	0.14	0.67	2.05	0.96	1.22

[HSO_3]-	2.01	1.12	2.12	0.83	0.86	0.04	0.06	0.48	1.58	0.73	0.86
[HSO4]-	3.43	2.41	3.34	1.68	1.70	0.28	0.53	1.11	1.59	1.38	1.95
[MetA]-	2.94	1.80	3.08	1.39	1.43	0.12	0.32	0.99	2.36	1.28	1.44
[$MeSO_4$]-	2.93	1.76	3.00	1.18	1.18	0.07	0.18	0.66	1.81	0.94	1.36
[$MeSO_3$]-	2.17	1.46	2.00	0.84	0.77	0.11	0.15	0.26	0.56	0.45	1.18
[F_9BSO_3]-	1.97	0.91	2.06	0.88	0.89	0.01	0.11	0.67	1.75	0.88	0.67
[$OctSO_3$]-	1.73	0.95	1.84	0.73	0.75	0.02	0.03	0.42	1.39	0.64	0.73
[NH_2SO_3]-	2.26	1.78	1.85	1.09	0.99	0.22	0.38	0.49	0.05	0.62	1.51
[Tau]-	2.39	1.56	2.34	1.02	0.99	0.15	0.25	0.52	1.19	0.73	1.27
[Tosy]-	2.28	1.25	2.37	0.90	0.92	-0.02	0.03	0.53	1.77	0.78	0.96
[CF_3SO_3]-	3.34	1.64	3.64	1.37	1.43	0.02	0.15	0.99	3.09	1.35	1.20

Table S3 (continued…): COSMO-RS predicted logarthmic activity coefficients of PET in different ILs at 363.15 K

	[DMIM]+	[AMIM]+	[BzBIM]+	[BzMIM]+	[BDMIM]+	[BMIM]+	[1-BIM]+	[EDMIM]+	[EMBzIM]+	[EMIM]+	[HMIM]+
[Ala]-	1.31	1.33	0.76	1.06	0.52	1.20	2.20	0.59	0.81	1.26	1.09
[Arg]-	1.68	1.53	0.89	1.22	0.83	1.34	2.06	1.01	1.08	1.52	1.19
[Aspg]-	1.76	1.74	1.05	1.43	0.93	1.55	2.52	1.04	1.23	1.67	1.38
[Cyst]-	1.61	1.44	0.71	1.10	0.59	1.19	2.04	0.78	0.92	1.40	1.01
[Glumn]-	1.71	1.60	0.93	1.29	0.83	1.41	2.26	0.99	1.11	1.57	1.25
[Gly]-	0.87	1.18	0.78	1.01	0.41	1.16	2.31	0.32	0.69	1.02	1.11
[His]-	2.03	1.79	0.98	1.41	0.97	1.51	2.26	1.23	1.28	1.79	1.29
[Isole]-	1.45	1.24	0.63	0.92	0.53	1.07	1.76	0.74	0.78	1.26	0.92
[Leu]-	1.45	1.22	0.60	0.90	0.52	1.04	1.71	0.75	0.77	1.25	0.89
[Lys]-	1.40	1.24	0.65	0.94	0.54	1.08	1.80	0.72	0.78	1.24	0.95
[Met]-	1.43	1.22	0.58	0.91	0.48	1.01	1.71	0.70	0.76	1.22	0.86
[Phe]-	1.44	1.18	0.53	0.87	0.49	0.96	1.57	0.73	0.75	1.21	0.79
[Pro]-	1.35	1.25	0.68	0.96	0.48	1.11	1.99	0.62	0.75	1.23	0.99

[AspMA]-	2.22	1.99	1.13	1.58	1.11	1.71	2.61	1.35	1.44	1.98	1.47
[GluMA]-	2.13	1.87	1.07	1.48	1.06	1.61	2.41	1.32	1.36	1.89	1.39
[Ser]-	1.72	1.75	1.07	1.44	0.91	1.58	2.63	0.99	1.21	1.66	1.43
[Thr]-	1.60	1.44	0.74	1.11	0.62	1.22	2.11	0.80	0.92	1.41	1.06
[Try]-	1.65	1.36	0.67	1.02	0.71	1.10	1.60	0.99	0.97	1.40	0.91
[Tyro]-	2.01	1.69	0.91	1.31	0.97	1.41	2.01	1.27	1.24	1.74	1.19
[Val]-	1.54	1.33	0.67	1.00	0.57	1.13	1.89	0.78	0.84	1.34	0.98
[2AIm]-	1.32	1.44	0.77	1.15	0.56	1.26	2.32	0.60	0.89	1.31	1.12
[2MIm]-	1.68	1.48	0.67	1.09	0.57	1.19	2.04	0.79	0.92	1.45	1.00
[45DCIm]-	2.01	1.41	0.42	0.95	0.59	0.95	1.35	1.05	0.93	1.51	0.64
[56DMBeIm]-	1.44	1.13	0.42	0.79	0.43	0.86	1.38	0.71	0.71	1.16	0.67
[BeIm]-	1.82	1.42	0.53	1.01	0.57	1.06	1.68	0.90	0.92	1.45	0.81
[Sac]-	1.90	1.53	0.64	1.13	0.68	1.15	1.84	1.01	1.02	1.54	0.90
[2-Mbut]-	1.37	1.25	0.65	0.96	0.47	1.08	1.92	0.63	0.75	1.22	0.95
[2-BrMAcr]-	1.74	1.40	0.57	1.01	0.52	1.06	1.76	0.83	0.88	1.41	0.83
[2-BOA]-	0.98	0.85	0.45	0.61	0.35	0.77	1.28	0.51	0.50	0.89	0.69
[2-ClAce]-	1.58	1.54	0.79	1.20	0.62	1.29	2.32	0.75	0.98	1.45	1.11
[2-EBA]-	1.35	1.19	0.63	0.89	0.49	1.04	1.76	0.68	0.73	1.20	0.91
[2-EHA]-	1.22	1.05	0.55	0.77	0.44	0.93	1.54	0.63	0.64	1.08	0.82
[2-HOA]-	0.83	0.72	0.37	0.50	0.29	0.66	1.10	0.43	0.42	0.76	0.59
[2-(OH)MAcr]-	1.72	1.52	0.73	1.16	0.63	1.24	2.14	0.84	0.97	1.49	1.04
[22-DMB]-	1.40	1.22	0.64	0.91	0.51	1.06	1.78	0.71	0.76	1.24	0.93
[3-$(OH)_2$-MBut]-	1.96	1.73	0.94	1.35	0.89	1.46	2.29	1.13	1.21	1.73	1.26
[4-EOA]-	1.10	0.95	0.49	0.69	0.39	0.85	1.42	0.56	0.56	0.98	0.75
[Abt]-	0.77	0.64	0.30	0.44	0.24	0.58	0.96	0.38	0.37	0.68	0.51
[Ace]-	0.67	1.07	0.76	0.95	0.33	1.09	2.29	0.19	0.60	0.89	1.08
[AceSal]-	1.55	1.28	0.58	0.96	0.54	1.01	1.67	0.80	0.83	1.29	0.83
[Acryl]-	1.19	1.30	0.75	1.06	0.46	1.17	2.25	0.49	0.78	1.19	1.07
[Benzoate]-	1.57	1.34	0.62	1.00	0.52	1.08	1.85	0.75	0.84	1.33	0.90

[But]-	1.30	1.25	0.70	0.97	0.48	1.12	2.03	0.59	0.74	1.21	1.01
[C3C]-	1.56	1.32	0.63	1.01	0.57	1.06	1.76	0.81	0.87	1.32	0.87
[Crotonate]-	1.22	1.22	0.68	0.97	0.43	1.09	2.06	0.51	0.72	1.15	0.99
[Dec]-	1.07	0.92	0.48	0.67	0.38	0.83	1.39	0.55	0.55	0.96	0.74
[For]-	0.05	0.91	0.80	0.94	0.24	1.07	2.49	-0.12	0.50	0.60	1.12
[Gen]-	2.62	2.36	1.44	1.93	1.49	2.05	2.94	1.75	1.82	2.37	1.79
[Glyco]-	0.64	1.23	1.05	1.18	0.60	1.36	2.65	0.35	0.82	1.02	1.39
[Hex]-	1.31	1.16	0.62	0.87	0.47	1.03	1.77	0.65	0.70	1.17	0.91
[Im2C]-	1.36	1.42	0.81	1.16	0.59	1.25	2.26	0.66	0.91	1.31	1.12
[I3A]-	1.74	1.45	0.73	1.11	0.75	1.19	1.77	1.02	1.02	1.48	0.99
[Lac]-	1.12	1.38	0.99	1.20	0.66	1.37	2.50	0.59	0.91	1.25	1.32
[MCb]-	1.17	1.35	0.79	1.11	0.49	1.22	2.40	0.49	0.81	1.21	1.12
[N-MCb]-	0.81	1.11	0.74	0.95	0.36	1.10	2.25	0.27	0.63	0.96	1.07
[NMeO]-	1.27	1.30	0.72	1.05	0.47	1.14	2.17	0.54	0.78	1.20	1.02
[Oct]-	1.20	1.04	0.55	0.77	0.43	0.93	1.56	0.61	0.63	1.07	0.82
[Oxa]-	1.30	1.57	0.97	1.34	0.72	1.45	2.65	0.68	1.05	1.40	1.32
[Prop]-	1.16	1.24	0.74	1.00	0.45	1.15	2.17	0.49	0.73	1.16	1.06
[Sal]-	1.98	1.83	1.07	1.47	1.00	1.59	2.49	1.19	1.31	1.80	1.39
[ThioSal]-	1.65	1.36	0.59	1.01	0.55	1.06	1.74	0.82	0.88	1.36	0.85
[TFA]-	2.28	1.77	0.70	1.26	0.77	1.31	2.10	1.16	1.16	1.81	1.00
[TSAC]-	1.04	0.68	0.12	0.42	0.34	0.44	0.51	0.62	0.46	0.78	0.24
[B(F_5)SI]-	0.54	0.34	-0.01	0.16	0.14	0.20	0.15	0.32	0.22	0.41	0.08
[MSA]-	1.93	1.64	0.75	1.25	0.76	1.29	2.12	1.03	1.11	1.62	1.05
[TFMI]	1.09	0.73	0.15	0.46	0.38	0.48	0.55	0.67	0.50	0.83	0.27
[DCN]-	2.38	1.88	0.63	1.31	0.68	1.31	2.19	1.10	1.17	1.87	0.95
[SbF_6]-	2.27	1.44	0.31	0.92	0.68	0.89	0.98	1.27	0.97	1.64	0.50
[PF_6]-	3.04	1.99	0.52	1.30	0.90	1.26	1.60	1.59	1.33	2.18	0.76
[NO_3]-	1.32	1.72	0.93	1.44	0.70	1.50	2.91	0.66	1.12	1.48	1.30
[WOF_5]-	2.62	1.70	0.44	1.11	0.80	1.08	1.32	1.43	1.15	1.90	0.65

[Phenolate]-	1.74	1.45	0.64	1.07	0.59	1.15	1.88	0.85	0.93	1.45	0.93
$[BF_4]$-	2.83	2.36	0.88	1.72	1.02	1.70	2.73	1.46	1.55	2.33	1.24
[SCN]-	2.12	1.97	0.73	1.45	0.74	1.45	2.56	1.01	1.25	1.85	1.10
[PhS]-	1.79	1.44	0.56	1.03	0.56	1.09	1.83	0.86	0.91	1.45	0.85
[TFMSM]-	0.70	0.46	0.07	0.28	0.28	0.30	0.25	0.47	0.33	0.53	0.15
[TCN]-	2.11	1.44	0.31	0.93	0.48	0.88	1.34	0.99	0.89	1.52	0.52
$[DBPO_4]$-	1.11	0.92	0.43	0.67	0.37	0.78	1.33	0.56	0.56	0.95	0.67
$[DEPO_4]$-	1.44	1.24	0.60	0.92	0.50	1.04	1.80	0.70	0.76	1.24	0.89
$[DIsoPrPO_4]$-	1.33	1.11	0.53	0.81	0.46	0.93	1.57	0.68	0.69	1.14	0.79
$[DMPO_4]$-	1.50	1.39	0.71	1.07	0.55	1.17	2.11	0.70	0.86	1.34	1.02
[22-(ME)OHES]-	1.52	1.22	0.53	0.91	0.56	0.96	1.54	0.82	0.82	1.25	0.77
[BzS]-	1.77	1.47	0.65	1.10	0.62	1.15	1.93	0.90	0.96	1.47	0.92
$[EtSO_4]$-	1.88	1.61	0.72	1.21	0.68	1.26	2.17	0.95	1.04	1.58	1.02
$[HSO_3]$-	1.38	1.15	0.53	0.84	0.47	0.96	1.65	0.69	0.71	1.17	0.81
[HSO4]-	2.33	2.40	1.28	1.94	1.25	2.02	3.38	1.41	1.70	2.25	1.70
[MetA]-	2.21	1.88	0.93	1.46	0.98	1.52	2.33	1.29	1.34	1.88	1.24
$[MeSO_4]$-	1.91	1.75	0.81	1.35	0.74	1.39	2.45	0.96	1.14	1.67	1.14
$[MeSO_3]$-	1.15	1.38	0.81	1.15	0.51	1.25	2.49	0.49	0.84	1.21	1.15
$[F_9BSO_3]$-	1.37	1.00	0.33	0.67	0.50	0.74	1.09	0.80	0.68	1.09	0.52
$[OctSO_3]$-	1.19	0.98	0.44	0.71	0.39	0.82	1.41	0.60	0.60	1.01	0.69
$[NH_2SO_3]$-	1.17	1.67	1.08	1.47	0.81	1.59	2.98	0.68	1.14	1.43	1.47
[Tau]-	1.46	1.51	0.87	1.23	0.68	1.34	2.41	0.74	0.99	1.41	1.20
[Tosy]-	1.58	1.31	0.56	0.97	0.53	1.02	1.74	0.79	0.84	1.31	0.82
$[CF_3SO_3]$-	2.40	1.75	0.61	1.22	0.80	1.24	1.87	1.28	1.17	1.84	0.88

