Analytical and Bioanalytical Chemistry

Electronic Supplementary Material

Predicting the partitioning of biological compounds between room-temperature ionic liquids and water by means of the Solvation-Parameter Model

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Figure S1: NMR Spectra of the synthesized RTILs

a). 1-octyl-3-methyl-imidazolium tetrafluorborate, [OMIm][BF_4] spectra:

-^{1}H NMR (200 MHz, acetone-6D): (chemical shifts (δ) indicated in parts per million and coupling constants [J] in Hertz) δ 9.12 (s, 1H, CH), 7.77 (t, 1H, J = 1.7, CH), 7.70 (t, 1H, J = 1.7, CH), 4.34 (t, 2H, J = 7.5, CH_2), 4.03 (s, 3H, CH_3), 1.93 (m, 2H, CH_2), 1.20-1.41 (m, 10H, 5xCH_2), 0.86 (t, 3H, J = 6.9, CH_3).

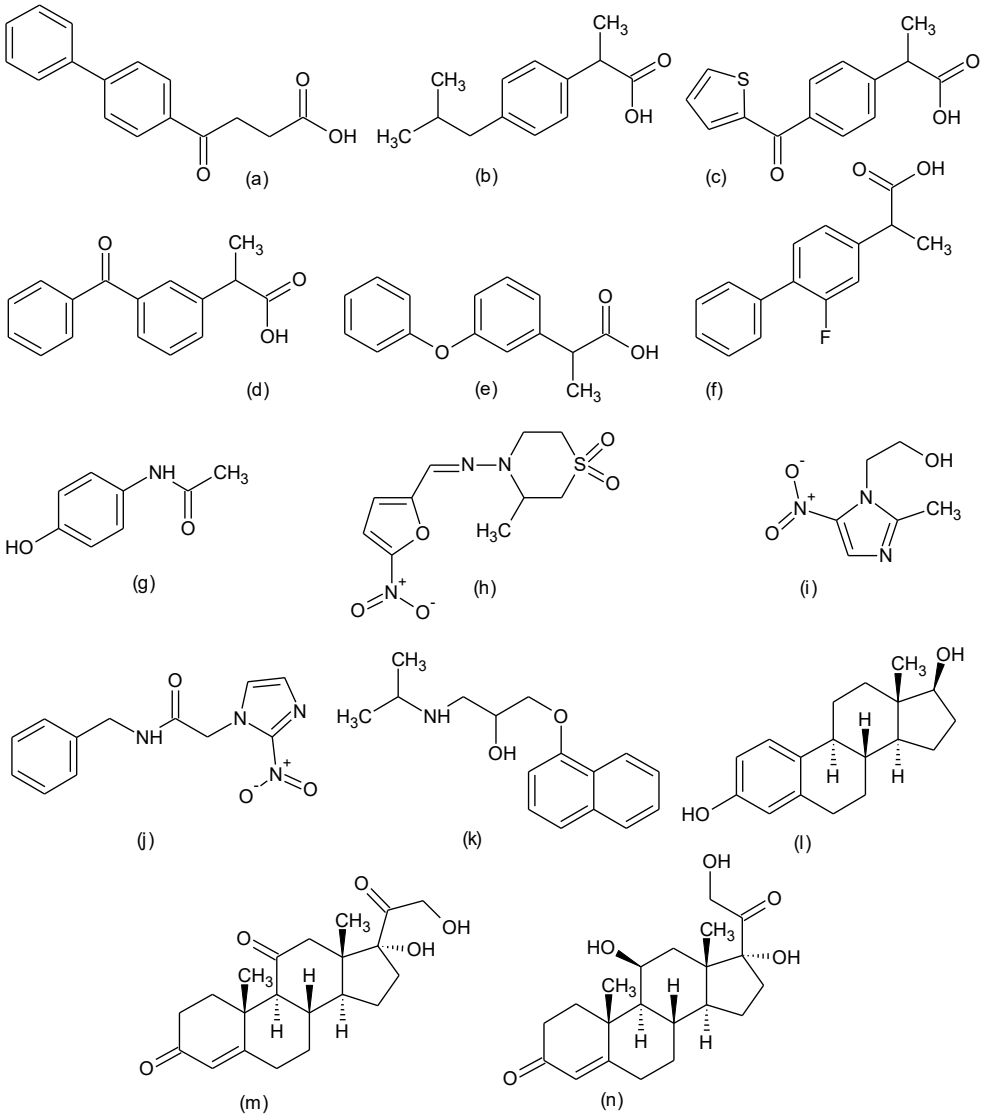
- ^{13}C NMR (50 MHz, acetone-6D): δ 137.14, 123.97, 122.65, 49.62, 35.90, 31.82, 30.24, 29.29, 29.04, 26.14, 22.62, 13.72.

b) 1-butyl-3-methylimidazolium hexafluorophosphate, [BMIM][PF_6] spectra:

-^{1}H NMR (200 MHz, acetone-d6): δ 8.92 (s, 1H, CH), 7.70 (s, 1H, CH), 7.65 (s, 1H, CH), 4.34 (t, 2H, CH_2), 4.03(s, 3H, CH_3), 1.93 (m, 2H, CH_2), 1.41 (m, 2H, CH_2), 0.96 (t, 3H, CH_3).

-^{13}C NMR (50 MHz, acetone-d6): δ 137.14, 124.47, 123.15, 49.82, 36.90, 32.32, 19.62, 13.72.

Figure S2: Chemical Structures of the Test set



(a) fenbufen, (b) ibuprofen, (c) suprofen, (d) ketoprofen, (e) fenoprofen, (f) flurbiprofen, (g) acetaminophen, (h) nifurtimox, (i) metronidazole, (j) benznidazole, (k) propranolol, (l) β-estradiol, (m) cortisone and (n) hydrocortisone.

Figure S3: Covariance matrix for the solute parameters of the training set

[OMIM][BF_4]					
	E	**S**	**A**	**B**	**V**
E	1				
S	0.3822	1			
A	0.0132	0.0017	1		
B	0.0014	0.0125	0.0697	1	
V	0.2752	0.1637	0.1022	0.0465	1
[BMIM][PF_6]					
E	1				
S	0.3466	1			
A	0.0003	0.0133	1		
B	0.0055	0.0389	0.0277	1	
V	0.2541	0.1497	0.0319	0.0181	1
[HMIM][PF_6]					
E	1				
S	0.3053	1			
A	0.0361	0.0870	1		
B	0.1449	0.1137	0.0129	1	
V	0.1079	0.0706	0.0015	0.0052	1