Table S3 (continued…): COSMO-RS predicted logarithmic activity coefficients of PET in different ILs at 363.15 K

	[OMIM]+	[PMIM]+	[DMEIM]+	[DIsoPIM]+	[AQunz]+	[BMPip]+	[4AB124Tz]+	[EMPip]+	[EMBzTz]+	[1-EQ]+	[1-MQ]+
[Ala]-	0.97	1.22	0.59	0.82	1.61	0.62	2.48	0.58	0.63	0.79	1.20
[Arg]-	1.05	1.41	1.01	1.04	1.74	0.90	2.26	1.00	0.92	1.06	1.40
[Aspg]-	1.20	1.60	1.04	1.16	2.04	1.00	2.82	1.01	1.06	1.21	1.62
[Cyst]-	0.86	1.28	0.78	0.81	1.78	0.63	2.28	0.72	0.74	0.90	1.33
[Glumn]-	1.09	1.47	0.99	1.06	1.86	0.90	2.51	0.97	0.95	1.10	1.48
[Gly]-	1.01	1.11	0.32	0.76	1.46	0.52	2.68	0.31	0.49	0.67	1.07
[His]-	1.10	1.62	1.22	1.18	2.07	1.02	2.46	1.19	1.12	1.26	1.66
[Isole]-	0.80	1.14	0.74	0.78	1.44	0.62	1.90	0.75	0.63	0.76	1.10
[Leu]-	0.77	1.12	0.74	0.76	1.42	0.61	1.84	0.75	0.62	0.75	1.08
[Lys]-	0.83	1.14	0.72	0.77	1.44	0.63	2.00	0.73	0.63	0.77	1.11
[Met]-	0.73	1.09	0.69	0.68	1.48	0.53	1.90	0.66	0.61	0.75	1.11
[Phe]-	0.66	1.05	0.73	0.67	1.42	0.53	1.73	0.70	0.62	0.73	1.07
[Pro]-	0.88	1.15	0.62	0.76	1.49	0.58	2.23	0.62	0.59	0.74	1.12
[AspMA]-	1.27	1.82	1.34	1.32	2.30	1.18	2.88	1.33	1.28	1.40	1.83
[GluMA]-	1.21	1.72	1.31	1.27	2.13	1.14	2.63	1.31	1.22	1.33	1.72
[Ser]-	1.26	1.62	0.99	1.19	2.03	1.01	2.95	0.99	1.03	1.18	1.61
[Thr]-	0.91	1.30	0.79	0.85	1.73	0.70	2.39	0.79	0.76	0.89	1.30
[Try]-	0.75	1.22	0.99	0.86	1.57	0.74	1.69	0.95	0.84	0.94	1.24
[Tyro]-	1.02	1.54	1.27	1.14	1.92	1.01	2.13	1.24	1.11	1.22	1.56
[Val]-	0.84	1.21	0.78	0.82	1.57	0.66	2.06	0.78	0.68	0.82	1.19
[2AIm]-	0.97	1.29	0.60	0.82	1.79	0.63	2.70	0.56	0.68	0.86	1.31
[2MIm]-	0.83	1.29	0.79	0.81	1.82	0.63	2.31	0.75	0.73	0.89	1.33
[45DCIm]-	0.44	1.17	1.04	0.67	1.77	0.61	1.45	1.00	0.79	0.89	1.27
[56DMBeIm]-	0.53	0.98	0.71	0.58	1.38	0.45	1.52	0.67	0.56	0.68	1.01
[BeIm]-	0.63	1.21	0.90	0.71	1.78	0.58	1.87	0.84	0.75	0.88	1.29
[Sac]-	0.70	1.31	1.00	0.78	1.88	0.68	2.11	0.93	0.91	1.00	1.41
[2-Mbut]-	0.83	1.13	0.63	0.74	1.51	0.54	2.14	0.60	0.60	0.75	1.12

[2-BrMAcr]-	0.66	1.19	0.83	0.71	1.76	0.51	1.90	0.71	0.73	0.88	1.30
[2-BOA]-	0.62	0.81	0.51	0.59	0.91	0.43	1.30	0.53	0.39	0.50	0.73
[2-ClAce]-	0.94	1.36	0.75	0.88	1.90	0.71	2.66	0.72	0.80	0.94	1.39
[2-EBA]-	0.81	1.10	0.67	0.76	1.36	0.58	1.88	0.68	0.58	0.72	1.05
[2-EHA]-	0.72	0.99	0.63	0.69	1.17	0.53	1.61	0.64	0.51	0.63	0.92
[2-HOA]-	0.53	0.70	0.42	0.50	0.75	0.36	1.11	0.44	0.31	0.41	0.61
[2-(OH)MAcr]-	0.87	1.34	0.84	0.85	1.87	0.69	2.44	0.80	0.82	0.94	1.38
[22-DMB]-	0.82	1.13	0.71	0.79	1.40	0.61	1.89	0.72	0.60	0.74	1.07
[3-$(OH)_2$-MBut]-	1.08	1.57	1.12	1.13	2.01	0.97	2.50	1.10	1.05	1.17	1.58
[4-EOA]-	0.67	0.90	0.56	0.62	1.05	0.46	1.50	0.58	0.45	0.56	0.82
[Abt]-	0.45	0.62	0.38	0.44	0.68	0.30	0.95	0.39	0.26	0.36	0.54
[Ace]-	1.00	1.02	0.20	0.72	1.32	0.45	2.62	0.18	0.40	0.59	0.97
[AceSal]-	0.68	1.12	0.79	0.70	1.56	0.57	1.90	0.74	0.72	0.81	1.17
[Acryl]-	0.94	1.18	0.49	0.77	1.63	0.54	2.58	0.45	0.60	0.76	1.19
[Benzoate]-	0.76	1.18	0.75	0.74	1.65	0.56	2.07	0.69	0.70	0.82	1.22
[But]-	0.91	1.15	0.59	0.79	1.48	0.58	2.24	0.59	0.58	0.74	1.11
[C3C]-	0.72	1.16	0.81	0.73	1.61	0.58	2.02	0.74	0.76	0.85	1.22
[Crotonate]-	0.88	1.11	0.51	0.72	1.50	0.51	2.35	0.47	0.56	0.71	1.10
[Dec]-	0.66	0.88	0.55	0.61	1.02	0.46	1.46	0.57	0.44	0.55	0.80
[For]-	1.05	0.91	-0.12	0.67	1.16	0.37	2.94	-0.14	0.28	0.48	0.85
[Gen]-	1.55	2.19	1.75	1.69	2.67	1.53	3.18	1.71	1.68	1.79	2.22
[Glyco]-	1.31	1.24	0.35	1.01	1.42	0.73	3.02	0.34	0.62	0.81	1.14
[Hex]-	0.81	1.08	0.64	0.74	1.33	0.56	1.92	0.65	0.56	0.70	1.02
[Im2C]-	0.98	1.28	0.65	0.86	1.74	0.64	2.59	0.58	0.74	0.90	1.32
[I3A]-	0.83	1.31	1.01	0.92	1.70	0.77	1.90	0.97	0.89	1.00	1.33
[Lac]-	1.22	1.33	0.59	1.02	1.60	0.77	2.81	0.59	0.73	0.90	1.26
[MCb]-	0.99	1.22	0.49	0.79	1.68	0.58	2.79	0.45	0.63	0.79	1.23
[N-MCb]-	0.98	1.05	0.27	0.71	1.37	0.46	2.60	0.25	0.44	0.62	1.01
[NMeO]-	0.89	1.16	0.54	0.73	1.63	0.53	2.54	0.48	0.63	0.77	1.20

[Oct]-	0.73	0.98	0.61	0.68	1.17	0.51	1.66	0.63	0.50	0.62	0.91
[Oxa]-	1.15	1.44	0.69	1.01	1.92	0.79	3.05	0.63	0.86	1.03	1.48
[Prop]-	0.96	1.15	0.49	0.79	1.50	0.56	2.43	0.48	0.55	0.72	1.11
[Sal]-	1.21	1.67	1.19	1.22	2.12	1.04	2.75	1.14	1.16	1.29	1.70
[ThioSal]-	0.68	1.18	0.82	0.72	1.69	0.55	1.93	0.73	0.73	0.87	1.26
[TFA]-	0.78	1.51	1.15	0.93	2.17	0.85	2.36	1.14	1.01	1.10	1.57
[TSAC]-	0.11	0.58	0.62	0.33	0.86	0.40	0.60	0.67	0.44	0.44	0.59
[$B(F_5)SI$]-	0.00	0.29	0.31	0.19	0.43	0.17	0.07	0.33	0.15	0.20	0.28
[MSA]-	0.84	1.42	1.03	0.87	2.01	0.80	2.46	0.98	0.98	1.07	1.51
[TFMI]	0.13	0.62	0.66	0.36	0.92	0.43	0.67	0.70	0.49	0.48	0.64
[DCN]-	0.69	1.54	1.10	0.81	2.47	0.67	2.48	0.96	0.98	1.15	1.74
[SbF_6]-	0.25	1.19	1.26	0.64	1.78	0.77	1.13	1.33	0.89	0.91	1.25
[PF_6]-	0.45	1.62	1.58	0.88	2.48	0.99	1.83	1.62	1.21	1.25	1.75
[NO_3]-	1.08	1.52	0.66	0.95	2.20	0.79	3.47	0.61	0.92	1.07	1.62
[WOF_5]-	0.38	1.40	1.42	0.78	2.10	0.89	1.50	1.47	1.07	1.09	1.49
[Phenolate]-	0.77	1.26	0.85	0.79	1.79	0.65	2.09	0.81	0.76	0.89	1.31
[BF_4]-	0.90	1.96	1.45	1.12	2.98	1.12	3.20	1.42	1.36	1.48	2.15
[SCN]-	0.81	1.63	1.00	0.87	2.59	0.74	2.98	0.88	1.03	1.21	1.84
[PhS]-	0.67	1.23	0.85	0.70	1.81	0.57	2.06	0.79	0.75	0.88	1.31
[TFMSM]-	0.05	0.40	0.47	0.25	0.58	0.32	0.34	0.51	0.34	0.32	0.40
[TCN]-	0.29	1.13	0.98	0.52	1.94	0.42	1.47	0.84	0.74	0.90	1.35
[$DBPO_4$]-	0.57	0.85	0.56	0.54	1.07	0.43	1.47	0.57	0.46	0.54	0.81
[$DEPO_4$]-	0.76	1.11	0.70	0.70	1.47	0.57	2.04	0.69	0.64	0.75	1.11
[$DIsoPrPO_4$]-	0.68	1.01	0.67	0.65	1.29	0.53	1.74	0.68	0.57	0.67	0.98
[$DMPO_4$]-	0.88	1.23	0.70	0.77	1.70	0.62	2.44	0.67	0.71	0.84	1.26
[22-(ME)OHES]-	0.62	1.07	0.82	0.65	1.47	0.61	1.78	0.81	0.72	0.78	1.10
[BzS]-	0.74	1.27	0.89	0.76	1.82	0.64	2.22	0.83	0.84	0.94	1.35
[$EtSO_4$]-	0.82	1.39	0.94	0.83	1.99	0.75	2.53	0.91	0.91	1.01	1.46

[HSO_3]-	0.68	1.04	0.68	0.64	1.36	0.54	1.88	0.69	0.59	0.69	1.02
[HSO4]-	1.40	2.14	1.41	1.45	2.89	1.33	3.88	1.36	1.52	1.66	2.26
[MetA]-	1.02	1.67	1.29	1.12	2.24	1.01	2.60	1.23	1.20	1.31	1.75
[$MeSO_4$]-	0.92	1.51	0.95	0.91	2.19	0.81	2.89	0.91	0.99	1.10	1.61
[$MeSO_3$]-	1.01	1.24	0.49	0.78	1.73	0.60	2.96	0.45	0.67	0.82	1.27
[F_9BSO_3]-	0.37	0.88	0.80	0.56	1.19	0.56	1.21	0.83	0.62	0.64	0.87
[$OctSO_3$]-	0.59	0.89	0.60	0.55	1.15	0.46	1.60	0.61	0.49	0.58	0.87
[NH_2SO_3]-	1.28	1.55	0.68	1.09	2.02	0.90	3.48	0.65	0.94	1.11	1.58
[Tau]-	1.04	1.37	0.74	0.91	1.83	0.76	2.80	0.72	0.82	0.96	1.39
[Tosy]-	0.67	1.13	0.79	0.67	1.61	0.56	2.00	0.74	0.72	0.81	1.19
[CF_3SO_3]-	0.64	1.48	1.27	0.87	2.15	0.86	2.12	1.27	1.06	1.11	1.56

Table S3 (continued…): COSMO-RS predicted logarthmic activity coefficients of PET in different ILs at 363.15 K

	[4AO124Tz]+	[1-OQ]+	[4AP124Tz]+	[3-MQunz]+	[4APh124Tz]+	[DEBS]+	[DEMS]+	[Qunz]+	[TES]+	[2EOMIM]+	[3SP2VPy]+
[Ala]-	1.72	0.51	2.27	1.05	1.59	0.77	1.06	1.39	0.88	2.01	2.26
[Arg]-	1.61	0.66	2.08	1.26	1.53	1.01	1.40	1.58	1.19	2.03	2.20
[Aspg]-	1.93	0.76	2.57	1.43	1.87	1.13	1.47	1.81	1.27	2.39	2.65
[Cyst]-	1.48	0.45	2.05	1.13	1.48	0.77	1.23	1.54	0.98	2.07	2.26
[Glumn]-	1.75	0.67	2.30	1.31	1.67	1.03	1.42	1.66	1.20	2.18	2.38
[Gly]-	1.87	0.53	2.47	0.94	1.74	0.68	0.72	1.25	0.65	1.98	2.34
[His]-	1.66	0.71	2.23	1.48	1.64	1.16	1.69	1.87	1.42	2.31	2.46
[Isole]-	1.34	0.40	1.75	0.98	1.21	0.74	1.18	1.29	0.96	1.74	1.86
[Leu]-	1.28	0.38	1.68	0.96	1.16	0.73	1.18	1.26	0.95	1.71	1.83
[Lys]-	1.42	0.43	1.85	0.97	1.28	0.74	1.14	1.28	0.93	1.76	1.91
[Met]-	1.28	0.35	1.73	0.95	1.23	0.66	1.11	1.30	0.87	1.75	1.90
[Phe]-	1.15	0.31	1.56	0.92	1.10	0.66	1.15	1.25	0.90	1.66	1.79
[Pro]-	1.59	0.44	2.06	0.98	1.43	0.73	1.09	1.31	0.89	1.84	2.03

[AspMA]-	1.95	0.83	2.60	1.63	1.87	1.32	1.85	2.05	1.57	2.54	2.67
[GluMA]-	1.82	0.79	2.39	1.54	1.73	1.26	1.78	1.92	1.51	2.36	2.46
[Ser]-	2.03	0.79	2.69	1.43	1.92	1.15	1.45	1.80	1.27	2.41	2.65
[Thr]-	1.61	0.47	2.17	1.10	1.50	0.84	1.28	1.49	1.04	2.06	2.26
[Try]-	1.12	0.45	1.52	1.12	1.12	0.86	1.37	1.42	1.12	1.76	1.85
[Tyro]-	1.46	0.67	1.93	1.41	1.43	1.14	1.69	1.75	1.42	2.10	2.18
[Val]-	1.42	0.43	1.88	1.05	1.31	0.79	1.25	1.38	1.01	1.88	2.02
[2AIm]-	1.73	0.50	2.42	1.10	1.69	0.80	1.07	1.51	0.89	2.21	2.51
[2MIm]-	1.44	0.41	2.05	1.12	1.42	0.81	1.33	1.55	1.04	2.13	2.30
[45DCIm]-	0.69	0.16	1.19	1.05	0.79	0.76	1.61	1.49	1.19	1.94	2.01
[56DMBeIm]-	0.92	0.21	1.33	0.85	0.92	0.59	1.14	1.19	0.86	1.60	1.71
[BeIm]-	1.06	0.28	1.61	1.07	1.12	0.75	1.42	1.50	1.07	1.98	2.10
[Sac]-	1.26	0.36	1.85	1.18	1.31	0.83	1.49	1.62	1.15	2.06	2.21
[2-Mbut]-	1.48	0.41	1.95	0.99	1.39	0.71	1.09	1.33	0.87	1.84	2.02
[2-BrMAcr]-	1.15	0.31	1.66	1.12	1.25	0.68	1.28	1.56	0.97	1.95	2.08
[2-BOA]-	1.02	0.29	1.24	0.69	0.85	0.53	0.83	0.87	0.69	1.15	1.20
[2-ClAce]-	1.70	0.49	2.37	1.17	1.65	0.89	1.29	1.60	1.04	2.26	2.53
[2-EBA]-	1.36	0.41	1.74	0.95	1.23	0.72	1.11	1.23	0.91	1.67	1.80
[2-EHA]-	1.20	0.35	1.50	0.85	1.05	0.65	1.01	1.08	0.83	1.45	1.54
[2-HOA]-	0.88	0.23	1.06	0.58	0.71	0.45	0.70	0.73	0.58	0.97	1.02
[2-(OH)MAcr]-	1.56	0.45	2.18	1.16	1.51	0.85	1.37	1.59	1.08	2.16	2.36
[22-DMB]-	1.36	0.41	1.74	0.97	1.23	0.74	1.15	1.26	0.94	1.71	1.84
[3-$(OH)_2$-MBut]-	1.68	0.67	2.26	1.40	1.62	1.11	1.62	1.79	1.35	2.28	2.42
[4-EOA]-	1.14	0.31	1.41	0.76	0.97	0.58	0.58	0.98	0.75	1.31	1.38
[Abt]-	0.73	0.17	0.89	0.52	0.60	0.39	0.39	0.66	0.52	0.89	0.94
[Ace]-	1.87	0.52	2.43	0.88	1.74	0.62	0.62	1.15	0.55	1.89	2.26
[AceSal]-	1.23	0.33	1.70	0.99	1.21	0.71	0.71	1.35	0.96	1.77	1.91
[Acryl]-	1.74	0.48	2.34	1.03	1.67	0.73	0.73	1.40	0.79	2.05	2.35
[Benzoate]-	1.35	0.37	1.85	1.05	1.34	0.73	0.73	1.43	0.96	1.91	2.08

[But]-	1.60	0.46	2.07	0.99	1.46	0.74	0.74	1.31	0.87	1.86	2.05
[C3C]-	1.34	0.37	1.82	1.04	1.32	0.73	0.73	1.41	0.97	1.82	1.98
[Crotonate]-	1.63	0.44	2.15	0.96	1.53	0.68	0.68	1.31	0.78	1.89	2.13
[Dec]-	1.12	0.31	1.38	0.74	0.94	0.57	0.57	0.95	0.73	1.27	1.34
[For]-	2.05	0.54	2.72	0.78	1.94	0.55	0.55	1.00	0.28	1.89	2.44
[Gen]-	2.19	1.12	2.88	2.03	2.16	1.69	1.69	2.45	1.96	2.86	2.97
[Glyco]-	2.24	0.81	2.84	1.10	2.08	0.88	0.88	1.30	0.71	2.04	2.47
[Hex]-	1.41	0.40	1.78	0.93	1.24	0.70	0.70	1.21	0.88	1.65	1.78
[Im2C]-	1.74	0.55	2.35	1.15	1.72	0.81	0.81	1.52	0.91	2.11	2.40
[I3A]-	1.26	0.50	1.71	1.19	1.27	0.91	0.91	1.53	1.17	1.90	2.01
[Lac]-	2.06	0.74	2.62	1.17	1.90	0.93	0.93	1.44	0.91	2.08	2.39
[MCb]-	1.88	0.51	2.54	1.05	1.78	0.75	0.75	1.44	0.80	2.13	2.47
[N-MCb]-	1.85	0.51	2.41	0.89	1.71	0.63	0.63	1.19	0.60	1.89	2.24
[NMeO]-	1.71	0.45	2.31	1.01	1.64	0.70	0.70	1.40	0.80	2.01	2.30
[Oct]-	1.25	0.35	1.56	0.83	1.08	0.64	0.64	1.08	0.82	1.45	1.54
[Oxa]-	2.01	0.68	2.75	1.29	1.98	0.96	0.96	1.68	0.97	2.38	2.76
[Prop]-	1.71	0.50	2.23	0.99	1.59	0.73	0.73	1.31	0.80	1.94	2.19
[Sal]-	1.90	0.79	2.50	1.52	1.85	1.21	1.21	1.92	1.41	2.38	2.55
[ThioSal]-	1.20	0.34	1.70	1.08	1.26	0.71	0.71	1.48	0.97	1.90	2.05
[TFA]-	1.36	0.38	2.02	1.30	1.34	1.03	1.03	1.82	1.42	2.41	2.57
[TSAC]-	0.15	-0.01	0.44	0.49	0.12	0.46	0.46	0.68	0.72	1.06	1.04
[B(F_5)SI]-	-0.17	-0.08	-0.02	0.27	-0.12	0.23	0.23	0.36	0.39	0.59	0.70
[MSA]-	1.51	0.45	2.17	1.24	1.50	0.92	0.92	1.70	1.20	2.24	2.43
[TFMI]	0.19	0.02	0.50	0.53	0.16	0.48	0.48	0.73	0.75	1.08	1.01
[DCN]-	1.25	0.29	2.07	1.40	1.44	0.87	0.87	2.07	1.28	2.62	2.80
[SbF_6]-	0.34	0.05	0.85	1.00	0.37	0.90	0.90	1.44	1.47	1.99	1.88
[PF_6]-	0.70	0.17	1.42	1.37	0.78	1.16	1.16	2.01	1.82	2.61	2.47
[NO_3]-	2.07	0.57	3.04	1.31	2.07	0.96	0.96	1.84	0.98	2.67	3.10
[WOF_5]-	0.57	0.14	1.17	1.19	0.62	1.02	2.19	1.71	1.62	2.26	2.15

[Phenolate]-	1.28	0.38	1.84	1.10	1.29	0.81	1.38	1.52	1.07	2.05	2.20
[BF_4]-	1.59	0.45	2.64	1.67	1.68	1.33	2.29	2.43	1.77	3.16	3.36
[SCN]-	1.49	0.38	2.48	1.44	1.70	0.94	1.62	2.13	1.23	2.82	3.07
[PhS]-	1.22	0.30	1.80	1.08	1.26	0.74	1.38	1.53	1.04	2.04	2.20
[TFMSM]-	0.00	0.00	0.22	0.34	-0.04	0.35	0.66	0.45	0.53	0.71	0.59
[TCN]-	0.58	0.05	1.17	1.09	0.82	0.57	1.51	1.64	1.05	2.03	2.12
[$DBPO_4$]-	1.06	0.25	1.37	0.71	0.91	0.53	0.91	0.95	0.72	1.30	1.41
[$DEPO_4$]-	1.42	0.37	1.87	0.94	1.29	0.70	1.15	1.29	0.91	1.76	1.92
[$DIsoPrPO_4$]-	1.22	0.31	1.60	0.86	1.09	0.64	1.08	1.15	0.86	1.55	1.68
[$DMPO_4$]-	1.65	0.45	2.22	1.06	1.54	0.77	1.19	1.45	0.95	2.02	2.25
[22-(ME)OHES]-	1.14	0.30	1.59	0.91	1.07	0.70	1.22	1.24	0.95	1.69	1.83
[BzS]-	1.38	0.37	1.97	1.12	1.39	0.80	1.39	1.56	1.07	2.04	2.24
[$EtSO_4$]-	1.55	0.42	2.23	1.19	1.51	0.88	1.48	1.67	1.15	2.25	2.46
[HSO_3]-	1.30	0.31	1.72	0.86	1.15	0.65	1.11	1.19	0.87	1.63	1.78
[HSO4]-	2.33	0.88	3.39	1.90	2.33	1.50	1.97	2.51	1.70	3.20	3.48
[MetA]-	1.65	0.62	2.31	1.51	1.67	1.16	1.80	1.98	1.46	2.45	2.63
[$MeSO_4$]-	1.74	0.49	2.53	1.30	1.72	0.96	1.51	1.82	1.19	2.48	2.74
[$MeSO_3$]-	1.96	0.52	2.69	1.05	1.86	0.76	0.94	1.46	0.79	2.19	2.58
[F_9BSO_3]-	0.64	0.15	1.02	0.75	0.57	0.66	1.21	1.01	0.95	1.38	1.46
[$OctSO_3$]-	1.13	0.25	1.48	0.74	0.97	0.56	0.96	1.01	0.75	1.40	1.53
[NH_2SO_3]-	2.26	0.76	3.14	1.36	2.21	1.06	1.05	1.75	1.00	2.55	3.02
[Tau]-	1.89	0.58	2.55	1.17	1.79	0.90	1.19	1.57	1.00	2.23	2.55
[Tosy]-	1.28	0.31	1.79	0.99	1.25	0.70	1.24	1.38	0.95	1.84	2.02
[CF_3SO_3]-	1.12	0.30	1.78	1.27	1.12	1.01	1.94	1.79	1.47	2.33	2.41

Table S3 (continued…): COSMO-RS predicted logarthmic activity coefficients of PET in different ILs at 363.15 K

	[4SB3MIM]+	[CMBIM]+	[CMMIM]+	[EUMIM]+	[(OH)MIM]+	[M33CEIM]+	[VCBIM]+	[DM(2OHE)A]+	[TE(3SP)A]+
[Ala]-	2.29	2.72	3.66	2.09	3.21	2.49	1.84	3.09	2.12
[Arg]-	2.24	2.51	3.29	2.03	3.00	2.44	1.84	2.83	2.09
[Aspg]-	2.65	3.04	4.14	2.45	3.70	2.89	2.15	3.46	2.46
[Cyst]-	2.31	2.54	3.64	2.08	3.30	2.56	1.81	2.98	2.09
[Glumn]-	2.41	2.74	3.67	2.22	3.32	2.63	1.96	3.11	2.24
[Gly]-	2.31	2.93	3.82	2.09	3.15	2.43	1.87	3.19	2.13
[His]-	2.53	2.69	3.74	2.33	3.50	2.79	2.04	3.15	2.34
[Isole]-	1.95	2.15	2.85	1.75	2.63	2.14	1.58	2.51	1.82
[Leu]-	1.93	2.09	2.80	1.71	2.59	2.11	1.55	2.46	1.79
[Lys]-	1.98	2.25	2.93	1.76	2.66	2.15	1.60	2.55	1.85
[Met]-	1.96	2.15	2.95	1.74	2.68	2.16	1.55	2.48	1.79
[Phe]-	1.87	1.96	2.71	1.66	2.50	2.05	1.47	2.30	1.71
[Pro]-	2.08	2.45	3.21	1.90	2.89	2.27	1.69	2.77	1.93
[AspMA]-	2.75	2.99	4.19	2.64	3.92	3.06	2.24	3.57	2.56
[GluMA]-	2.55	2.75	3.76	2.44	3.54	2.83	2.10	3.27	2.38
[Ser]-	2.67	3.12	4.22	2.51	3.77	2.92	2.18	3.59	2.50
[Thr]-	2.32	2.60	3.61	2.12	3.27	2.56	1.83	3.06	2.16
[Try]-	1.95	1.92	2.68	1.73	2.53	2.12	1.56	2.30	1.79
[Tyro]-	2.28	2.31	3.19	2.12	3.05	2.51	1.86	2.77	2.11
[Val]-	2.11	2.31	3.15	1.90	2.89	2.32	1.69	2.73	1.96
[2AIm]-	2.50	2.94	4.18	2.27	3.61	2.72	1.95	3.40	2.29
[2MIm]-	2.38	2.53	3.77	2.15	3.44	2.65	1.82	3.11	2.17
[45DCIm]-	2.20	1.77	2.95	1.86	2.83	2.44	1.57	2.49	1.99
[56DMBeIm]-	1.82	1.76	2.61	1.57	2.41	1.99	1.38	2.20	1.65
[BeIm]-	2.22	2.11	3.33	1.96	3.13	2.48	1.65	2.72	2.00
[Sac]-	2.29	2.29	3.46	2.10	3.24	2.56	1.74	2.81	2.07
[2-Mbut]-	2.08	2.35	3.20	1.89	2.89	2.27	1.66	2.70	1.90

[2-BrMAcr]-	2.16	2.17	3.31	1.93	3.11	2.43	1.66	2.62	1.90
[2-BOA]-	1.29	1.49	1.76	1.15	1.68	1.40	1.12	1.65	1.22
[2-ClAce]-	2.58	2.86	4.20	2.36	3.77	2.83	1.99	3.43	2.37
[2-EBA]-	1.89	2.11	2.75	1.70	2.53	2.06	1.55	2.44	1.76
[2-EHA]-	1.63	1.83	2.29	1.46	2.14	1.78	1.36	2.09	1.53
[2-HOA]-	1.09	1.28	1.48	0.97	1.43	1.20	0.96	1.41	1.04
[2-(OH)MAcr]-	2.43	2.62	3.84	2.24	3.51	2.70	1.88	3.17	2.23
[22-DMB]-	1.94	2.13	2.81	1.74	2.59	2.11	1.58	2.49	1.80
[3-$(OH)_2$-MBut]-	2.50	2.67	3.78	2.34	3.52	2.77	2.01	3.21	2.32
[4-EOA]-	1.46	1.69	2.05	1.32	1.93	1.60	1.24	1.88	1.38
[Abt]-	1.03	1.14	1.36	0.88	1.30	1.11	0.88	1.29	0.96
[Ace]-	2.23	2.88	3.70	2.02	2.99	2.31	1.82	3.09	2.06
[AceSal]-	1.98	2.06	2.93	1.81	2.70	2.18	1.54	2.45	1.80
[Acryl]-	2.36	2.80	3.88	2.15	3.36	2.54	1.87	3.17	2.15
[Benzoate]-	2.15	2.27	3.28	1.95	3.01	2.37	1.67	2.70	1.94
[But]-	2.11	2.47	3.26	1.92	2.91	2.29	1.71	2.80	1.96
[C3C]-	2.03	2.17	3.03	1.88	2.78	2.23	1.59	2.50	1.84
[Crotonate]-	2.15	2.56	3.44	1.97	3.02	2.33	1.73	2.87	1.97
[Dec]-	1.42	1.65	1.98	1.28	1.87	1.55	1.21	1.83	1.34
[For]-	2.33	3.21	4.00	2.08	2.87	2.29	1.91	3.30	2.14
[Gen]-	3.04	3.24	4.52	2.96	4.30	3.38	2.53	3.83	2.82
[Glyco]-	2.39	3.23	3.84	2.21	3.00	2.41	2.05	3.31	2.23
[Hex]-	1.86	2.13	2.72	1.68	2.50	2.03	1.53	2.42	1.73
[Im2C]-	2.39	2.81	3.88	2.19	3.40	2.59	1.91	3.13	2.17
[I3A]-	2.10	2.11	2.99	1.90	2.80	2.30	1.67	2.52	1.92
[Lac]-	2.37	3.00	3.76	2.21	3.18	2.50	1.99	3.23	2.21
[MCb]-	2.46	3.00	4.11	2.26	3.53	2.66	1.95	3.37	2.26
[N-MCb]-	2.21	2.85	3.65	2.00	3.00	2.32	1.80	3.05	2.04
[NMeO]-	2.29	2.74	3.75	2.11	3.27	2.49	1.82	3.06	2.09

[Oct]-	1.62	1.86	2.31	1.47	2.15	1.77	1.36	2.09	1.52
[Oxa]-	2.71	3.26	4.54	2.51	3.87	2.92	2.17	3.66	2.49
[Prop]-	2.23	2.67	3.55	2.02	3.09	2.39	1.80	3.01	2.06
[Sal]-	2.59	2.88	3.95	2.47	3.66	2.85	2.12	3.31	2.39
[ThioSal]-	2.11	2.15	3.20	1.90	2.97	2.35	1.63	2.58	1.89
[TFA]-	2.73	2.59	4.16	2.47	4.02	3.09	2.01	3.43	2.52
[TSAC]-	1.23	0.74	1.36	1.01	1.16	1.28	0.85	1.31	1.12
[B(F_5)SI]-	0.82	0.41	0.78	0.49	0.67	0.80	0.56	0.73	0.76
[MSA]-	2.50	2.62	3.91	2.31	3.61	2.79	1.90	3.21	2.29
[TFMI]	1.19	0.70	1.35	1.05	1.13	1.28	0.83	1.32	1.08
[DCN]-	2.90	2.80	4.86	2.62	4.73	3.39	2.10	3.67	2.57
[SbF_6]-	2.19	1.30	2.39	1.88	2.21	2.43	1.48	2.35	2.02
[PF_6]-	2.80	1.93	3.66	2.56	3.67	3.27	1.90	3.30	2.56
[NO_3]-	3.05	3.59	5.50	2.87	4.69	3.36	2.34	4.29	2.80
[WOF_5]-	2.47	1.65	2.95	2.20	2.86	2.79	1.70	2.75	2.27
[Phenolate]-	2.30	2.32	3.54	2.06	3.28	2.56	1.74	2.92	2.10
[BF_4]-	3.50	3.36	6.13	3.30	6.01	4.13	2.50	4.72	3.21
[SCN]-	3.12	3.19	5.66	2.88	5.30	3.62	2.26	4.20	2.77
[PhS]-	2.29	2.32	3.55	2.03	3.32	2.56	1.72	2.87	2.06
[TFMSM]-	0.74	0.28	0.71	0.68	0.48	0.78	0.52	0.82	0.66
[TCN]-	2.25	1.87	3.33	1.92	3.23	2.61	1.59	2.54	1.96
[$DBPO_4$]-	1.48	1.67	2.11	1.32	1.95	1.62	1.21	1.88	1.39
[$DEPO_4$]-	1.98	2.24	2.98	1.81	2.72	2.18	1.58	2.57	1.84
[$DIsoPrPO_4$]-	1.76	1.95	2.55	1.58	2.35	1.93	1.42	2.24	1.64
[$DMPO_4$]-	2.29	2.63	3.62	2.11	3.24	2.52	1.80	3.03	2.11
[22-(ME)OHES]-	1.92	1.95	2.79	1.72	2.56	2.10	1.45	2.38	1.77
[BzS]-	2.30	2.42	3.56	2.10	3.29	2.56	1.76	2.88	2.09
[$EtSO_4$]-	2.53	2.70	4.05	2.34	3.74	2.84	1.92	3.32	2.32

[HSO_3]-	1.85	2.09	2.76	1.67	2.54	2.04	1.47	2.39	1.73
[HSO4]-	3.50	3.90	6.05	3.40	5.54	3.96	2.73	4.81	3.22
[MetA]-	2.69	2.80	4.10	2.49	3.86	3.00	2.10	3.35	2.46
[$MeSO_4$]-	2.79	3.03	4.65	2.60	4.25	3.13	2.10	3.73	2.55
[$MeSO_3$]-	2.53	3.15	4.29	2.34	3.65	2.73	2.00	3.50	2.33
[F_9BSO_3]-	1.61	1.39	2.15	1.38	2.05	1.75	1.18	1.89	1.51
[$OctSO_3$]-	1.60	1.80	2.33	1.42	2.14	1.76	1.28	2.04	1.50
[NH_2SO_3]-	2.93	3.68	4.99	2.72	4.12	3.11	2.35	4.07	2.71
[Tau]-	2.54	3.02	4.11	2.32	3.59	2.75	2.01	3.41	2.35
[Tosy]-	2.08	2.21	3.16	1.88	2.91	2.30	1.60	2.60	1.89
[CF_3SO_3]-	2.61	2.30	3.83	2.37	3.74	2.97	1.88	3.19	2.39

Table S3 (continued…): COSMO-RS predicted logarthmic activity coefficients of PET in different ILs at 363.15 K

	[2ETeG]+	[TMGH]+	[BAMDMG]+	[C(NH2)3]+	[HMG]+	[TeMDBG]+	[TeMDOG]+	[C2(OH)DMIM]+	[APrMIM]+	[MAEIM]+
[Ala]-	1.07	0.84	0.23	5.16	0.70	0.29	0.12	1.40	1.28	1.44
[Arg]-	1.25	1.26	0.38	4.10	1.03	0.53	0.27	1.63	1.48	1.65
[Aspg]-	1.44	1.28	0.44	5.93	1.10	0.61	0.31	1.78	1.63	1.82
[Cyst]-	1.06	1.08	0.17	4.67	0.80	0.26	0.05	1.56	1.37	1.57
[Glumn]-	1.30	1.26	0.38	4.98	1.02	0.53	0.27	1.69	1.53	1.72
[Gly]-	1.02	0.44	0.24	5.86	0.52	0.27	0.13	1.15	1.09	1.19
[His]-	1.41	1.56	0.41	4.70	1.21	0.59	0.29	1.92	1.73	1.94
[Isole]-	0.96	1.04	0.19	3.42	0.76	0.26	0.09	1.42	1.26	1.43
[Leu]-	0.94	1.05	0.18	3.30	0.75	0.24	0.08	1.41	1.25	1.42
[Lys]-	0.96	0.99	0.19	3.69	0.75	0.27	0.09	1.38	1.23	1.40
[Met]-	0.89	0.99	0.11	3.57	0.70	0.18	0.01	1.37	1.20	1.38
[Phe]-	0.86	1.04	0.10	3.20	0.71	0.17	0.00	1.37	1.20	1.37
[Pro]-	0.97	0.90	0.18	4.39	0.68	0.24	0.08	1.36	1.23	1.41

[AspMA]-	1.62	1.72	0.53	6.04	1.36	0.72	0.40	2.10	1.92	2.17
[GluMA]-	1.53	1.68	0.52	5.17	1.31	0.69	0.40	2.01	1.84	2.06
[Ser]-	1.48	1.25	0.48	6.32	1.09	0.62	0.36	1.78	1.65	1.84
[Thr]-	1.10	1.13	0.22	5.03	0.84	0.31	0.10	1.58	1.41	1.62
[Try]-	1.04	1.29	0.24	2.91	0.94	0.36	0.13	1.56	1.37	1.54
[Tyro]-	1.35	1.61	0.43	3.78	1.22	0.59	0.31	1.88	1.69	1.89
[Val]-	1.03	1.10	0.21	3.88	0.81	0.28	0.10	1.51	1.34	1.53
[2AIm]-	1.13	0.83	0.19	6.32	0.73	0.27	0.06	1.45	1.33	1.50
[2MIm]-	1.07	1.16	0.15	5.07	0.83	0.23	0.02	1.62	1.43	1.66
[45DCIm]-	0.93	1.57	0.01	2.24	0.94	0.13	-0.09	1.82	1.51	1.79
[56DMBeIm]-	0.79	1.05	0.03	2.87	0.67	0.09	-0.08	1.36	1.17	1.34
[BeIm]-	0.98	1.33	0.06	3.84	0.85	0.15	-0.07	1.67	1.43	1.67
[Sac]-	1.05	1.43	0.09	4.54	0.94	0.24	-0.02	1.74	1.50	1.75
[2-Mbut]-	0.95	0.91	0.17	4.22	0.67	0.21	0.06	1.37	1.23	1.40
[2-BrMAcr]-	0.93	1.18	0.06	3.74	0.77	0.13	-0.05	1.58	1.34	1.57
[2-BOA]-	0.67	0.69	0.13	1.90	0.52	0.16	0.05	0.98	0.89	0.98
[2-ClAce]-	1.18	1.09	0.23	6.28	0.84	0.32	0.10	1.63	1.46	1.67
[2-EBA]-	0.93	0.95	0.20	3.24	0.70	0.24	0.10	1.35	1.20	1.36
[2-EHA]-	0.83	0.87	0.17	2.58	0.64	0.21	0.08	1.21	1.09	1.22
[2-HOA]-	0.58	0.57	0.10	1.58	0.43	0.12	0.03	0.84	0.76	0.83
[2-(OH)MAcr]-	1.13	1.22	0.20	5.44	0.87	0.29	0.08	1.67	1.48	1.71
[22-DMB]-	0.96	1.00	0.21	3.27	0.73	0.26	0.11	1.39	1.24	1.41
[3-$(OH)_2$-MBut]-	1.38	1.49	0.41	5.08	1.14	0.55	0.29	1.87	1.69	1.91
[4-EOA]-	0.73	0.77	0.13	2.39	0.57	0.16	0.04	1.09	0.98	1.10
[Abt]-	0.52	0.53	0.07	1.30	0.38	0.08	0.00	0.78	0.69	0.76
[Ace]-	0.96	0.27	0.24	5.71	0.41	0.24	0.13	1.02	0.99	1.06
[AceSal]-	0.91	1.14	0.11	3.83	0.77	0.20	0.00	1.46	1.28	1.48
[Acryl]-	1.04	0.71	0.21	5.89	0.61	0.25	0.09	1.33	1.22	1.37
[Benzoate]-	0.96	1.09	0.13	4.21	0.75	0.20	0.02	1.49	1.31	1.52

[But]-	0.99	0.85	0.22	4.30	0.67	0.26	0.11	1.35	1.23	1.39
[C3C]-	0.94	1.14	0.12	4.14	0.78	0.23	0.01	1.47	1.29	1.49
[Crotonate]-	0.95	0.75	0.18	4.92	0.59	0.21	0.06	1.29	1.17	1.33
[Dec]-	0.72	0.75	0.13	2.30	0.56	0.16	0.04	1.07	0.96	1.07
[For]-	0.95	-0.25	0.26	7.15	0.22	0.25	0.13	0.73	0.79	0.76
[Gen]-	1.99	2.12	0.79	6.41	1.73	1.04	0.64	2.45	2.26	2.51
[Glyco]-	1.27	0.31	0.52	6.32	0.61	0.57	0.39	1.09	1.12	1.14
[Hex]-	0.90	0.91	0.18	3.35	0.68	0.23	0.08	1.31	1.18	1.33
[Im2C]-	1.12	0.87	0.25	5.75	0.74	0.33	0.12	1.43	1.30	1.47
[I3A]-	1.12	1.34	0.27	3.46	0.97	0.39	0.16	1.63	1.44	1.63
[Lac]-	1.26	0.71	0.46	5.80	0.75	0.52	0.34	1.34	1.29	1.39
[MCb]-	1.08	0.69	0.22	6.63	0.63	0.27	0.09	1.36	1.25	1.41
[N-MCb]-	0.96	0.38	0.22	5.67	0.45	0.24	0.11	1.07	1.03	1.12
[NMeO]-	0.99	0.78	0.17	5.75	0.62	0.22	0.05	1.35	1.22	1.39
[Oct]-	0.81	0.85	0.15	2.73	0.62	0.19	0.06	1.19	1.07	1.21
[Oxa]-	1.33	0.83	0.35	7.42	0.83	0.47	0.22	1.52	1.42	1.56
[Prop]-	1.02	0.71	0.24	4.97	0.62	0.27	0.12	1.30	1.19	1.34
[Sal]-	1.49	1.50	0.49	5.61	1.20	0.64	0.36	1.90	1.74	1.95
[ThioSal]-	0.95	1.17	0.09	3.84	0.78	0.18	-0.03	1.53	1.32	1.53
[TFA]-	1.25	1.75	0.18	5.21	1.12	0.33	0.06	2.09	1.78	2.12
[TSAC]-	0.44	0.94	-0.06	1.06	0.57	0.09	-0.06	1.05	0.92	1.04
[B(F_5)SI]-	0.28	0.46	-0.05	-0.14	0.27	-0.01	-0.10	0.66	0.52	0.55
[MSA]-	1.19	1.45	0.16	5.53	1.01	0.33	0.06	1.81	1.59	1.85
[TFMI]	0.46	0.99	-0.05	1.26	0.61	0.11	-0.04	1.06	0.96	1.07
[DCN]-	1.18	1.64	-0.01	5.62	1.04	0.13	-0.15	2.11	1.76	2.13
[SbF_6]-	0.84	1.95	-0.08	0.27	1.14	0.18	-0.08	2.02	1.72	2.04
[PF_6]-	1.18	2.47	-0.03	0.48	1.44	0.28	-0.06	2.52	2.13	2.60
[NO_3]-	1.36	0.84	0.24	10.70	0.84	0.38	0.11	1.65	1.53	1.71
[WOF_5]-	1.04	2.20	-0.02	0.89	1.29	0.25	-0.04	2.26	1.92	2.30

[Phenolate]-	1.05	1.25	0.16	4.49	0.85	0.24	0.04	1.65	1.43	1.67
$[BF_4]$-	1.56	2.10	0.13	7.72	1.43	0.42	0.04	2.58	2.22	2.67
[SCN]-	1.32	1.44	0.03	8.12	1.03	0.19	-0.11	2.04	1.77	2.09
[PhS]-	1.00	1.27	0.04	4.40	0.83	0.13	-0.08	1.65	1.41	1.66
[TFMSM]-	0.28	0.67	-0.06	0.66	0.43	0.10	-0.02	0.69	0.67	0.73
[TCN]-	0.78	1.50	-0.19	2.61	0.83	-0.06	-0.28	1.81	1.45	1.77
$[DBPO_4]$-	0.68	0.80	0.08	2.67	0.56	0.13	0.00	1.10	0.97	1.10
$[DEPO_4]$-	0.91	1.02	0.14	4.07	0.71	0.21	0.04	1.40	1.24	1.43
$[DIsoPrPO_4]$-	0.82	0.96	0.12	3.25	0.67	0.18	0.03	1.30	1.14	1.30
$[DMPO_4]$-	1.03	1.02	0.18	5.33	0.75	0.26	0.07	1.50	1.34	1.54
[22-(ME)OHES]-	0.89	1.18	0.09	3.63	0.80	0.23	0.02	1.44	1.26	1.45
[BzS]-	1.03	1.29	0.10	4.82	0.87	0.23	0.00	1.66	1.44	1.68
$[EtSO_4]$-	1.15	1.38	0.15	5.93	0.95	0.29	0.04	1.79	1.57	1.83
$[HSO_3]$-	0.84	0.99	0.10	3.73	0.68	0.17	0.01	1.34	1.18	1.35
[HSO4]-	1.89	1.74	0.47	11.09	1.49	0.74	0.33	2.37	2.18	2.47
[MetA]-	1.41	1.69	0.29	5.48	1.24	0.51	0.16	2.04	1.80	2.07
$[MeSO_4]$-	1.27	1.36	0.18	7.35	0.99	0.34	0.07	1.87	1.65	1.92
$[MeSO_3]$-	1.11	0.68	0.21	7.29	0.64	0.29	0.09	1.36	1.26	1.42
$[F_9BSO_3]$-	0.74	1.16	0.05	2.54	0.75	0.20	0.00	1.33	1.15	1.32
$[OctSO_3]$-	0.72	0.86	0.07	3.05	0.59	0.13	-0.01	1.17	1.03	1.17
$[NH_2SO_3]$-	1.47	0.75	0.38	8.87	0.89	0.55	0.24	1.55	1.49	1.59
[Tau]-	1.22	0.99	0.27	6.26	0.84	0.39	0.15	1.55	1.42	1.60
[Tosy]-	0.91	1.15	0.07	4.20	0.76	0.18	-0.03	1.50	1.29	1.51
$[CF_3SO_3]$-	1.19	1.92	0.10	4.61	1.19	0.31	0.02	2.14	1.83	2.17

Table S3 (continued…): COSMO-RS predicted logarithmic activity coefficients of PET in different ILs at 363.15 K

	[BzTPhP]+	[TeBP]+	[TeEP]+	[TEMP]+	[TMBP]+	[TMEOHP]+	[TMEP]+	[TBMP]+	[THTeDP]+	[A34DMPy]+	[A35DMPy]+
[Ala]-	0.40	0.13	0.31	0.52	0.91	1.81	0.82	0.42	0.01	0.71	0.63
[Arg]-	0.54	0.35	0.70	0.89	1.14	2.01	1.24	0.61	0.10	0.98	0.91
[Aspg]-	0.66	0.41	0.74	0.94	1.28	2.17	1.24	0.70	0.12	1.10	1.02
[Cyst]-	0.38	0.07	0.39	0.60	0.92	1.97	1.00	0.34	-0.06	0.77	0.69
[Glumn]-	0.57	0.34	0.68	0.87	1.17	2.09	1.22	0.62	0.10	0.99	0.92
[Gly]-	0.43	0.12	0.16	0.33	0.79	1.44	0.45	0.42	0.00	0.61	0.52
[His]-	0.62	0.38	0.83	1.05	1.30	2.35	1.48	0.66	0.12	1.14	1.07
[Isole]-	0.30	0.10	0.41	0.62	0.88	1.84	1.03	0.36	0.01	0.69	0.63
[Leu]-	0.28	0.09	0.41	0.62	0.86	1.84	1.03	0.34	0.00	0.68	0.61
[Lys]-	0.32	0.12	0.41	0.61	0.88	1.79	0.98	0.38	-0.01	0.69	0.62
[Met]-	0.27	0.02	0.33	0.53	0.79	1.76	0.93	0.26	-0.08	0.64	0.57
[Phe]-	0.24	0.01	0.36	0.56	0.77	1.75	0.97	0.24	-0.08	0.64	0.57
[Pro]-	0.33	0.07	0.31	0.53	0.86	1.79	0.89	0.36	-0.02	0.66	0.58
[AspMA]-	0.71	0.50	0.96	1.19	1.49	2.60	1.63	0.80	0.22	1.27	1.19
[GluMA]-	0.67	0.49	0.94	1.16	1.42	2.48	1.61	0.77	0.23	1.22	1.14
[Ser]-	0.67	0.43	0.72	0.92	1.30	2.20	1.22	0.74	0.18	1.09	1.00
[Thr]-	0.37	0.14	0.45	0.67	1.00	2.06	1.08	0.41	0.00	0.78	0.70
[Try]-	0.38	0.19	0.63	0.81	0.96	1.90	1.22	0.41	0.02	0.85	0.80
[Tyro]-	0.57	0.40	0.88	1.09	1.26	2.29	1.53	0.64	0.18	1.12	1.05
[Val]-	0.34	0.12	0.44	0.66	0.93	1.97	1.07	0.38	0.01	0.74	0.67
[2AIm]-	0.40	0.07	0.30	0.50	0.93	1.82	0.77	0.38	-0.08	0.74	0.65
[2MIm]-	0.33	0.03	0.38	0.61	0.94	2.12	1.06	0.31	-0.06	0.76	0.67
[45DCIm]-	0.13	-0.05	0.52	0.76	0.88	2.38	1.39	0.15	-0.11	0.73	0.66
[56DMBeIm]-	0.15	-0.08	0.31	0.51	0.69	1.75	0.95	0.14	-0.13	0.57	0.51
[BeIm]-	0.22	-0.05	0.41	0.65	0.87	2.16	1.18	0.19	-0.12	0.73	0.65
[Sac]-	0.31	0.04	0.53	0.75	0.97	2.19	1.27	0.28	-0.12	0.83	0.75
[2-Mbut]-	0.34	0.05	0.29	0.50	0.82	1.77	0.87	0.33	-0.02	0.66	0.58

[2-BrMAcr]-	0.30	-0.05	0.34	0.56	0.79	1.97	1.03	0.19	-0.11	0.73	0.65
[2-BOA]-	0.18	0.04	0.27	0.44	0.62	1.26	0.73	0.25	0.01	0.48	0.44
[2-ClAce]-	0.42	0.14	0.42	0.64	1.02	2.09	1.00	0.43	0.00	0.81	0.72
[2-EBA]-	0.31	0.09	0.36	0.57	0.83	1.75	0.95	0.36	0.02	0.66	0.60
[2-EHA]-	0.25	0.07	0.34	0.54	0.75	1.56	0.89	0.31	0.02	0.60	0.54
[2-HOA]-	0.13	0.02	0.22	0.37	0.52	1.07	0.62	0.21	0.00	0.40	0.36
[2-(OH)MAcr]-	0.38	0.11	0.45	0.68	1.00	2.16	1.12	0.38	-0.01	0.80	0.72
[22-DMB]-	0.32	0.11	0.39	0.61	0.86	1.81	0.99	0.37	0.03	0.69	0.62
[3-$(OH)_2$-MBut]-	0.57	0.36	0.75	0.98	1.25	2.34	1.40	0.63	0.16	1.07	0.99
[4-EOA]-	0.20	0.03	0.29	0.47	0.68	1.41	0.80	0.26	-0.01	0.53	0.47
[Abt]-	0.09	-0.01	0.18	0.32	0.45	0.99	0.56	0.16	-0.02	0.35	0.32
[Ace]-	0.43	0.10	0.07	0.23	0.71	1.26	0.29	0.40	0.01	0.55	0.46
[AceSal]-	0.28	0.03	0.40	0.60	0.83	1.85	1.04	0.26	-0.08	0.69	0.62
[Acryl]-	0.41	0.08	0.22	0.41	0.83	1.68	0.65	0.37	-0.02	0.67	0.58
[Benzoate]-	0.32	0.02	0.35	0.56	0.84	1.90	0.98	0.28	-0.06	0.70	0.63
[But]-	0.37	0.10	0.30	0.51	0.85	1.76	0.84	0.39	0.01	0.67	0.59
[C3C]-	0.33	0.05	0.41	0.61	0.85	1.83	1.02	0.29	-0.09	0.72	0.65
[Crotonate]-	0.36	0.05	0.21	0.41	0.79	1.66	0.71	0.33	-0.03	0.62	0.54
[Dec]-	0.19	0.03	0.29	0.47	0.67	1.37	0.79	0.26	-0.01	0.51	0.46
[For]-	0.47	0.11	-0.08	0.03	0.61	0.76	-0.19	0.42	0.01	0.46	0.37
[Gen]-	1.00	0.79	1.35	1.57	1.83	2.89	2.00	1.10	0.40	1.66	1.58
[Glyco]-	0.70	0.42	0.34	0.46	0.95	1.21	0.36	0.73	0.21	0.80	0.73
[Hex]-	0.30	0.07	0.34	0.55	0.82	1.70	0.92	0.34	0.01	0.64	0.57
[Im2C]-	0.48	0.15	0.36	0.54	0.91	1.74	0.79	0.43	-0.01	0.79	0.70
[I3A]-	0.43	0.22	0.63	0.83	1.01	2.00	1.24	0.45	0.05	0.90	0.84
[Lac]-	0.63	0.37	0.44	0.61	1.02	1.62	0.73	0.67	0.18	0.86	0.78
[MCb]-	0.42	0.10	0.23	0.43	0.88	1.72	0.66	0.40	-0.02	0.68	0.59
[N-MCb]-	0.41	0.09	0.10	0.27	0.73	1.35	0.39	0.39	-0.01	0.56	0.48
[NMeO]-	0.38	0.06	0.23	0.43	0.82	1.72	0.72	0.34	-0.05	0.65	0.57

[Oct]-	0.24	0.05	0.32	0.52	0.75	1.54	0.87	0.30	0.00	0.58	0.52
[Oxa]-	0.59	0.28	0.46	0.64	1.08	1.80	0.78	0.58	0.06	0.92	0.83
[Prop]-	0.40	0.11	0.24	0.44	0.84	1.67	0.70	0.41	0.02	0.66	0.58
[Sal]-	0.70	0.43	0.82	1.03	1.33	2.30	1.41	0.72	0.18	1.17	1.09
[ThioSal]-	0.30	-0.01	0.38	0.59	0.82	1.91	1.03	0.23	-0.11	0.73	0.65
[TFA]-	0.32	0.13	0.65	0.93	1.18	2.78	1.56	0.39	0.00	0.93	0.84
[TSAC]-	-0.08	0.02	0.39	0.51	0.52	1.40	0.86	0.09	-0.01	0.37	0.34
[$B(F_5)SI$]-	-0.12	-0.05	0.18	0.25	0.23	0.82	0.43	-0.01	-0.03	0.19	0.17
[MSA]-	0.37	0.13	0.59	0.82	1.11	2.32	1.31	0.39	-0.07	0.89	0.81
[TFMI]	-0.06	0.03	0.42	0.55	0.55	1.40	0.90	0.11	-0.01	0.41	0.38
[DCN]-	0.27	-0.12	0.45	0.73	1.05	2.74	1.39	0.16	-0.21	0.89	0.79
[SbF_6]-	-0.01	0.03	0.74	1.01	1.04	2.79	1.79	0.18	-0.05	0.75	0.69
[PF_6]-	0.11	0.07	0.91	1.24	1.36	3.52	2.21	0.28	-0.07	1.02	0.93
[NO_3]-	0.51	0.17	0.40	0.60	1.14	1.99	0.77	0.49	-0.01	0.89	0.78
[WOF_5]-	0.08	0.07	0.84	1.13	1.19	3.10	1.99	0.25	-0.04	0.90	0.82
[Phenolate]-	0.32	0.06	0.43	0.66	0.94	2.14	1.13	0.31	-0.03	0.76	0.68
[BF_4]-	0.39	0.16	0.86	1.18	1.57	3.42	1.91	0.47	-0.05	1.19	1.07
[SCN]-	0.34	-0.07	0.45	0.71	1.13	2.57	1.21	0.23	-0.21	0.94	0.82
[PhS]-	0.24	-0.07	0.37	0.60	0.86	2.13	1.12	0.19	-0.16	0.72	0.64
[TFMSM]-	-0.10	0.06	0.33	0.41	0.39	0.93	0.63	0.10	0.03	0.28	0.26
[TCN]-	0.05	-0.26	0.33	0.58	0.71	2.34	1.26	-0.07	-0.28	0.66	0.58
[$DBPO_4$]-	0.15	0.01	0.28	0.46	0.65	1.43	0.80	0.21	-0.05	0.48	0.43
[$DEPO_4$]-	0.28	0.05	0.35	0.56	0.84	1.83	0.98	0.30	-0.04	0.64	0.57
[$DIsoPrPO_4$]-	0.22	0.04	0.35	0.55	0.77	1.69	0.95	0.27	-0.03	0.59	0.53
[$DMPO_4$]-	0.36	0.09	0.35	0.57	0.92	1.95	0.96	0.37	-0.03	0.71	0.63
[22-(ME)OHES]-	0.22	0.08	0.47	0.66	0.85	1.87	1.09	0.28	-0.06	0.66	0.60
[BzS]-	0.32	0.04	0.45	0.67	0.94	2.11	1.15	0.29	-0.10	0.77	0.70
[$EtSO_4$]-	0.34	0.10	0.51	0.75	1.07	2.34	1.26	0.36	-0.05	0.83	0.74

[HSO_3]-	0.21	0.03	0.35	0.55	0.79	1.76	0.97	0.26	-0.06	0.59	0.53
[HSO4]-	0.76	0.47	1.00	1.26	1.72	2.87	1.64	0.83	0.12	1.43	1.32
[MetA]-	0.54	0.27	0.83	1.06	1.32	2.52	1.56	0.56	-0.02	1.14	1.06
[$MeSO_4$]-	0.41	0.14	0.53	0.77	1.15	2.41	1.23	0.42	-0.04	0.90	0.81
[$MeSO_3$]-	0.43	0.12	0.24	0.43	0.91	1.72	0.65	0.42	-0.04	0.69	0.60
[F_9BSO_3]-	0.06	0.08	0.51	0.67	0.74	1.73	1.08	0.22	0.00	0.56	0.52
[$OctSO_3$]-	0.15	0.00	0.30	0.48	0.69	1.54	0.86	0.21	-0.06	0.50	0.45
[NH_2SO_3]-	0.65	0.33	0.52	0.69	1.21	1.78	0.74	0.67	0.04	0.99	0.89
[Tau]-	0.48	0.21	0.46	0.65	1.06	1.96	0.95	0.50	-0.01	0.83	0.75
[Tosy]-	0.26	0.01	0.38	0.59	0.83	1.92	1.04	0.24	-0.11	0.67	0.60
[CF_3SO_3]-	0.23	0.11	0.73	1.01	1.18	2.86	1.71	0.34	-0.02	0.93	0.85

Table S3 (continued…): COSMO-RS predicted logarthmic activity coefficients of PET in different ILs at 363.15 K

	[B-3-MPy]+	[B-4-MPy]+	[BPy]+	[EPy]+	[HPy]+	[OPy]+	[DMPyrr]+	[DprPyrr]+	[12MeoEMPyrr]+
[Ala]-	0.88	0.97	1.26	1.34	1.14	0.91	0.69	0.36	0.98
[Arg]-	1.08	1.15	1.40	1.60	1.24	1.01	1.25	0.71	1.26
[Aspg]-	1.22	1.31	1.61	1.76	1.43	1.17	1.14	0.78	1.36
[Cyst]-	0.88	0.96	1.27	1.52	1.08	0.82	0.99	0.41	1.07
[Glumn]-	1.11	1.19	1.46	1.66	1.30	1.05	1.19	0.70	1.28
[Gly]-	0.83	0.94	1.21	1.08	1.17	0.94	0.14	0.25	0.78
[His]-	1.22	1.28	1.57	1.90	1.34	1.08	1.52	0.82	1.46
[Isole]-	0.80	0.87	1.11	1.34	0.96	0.74	1.06	0.41	1.02
[Leu]-	0.78	0.85	1.08	1.33	0.92	0.71	1.08	0.41	1.02
[Lys]-	0.81	0.88	1.13	1.32	0.99	0.78	1.00	0.42	1.01
[Met]-	0.74	0.81	1.07	1.32	0.91	0.69	0.97	0.33	0.94
[Phe]-	0.71	0.77	1.01	1.30	0.83	0.62	1.04	0.35	0.95
[Pro]-	0.81	0.89	1.16	1.31	1.04	0.82	0.84	0.34	0.96

[AspMA]-	1.37	1.45	1.77	2.08	1.52	1.24	1.65	0.97	1.64
[GluMA]-	1.30	1.37	1.66	1.98	1.44	1.17	1.66	0.94	1.58
[Ser]-	1.24	1.33	1.64	1.74	1.48	1.21	1.08	0.77	1.37
[Thr]-	0.90	0.98	1.28	1.51	1.11	0.86	1.07	0.48	1.14
[Try]-	0.88	0.93	1.15	1.49	0.94	0.73	1.31	0.59	1.15
[Tyro]-	1.16	1.21	1.46	1.83	1.23	0.99	1.63	0.85	1.45
[Val]-	0.85	0.92	1.18	1.43	1.02	0.78	1.10	0.44	1.09
[2AIm]-	0.91	1.01	1.34	1.41	1.19	0.93	0.59	0.36	1.01
[2MIm]-	0.87	0.95	1.27	1.56	1.05	0.79	1.07	0.39	1.13
[45DCIm]-	0.70	0.73	1.03	1.66	0.69	0.44	1.67	0.47	1.27
[56DMBeIm]-	0.62	0.67	0.92	1.26	0.71	0.51	1.07	0.28	0.91
[BeIm]-	0.77	0.82	1.13	1.58	0.86	0.61	1.33	0.39	1.14
[Sac]-	0.85	0.90	1.23	1.67	0.95	0.69	1.39	0.52	1.21
[2-Mbut]-	0.79	0.87	1.13	1.31	0.99	0.77	0.82	0.31	0.93
[2-BrMAcr]-	0.77	0.84	1.14	1.55	0.89	0.63	1.10	0.31	1.00
[2-BOA]-	0.59	0.64	0.79	0.92	0.71	0.55	0.73	0.26	0.70
[2-ClAce]-	0.94	1.03	1.36	1.55	1.17	0.90	0.89	0.47	1.15
[2-EBA]-	0.78	0.86	1.08	1.27	0.95	0.74	0.95	0.37	0.96
[2-EHA]-	0.70	0.77	0.96	1.13	0.84	0.66	0.90	0.34	0.87
[2-HOA]-	0.50	0.55	0.68	0.78	0.61	0.47	0.62	0.21	0.59
[2-(OH)MAcr]-	0.91	0.98	1.31	1.60	1.09	0.83	1.12	0.47	1.18
[22-DMB]-	0.81	0.88	1.10	1.30	0.96	0.75	1.00	0.40	1.00
[3-$(OH)_2$-MBut]-	1.16	1.23	1.52	1.82	1.30	1.04	1.43	0.76	1.41
[4-EOA]-	0.64	0.69	0.88	1.03	0.78	0.60	0.81	0.28	0.78
[Abt]-	0.43	0.48	0.59	0.70	0.52	0.39	0.56	0.16	0.53
[Ace]-	0.78	0.90	1.14	0.93	1.13	0.92	-0.10	0.16	0.65
[AceSal]-	0.74	0.80	1.07	1.39	0.87	0.65	1.11	0.39	1.01
[Acryl]-	0.84	0.94	1.23	1.27	1.12	0.88	0.44	0.28	0.88
[Benzoate]-	0.79	0.86	1.14	1.43	0.95	0.71	1.01	0.35	1.00

[But]-	0.83	0.92	1.17	1.28	1.06	0.84	0.76	0.33	0.94
[C3C]-	0.78	0.84	1.12	1.42	0.92	0.69	1.07	0.41	1.01
[Crotonate]-	0.78	0.87	1.15	1.23	1.04	0.82	0.58	0.26	0.85
[Dec]-	0.62	0.68	0.86	1.00	0.76	0.59	0.80	0.28	0.76
[For]-	0.75	0.88	1.11	0.59	1.18	0.97	-0.85	0.07	0.43
[Gen]-	1.73	1.80	2.12	2.47	1.84	1.53	2.02	1.34	1.97
[Glyco]-	1.06	1.18	1.39	1.02	1.43	1.22	-0.13	0.45	0.80
[Hex]-	0.77	0.84	1.07	1.24	0.95	0.75	0.91	0.35	0.93
[Im2C]-	0.93	1.02	1.32	1.41	1.18	0.94	0.63	0.40	0.97
[I3A]-	0.95	1.00	1.24	1.58	1.03	0.80	1.32	0.61	1.19
[Lac]-	1.06	1.17	1.41	1.29	1.36	1.14	0.44	0.52	0.99
[MCb]-	0.87	0.97	1.29	1.29	1.18	0.93	0.42	0.31	0.91
[N-MCb]-	0.78	0.89	1.15	1.01	1.12	0.91	0.08	0.19	0.70
[NMeO]-	0.80	0.90	1.20	1.30	1.08	0.84	0.58	0.29	0.89
[Oct]-	0.70	0.76	0.96	1.13	0.85	0.67	0.88	0.32	0.85
[Oxa]-	1.09	1.19	1.51	1.48	1.38	1.10	0.48	0.54	1.09
[Prop]-	0.84	0.94	1.20	1.22	1.11	0.88	0.51	0.30	0.88
[Sal]-	1.27	1.35	1.65	1.90	1.44	1.18	1.38	0.83	1.44
[ThioSal]-	0.78	0.84	1.13	1.49	0.90	0.66	1.10	0.36	1.01
[TFA]-	0.96	1.03	1.38	1.94	1.04	0.75	1.73	0.65	1.51
[TSAC]-	0.33	0.33	0.47	0.84	0.26	0.13	1.05	0.36	0.82
[B(F_5)SI]-	0.16	0.16	0.22	0.44	0.08	0.00	0.53	0.14	0.41
[MSA]-	0.95	1.01	1.36	1.75	1.10	0.83	1.40	0.61	1.32
[TFMI]	0.36	0.36	0.51	0.89	0.29	0.16	1.09	0.39	0.84
[DCN]-	0.92	0.99	1.44	2.09	1.04	0.70	1.52	0.44	1.37
[SbF_6]-	0.65	0.65	0.96	1.78	0.53	0.29	2.23	0.69	1.58
[PF_6]-	0.91	0.93	1.35	2.39	0.82	0.49	2.70	0.87	1.95
[NO_3]-	1.06	1.17	1.58	1.58	1.37	1.05	0.38	0.52	1.17
[WOF_5]-	0.80	0.81	1.16	2.06	0.69	0.42	2.45	0.79	1.75

[Phenolate]-	0.84	0.91	1.21	1.56	0.98	0.73	1.20	0.43	1.15
$[BF_4]$-	1.21	1.28	1.80	2.53	1.31	0.91	1.98	0.89	1.92
[SCN]-	1.01	1.09	1.59	2.05	1.20	0.84	1.15	0.48	1.37
[PhS]-	0.78	0.84	1.17	1.59	0.91	0.66	1.23	0.37	1.10
[TFMSM]-	0.24	0.23	0.32	0.57	0.16	0.08	0.76	0.32	0.60
[TCN]-	0.60	0.63	0.99	1.73	0.60	0.33	1.53	0.27	1.12
$[DBPO_4]$-	0.57	0.62	0.82	1.01	0.69	0.52	0.85	0.28	0.77
$[DEPO_4]$-	0.75	0.82	1.09	1.32	0.93	0.71	1.01	0.37	0.99
$[DIsoPrPO_4]$-	0.68	0.74	0.97	1.21	0.82	0.63	1.00	0.35	0.92
$[DMPO_4]$-	0.84	0.92	1.23	1.44	1.07	0.83	0.92	0.39	1.05
[22-(ME)OHES]-	0.70	0.75	1.01	1.33	0.81	0.60	1.21	0.47	1.06
[BzS]-	0.83	0.89	1.22	1.59	0.97	0.72	1.23	0.46	1.14
$[EtSO_4]$-	0.90	0.97	1.33	1.71	1.08	0.81	1.32	0.54	1.28
$[HSO_3]$-	0.68	0.74	1.00	1.25	0.85	0.64	1.03	0.36	0.95
[HSO4]-	1.55	1.65	2.12	2.39	1.78	1.40	1.43	1.07	1.84
[MetA]-	1.19	1.25	1.60	2.02	1.31	1.01	1.64	0.82	1.53
$[MeSO_4]$-	1.00	1.08	1.47	1.80	1.21	0.91	1.21	0.58	1.34
$[MeSO_3]$-	0.88	0.98	1.32	1.30	1.21	0.96	0.40	0.34	0.93
$[F_9BSO_3]$-	0.56	0.58	0.77	1.15	0.54	0.36	1.24	0.48	1.00
$[OctSO_3]$-	0.59	0.64	0.86	1.08	0.72	0.55	0.91	0.30	0.83
$[NH_2SO_3]$-	1.19	1.31	1.66	1.49	1.54	1.24	0.34	0.64	1.16
[Tau]-	0.99	1.08	1.41	1.50	1.26	1.01	0.83	0.52	1.13
[Tosy]-	0.73	0.79	1.08	1.42	0.87	0.64	1.12	0.38	1.02
$[CF_3SO_3]$-	0.91	0.95	1.31	1.99	0.93	0.64	1.99	0.71	1.58

Table S3 (continued…): COSMO-RS predicted logarithmic activity coefficients of PET in different ILs at 363.15 K

	[BEPyrr]+	[EMPyrr]+	[HMPyrr]+	[M12MThEPyrr]+	[tBTMGH]+	[ETBDH]+	[ITBDH]+	[MTBDH]+
[Ala]-	0.39	0.55	0.65	1.08	0.05	0.01	-0.08	0.05
[Arg]-	0.74	1.04	0.87	1.28	0.49	0.50	0.42	0.57
[Aspg]-	0.81	0.99	1.00	1.44	0.52	0.51	0.43	0.55
[Cyst]-	0.44	0.75	0.62	1.13	0.15	0.14	0.04	0.20
[Glumn]-	0.72	0.99	0.89	1.34	0.45	0.45	0.37	0.51
[Gly]-	0.28	0.17	0.62	0.92	-0.08	-0.17	-0.24	-0.19
[His]-	0.85	1.25	0.96	1.50	0.60	0.62	0.53	0.71
[Isole]-	0.44	0.81	0.58	1.04	0.16	0.17	0.08	0.26
[Leu]-	0.43	0.82	0.57	1.03	0.17	0.18	0.09	0.27
[Lys]-	0.45	0.77	0.61	1.04	0.17	0.17	0.09	0.24
[Met]-	0.36	0.72	0.50	0.98	0.09	0.10	0.01	0.18
[Phe]-	0.37	0.78	0.48	0.97	0.14	0.17	0.07	0.26
[Pro]-	0.37	0.64	0.59	1.03	0.03	0.01	-0.08	0.08
[AspMA]-	1.00	1.39	1.13	1.70	0.71	0.74	0.63	0.83
[GluMA]-	0.96	1.38	1.08	1.61	0.70	0.73	0.63	0.83
[Ser]-	0.79	0.95	1.02	1.47	0.48	0.45	0.37	0.49
[Thr]-	0.51	0.83	0.70	1.21	0.19	0.18	0.10	0.25
[Try]-	0.62	1.05	0.66	1.15	0.44	0.48	0.39	0.59
[Tyro]-	0.88	1.35	0.93	1.45	0.67	0.72	0.62	0.84
[Val]-	0.47	0.84	0.63	1.12	0.18	0.18	0.09	0.27
[2AIm]-	0.40	0.50	0.67	1.14	0.06	0.00	-0.07	0.03
[2MIm]-	0.43	0.80	0.61	1.21	0.11	0.10	0.00	0.18
[45DCIm]-	0.50	1.21	0.48	1.28	0.28	0.35	0.25	0.50
[56DMBeIm]-	0.31	0.77	0.39	0.93	0.10	0.13	0.04	0.23
[BeIm]-	0.43	0.96	0.51	1.18	0.17	0.21	0.11	0.33
[Sac]-	0.55	1.05	0.62	1.28	0.30	0.34	0.24	0.46
[2-Mbut]-	0.34	0.61	0.54	1.00	0.03	0.01	-0.08	0.08

[2-BrMAcr]-	0.34	0.79	0.45	1.05	0.10	0.13	0.01	0.23
[2-BOA]-	0.28	0.57	0.39	0.68	0.06	0.08	0.00	0.15
[2-ClAce]-	0.50	0.72	0.72	1.28	0.16	0.14	0.05	0.19
[2-EBA]-	0.39	0.72	0.55	0.98	0.10	0.10	0.00	0.18
[2-EHA]-	0.35	0.70	0.49	0.87	0.10	0.11	0.02	0.20
[2-HOA]-	0.22	0.48	0.32	0.56	0.04	0.06	-0.02	0.12
[2-(OH)MAcr]-	0.50	0.86	0.68	1.26	0.19	0.20	0.10	0.27
[22-DMB]-	0.42	0.77	0.58	1.02	0.13	0.13	0.04	0.22
[3-$(OH)_2$-MBut]-	0.78	1.17	0.92	1.46	0.52	0.53	0.43	0.62
[4-EOA]-	0.30	0.62	0.43	0.77	0.06	0.07	-0.02	0.15
[Abt]-	0.18	0.43	0.26	0.49	0.03	0.05	-0.02	0.11
[Ace]-	0.19	-0.01	0.56	0.81	-0.17	-0.28	-0.34	-0.30
[AceSal]-	0.42	0.83	0.52	1.07	0.18	0.22	0.12	0.31
[Acryl]-	0.31	0.37	0.59	1.02	-0.03	-0.09	-0.17	-0.07
[Benzoate]-	0.38	0.74	0.53	1.08	0.11	0.12	0.01	0.20
[But]-	0.36	0.58	0.59	1.01	0.03	-0.01	-0.10	0.05
[C3C]-	0.43	0.81	0.55	1.08	0.20	0.23	0.13	0.32
[Crotonate]-	0.28	0.44	0.54	0.96	-0.05	-0.09	-0.18	-0.05
[Dec]-	0.30	0.61	0.42	0.75	0.06	0.07	-0.01	0.15
[For]-	0.10	-0.48	0.55	0.66	-0.27	-0.43	-0.47	-0.53
[Gen]-	1.36	1.77	1.46	2.02	1.12	1.17	1.05	1.27
[Glyco]-	0.47	0.09	0.86	0.97	0.16	0.05	0.00	-0.01
[Hex]-	0.37	0.70	0.54	0.96	0.07	0.07	-0.03	0.15
[Im2C]-	0.43	0.53	0.67	1.09	0.14	0.10	0.02	0.13
[I3A]-	0.63	1.05	0.70	1.21	0.43	0.47	0.37	0.57
[Lac]-	0.54	0.46	0.84	1.11	0.22	0.16	0.08	0.15
[MCb]-	0.34	0.36	0.65	1.07	-0.02	-0.08	-0.16	-0.07
[N-MCb]-	0.22	0.10	0.56	0.85	-0.14	-0.23	-0.30	-0.24
[NMeO]-	0.32	0.45	0.58	1.02	-0.01	-0.05	-0.14	-0.02

[Oct]-	0.34	0.67	0.48	0.85	0.07	0.08	-0.01	0.16
[Oxa]-	0.57	0.50	0.85	1.24	0.25	0.19	0.11	0.18
[Prop]-	0.32	0.42	0.60	0.99	-0.02	-0.08	-0.17	-0.05
[Sal]-	0.86	1.17	1.01	1.51	0.59	0.61	0.50	0.68
[ThioSal]-	0.39	0.81	0.50	1.07	0.16	0.18	0.07	0.27
[TFA]-	0.68	1.31	0.76	1.59	0.38	0.43	0.32	0.56
[TSAC]-	0.37	0.81	0.30	0.79	0.25	0.32	0.27	0.42
[B(F_5)SI]-	0.14	0.40	0.09	0.38	0.12	0.16	0.13	0.22
[MSA]-	0.64	1.09	0.76	1.41	0.34	0.37	0.27	0.47
[TFMI]	0.40	0.85	0.34	0.82	0.29	0.35	0.31	0.46
[DCN]-	0.48	1.09	0.58	1.48	0.16	0.18	0.06	0.30
[SbF_6]-	0.71	1.66	0.59	1.57	0.46	0.56	0.48	0.76
[PF_6]-	0.90	1.99	0.80	1.97	0.58	0.68	0.58	0.89
[NO_3]-	0.55	0.46	0.86	1.39	0.16	0.09	0.02	0.07
[WOF_5]-	0.81	1.81	0.70	1.74	0.54	0.65	0.55	0.85
[Phenolate]-	0.46	0.90	0.60	1.21	0.18	0.19	0.09	0.29
[BF_4]-	0.93	1.58	1.02	2.08	0.51	0.53	0.43	0.65
[SCN]-	0.54	0.91	0.70	1.54	0.17	0.15	0.05	0.23
[PhS]-	0.40	0.89	0.51	1.16	0.13	0.15	0.05	0.26
[TFMSM]-	0.32	0.61	0.25	0.56	0.25	0.29	0.27	0.37
[TCN]-	0.30	1.04	0.29	1.14	0.08	0.13	0.02	0.29
[$DBPO_4$]-	0.30	0.64	0.40	0.78	0.08	0.10	0.03	0.18
[$DEPO_4$]-	0.39	0.76	0.55	1.04	0.10	0.11	0.02	0.19
[$DIsoPrPO_4$]-	0.37	0.75	0.49	0.94	0.12	0.15	0.06	0.23
[$DMPO_4$]-	0.42	0.70	0.63	1.15	0.10	0.08	-0.01	0.14
[22-(ME)OHES]-	0.50	0.93	0.57	1.09	0.26	0.30	0.22	0.40
[BzS]-	0.49	0.93	0.60	1.22	0.22	0.24	0.14	0.34
[$EtSO_4$]-	0.58	1.01	0.72	1.37	0.26	0.27	0.18	0.36

[HSO_3]-	0.38	0.77	0.51	0.98	0.11	0.13	0.05	0.22
[HSO4]-	1.11	1.33	1.31	2.00	0.72	0.71	0.61	0.76
[MetA]-	0.85	1.33	0.94	1.59	0.58	0.62	0.51	0.73
[$MeSO_4$]-	0.62	0.96	0.80	1.47	0.27	0.26	0.17	0.33
[$MeSO_3$]-	0.38	0.36	0.69	1.10	0.01	-0.06	-0.13	-0.06
[F_9BSO_3]-	0.49	0.97	0.47	1.01	0.34	0.41	0.35	0.53
[$OctSO_3$]-	0.32	0.69	0.43	0.83	0.09	0.11	0.03	0.20
[NH_2SO_3]-	0.67	0.47	1.00	1.35	0.31	0.23	0.17	0.20
[Tau]-	0.56	0.69	0.80	1.25	0.22	0.19	0.11	0.21
[Tosy]-	0.41	0.83	0.52	1.09	0.16	0.18	0.09	0.28
[CF_3SO_3]-	0.74	1.50	0.74	1.62	0.47	0.54	0.44	0.70

Table S3 (continued…): COSMO-RS predicted logarthmic activity coefficients of PET in different ILs at 363.15 K

	[DMPH]+	[DBNH]+	[DMANH]+	[DBUH]+	[TBDH]+	[TMGH]+	[PeMPipH]+	[DMAAH]+
[Ala]-	0.54	0.49	0.56	0.55	0.91	0.84	1.53	1.28
[Arg]-	1.05	0.98	0.79	0.91	1.20	1.19	1.62	1.37
[Aspg]-	1.02	0.98	0.93	0.99	1.35	1.28	1.86	1.60
[Cyst]-	0.77	0.68	0.59	0.62	0.96	0.95	1.50	1.18
[Glumn]-	1.02	0.95	0.82	0.91	1.24	1.21	1.71	1.45
[Gly]-	0.16	0.18	0.52	0.39	0.75	0.60	1.46	1.28
[His]-	1.30	1.20	0.92	1.07	1.41	1.42	1.83	1.50
[Isole]-	0.81	0.72	0.50	0.63	0.94	0.95	1.41	1.10
[Leu]-	0.83	0.73	0.49	0.63	0.93	0.95	1.39	1.07
[Lys]-	0.76	0.68	0.52	0.61	0.90	0.90	1.38	1.11
[Met]-	0.73	0.63	0.46	0.53	0.83	0.85	1.30	0.99
[Phe]-	0.81	0.71	0.45	0.57	0.87	0.90	1.27	0.94
[Pro]-	0.62	0.54	0.50	0.53	0.86	0.84	1.43	1.16

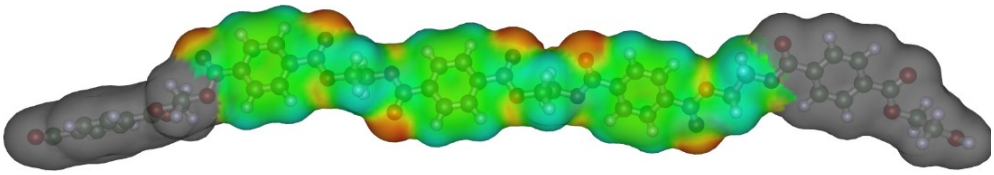
[AspMA]-	1.44	1.35	1.05	1.25	1.63	1.62	2.06	1.74
[GluMA]-	1.43	1.34	1.00	1.21	1.57	1.57	1.96	1.64
[Ser]-	0.97	0.94	0.92	0.99	1.37	1.28	1.92	1.67
[Thr]-	0.83	0.75	0.61	0.70	1.04	1.02	1.59	1.26
[Try]-	1.11	1.01	0.64	0.83	1.11	1.15	1.42	1.08
[Tyro]-	1.41	1.30	0.88	1.12	1.44	1.47	1.75	1.41
[Val]-	0.85	0.75	0.55	0.67	1.00	1.00	1.50	1.17
[2AIm]-	0.49	0.46	0.59	0.54	0.90	0.80	1.57	1.31
[2MIm]-	0.81	0.71	0.55	0.62	0.99	0.98	1.57	1.20
[45DCIm]-	1.26	1.08	0.48	0.74	1.02	1.16	1.46	0.90
[56DMBeIm]-	0.81	0.69	0.36	0.51	0.79	0.84	1.20	0.83
[BeIm]-	1.01	0.87	0.50	0.65	0.98	1.04	1.44	1.01
[Sac]-	1.11	0.97	0.62	0.76	1.09	1.15	1.49	1.08
[2-Mbut]-	0.64	0.55	0.49	0.52	0.88	0.86	1.40	1.11
[2-BrMAcr]-	0.88	0.74	0.50	0.57	0.93	0.97	1.37	0.97
[2-BOA]-	0.57	0.50	0.31	0.45	0.69	0.69	1.03	0.81
[2-ClAce]-	0.74	0.68	0.66	0.69	1.09	1.02	1.69	1.36
[2-EBA]-	0.73	0.64	0.48	0.58	0.91	0.90	1.38	1.09
[2-EHA]-	0.70	0.62	0.41	0.54	0.83	0.83	1.24	0.97
[2-HOA]-	0.49	0.43	0.24	0.38	0.60	0.59	0.89	0.69
[2-(OH)MAcr]-	0.89	0.79	0.63	0.72	1.09	1.08	1.62	1.26
[22-DMB]-	0.78	0.69	0.50	0.62	0.95	0.95	1.42	1.12
[3-$(OH)_2$-MBut]-	1.22	1.13	0.85	1.03	1.40	1.39	1.84	1.50
[4-EOA]-	0.62	0.54	0.35	0.47	0.73	0.74	1.12	0.87
[Abt]-	0.46	0.40	0.20	0.35	0.56	0.55	0.82	0.62
[Ace]-	0.01	0.04	0.47	0.31	0.69	0.51	1.40	1.24
[AceSal]-	0.88	0.77	0.51	0.63	0.94	0.97	1.33	0.98
[Acryl]-	0.40	0.37	0.54	0.48	0.87	0.76	1.50	1.24
[Benzoate]-	0.80	0.69	0.51	0.59	0.95	0.95	1.41	1.06

[But]-	0.58	0.52	0.51	0.54	0.89	0.85	1.46	1.19
[C3C]-	0.88	0.77	0.55	0.64	0.96	0.98	1.34	1.01
[Crotonate]-	0.45	0.40	0.48	0.45	0.81	0.75	1.40	1.14
[Dec]-	0.61	0.53	0.34	0.46	0.71	0.73	1.10	0.86
[For]-	-0.45	-0.32	0.46	0.16	0.55	0.24	1.37	1.29
[Gen]-	1.87	1.78	1.40	1.65	2.06	2.04	2.38	2.07
[Glyco]-	0.15	0.24	0.75	0.60	0.99	0.72	1.63	1.57
[Hex]-	0.69	0.60	0.46	0.55	0.86	0.86	1.35	1.07
[Im2C]-	0.58	0.54	0.64	0.60	0.98	0.89	1.53	1.28
[I3A]-	1.13	1.02	0.68	0.86	1.17	1.20	1.50	1.17
[Lac]-	0.50	0.51	0.74	0.70	1.08	0.92	1.66	1.51
[MCb]-	0.37	0.36	0.57	0.49	0.88	0.76	1.56	1.31
[N-MCb]-	0.11	0.12	0.47	0.33	0.69	0.55	1.39	1.22
[NMeO]-	0.46	0.41	0.53	0.47	0.83	0.76	1.44	1.17
[Oct]-	0.67	0.58	0.40	0.52	0.79	0.80	1.22	0.96
[Oxa]-	0.55	0.57	0.80	0.73	1.13	0.98	1.76	1.53
[Prop]-	0.42	0.39	0.52	0.49	0.86	0.78	1.49	1.25
[Sal]-	1.24	1.16	0.97	1.09	1.48	1.44	1.89	1.60
[ThioSal]-	0.88	0.76	0.52	0.60	0.94	0.97	1.36	0.99
[TFA]-	1.35	1.20	0.70	0.96	1.36	1.42	1.87	1.33
[TSAC]-	0.80	0.72	0.22	0.49	0.58	0.71	0.84	0.42
[B(F_5)SI]-	0.45	0.40	0.05	0.27	0.33	0.37	0.55	0.25
[MSA]-	1.10	0.99	0.72	0.83	1.17	1.20	1.65	1.27
[TFMI]	0.84	0.75	0.25	0.52	0.61	0.75	0.84	0.44
[DCN]-	1.13	0.95	0.62	0.70	1.12	1.20	1.75	1.19
[SbF_6]-	1.61	1.39	0.51	0.91	1.09	1.40	1.52	0.79
[PF_6]-	1.95	1.69	0.74	1.15	1.44	1.77	1.91	1.13
[NO_3]-	0.46	0.50	0.80	0.70	1.13	0.96	1.89	1.59
[WOF_5]-	1.80	1.56	0.64	1.05	1.30	1.60	1.72	0.99

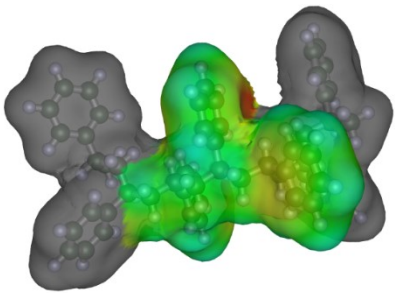
[Phenolate]-	0.93	0.82	0.56	0.69	1.05	1.06	1.54	1.15
$[BF_4]$-	1.50	1.36	0.98	1.15	1.58	1.67	2.28	1.64
[SCN]-	0.92	0.82	0.71	0.72	1.14	1.14	1.84	1.36
[PhS]-	0.93	0.80	0.50	0.61	0.95	1.00	1.46	1.05
[TFMSM]-	0.59	0.54	0.16	0.38	0.40	0.52	0.55	0.26
[TCN]-	1.10	0.87	0.38	0.50	0.79	0.98	1.29	0.69
$[DBPO_4]$-	0.64	0.56	0.33	0.46	0.70	0.72	1.07	0.80
$[DEPO_4]$-	0.75	0.66	0.48	0.57	0.87	0.89	1.36	1.05
$[DIsoPrPO_4]$-	0.76	0.66	0.42	0.55	0.83	0.85	1.25	0.95
$[DMPO_4]$-	0.70	0.62	0.57	0.60	0.95	0.92	1.51	1.20
[22-(ME)OHES]-	0.94	0.84	0.51	0.67	0.92	0.97	1.29	0.95
[BzS]-	0.97	0.85	0.59	0.69	1.03	1.07	1.49	1.10
$[EtSO_4]$-	1.01	0.90	0.66	0.77	1.12	1.15	1.66	1.26
$[HSO_3]$-	0.76	0.66	0.43	0.55	0.82	0.85	1.28	0.97
[HSO4]-	1.34	1.32	1.23	1.34	1.80	1.72	2.42	2.06
[MetA]-	1.38	1.26	0.92	1.08	1.43	1.47	1.86	1.47
$[MeSO_4]$-	0.96	0.87	0.75	0.81	1.19	1.18	1.79	1.40
$[MeSO_3]$-	0.35	0.35	0.60	0.50	0.87	0.75	1.58	1.34
$[F_9BSO_3]$-	1.01	0.91	0.38	0.69	0.90	0.97	1.16	0.76
$[OctSO_3]$-	0.68	0.59	0.35	0.48	0.72	0.75	1.12	0.83
$[NH_2SO_3]$-	0.48	0.54	0.90	0.80	1.20	0.98	1.90	1.72
[Tau]-	0.68	0.65	0.71	0.70	1.05	0.97	1.66	1.41
[Tosy]-	0.86	0.75	0.50	0.60	0.91	0.95	1.35	0.98
$[CF_3SO_3]$-	1.53	1.35	0.68	1.01	1.35	1.50	1.78	1.20

Table S3: Correlation between experimental and COSMO-RS predicted viscosities (η) of ionic liquids.

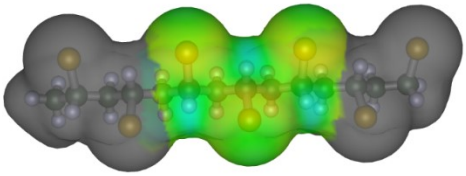
Cation	Anion	T (K)	η_{exp} (cP)	η_{pred} (cP)
1-butyl-3-methylimidazolium	Bis(trifluoromethylsulfonyl)imide	298.15	51.6	51.7
1-butyl-3-methylimidazolium	triflate	298.15	84.4	59.0
1-ethyl-3-methylimidazolium	Bis(trifluoromethylsulfonyl)imide	298.15	33.0	33.7
1-ethyl-3-methylimidazolium	hexafluorophosphate	353.15	17.1	16.0
1-ethyl-3-methylimidazolium	thiocyanate	298.15	22.7	20.5
1-ethyl-3-methylimidazolium	ethylsulfate	298.15	97.8	105.6
1-ethyl-3-methylimidazolium	methylsulfate	298.15	67.1	70.9
1-ethyl-3-methylimidazolium	triflate	298.15	42.9	40.1
1-butyl-3-methylpyridinium	Bis(trifluoromethylsulfonyl)imide	298.15	64.7	53.8
1-butyl-3-methylpyridinium	tetrafluoroborate	298.15	176.9	157.0
1-ethyl-3-methylimidazolium	acetate	298.15	128.5	101.7



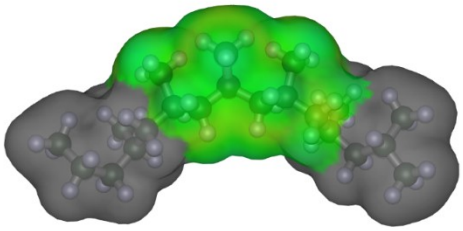
Polyethylene Terephthalate (PET)



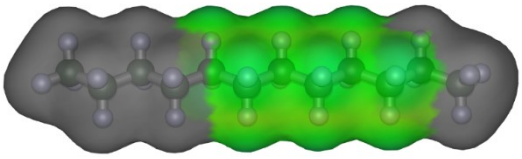
Polystyrene (PS)



Polyvinylchloride (PVC)



Polypropylene (PP)



Polyethylene (PE)

Figure S1: Chemical Structures and COSMO cavities of plastic molecules. In the COSMO cavity (charge distribution), red, blue, and green colors represent the negative, positive, and neutral charge on the surface of the molecule, respectively.

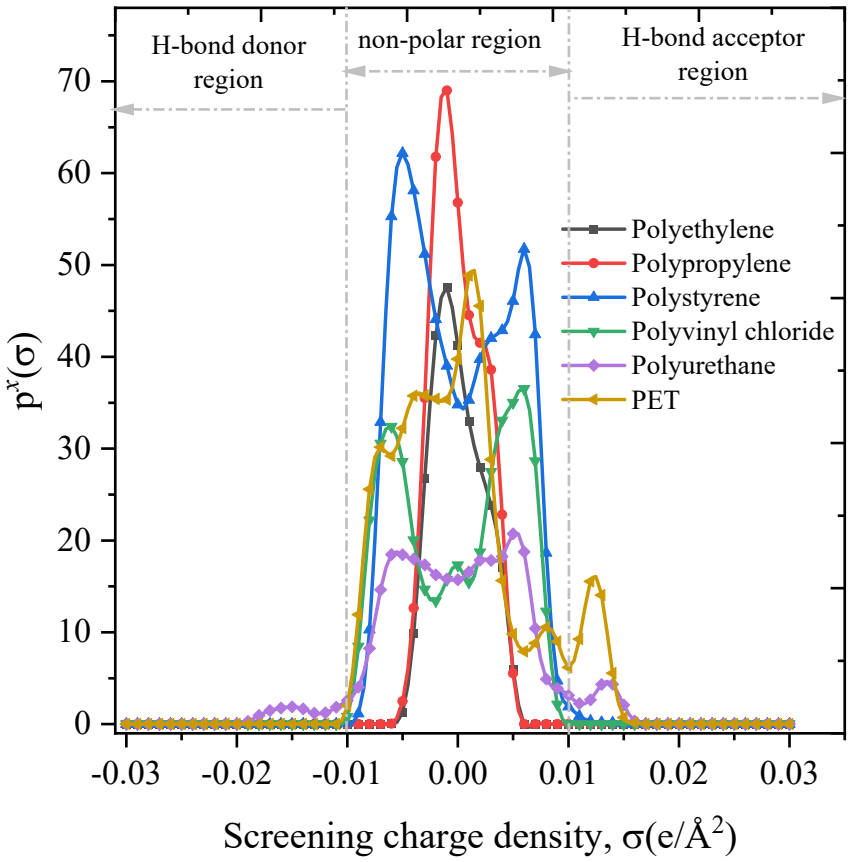


Figure S2: Sigma profiles of different plastics predicted by COSMO-RS