Electronic Supplementary Material (ESI) for RSC Advances

SUPPORTING INFORMATION

From the dissolution to the extraction of carbohydrates using ionic liquids

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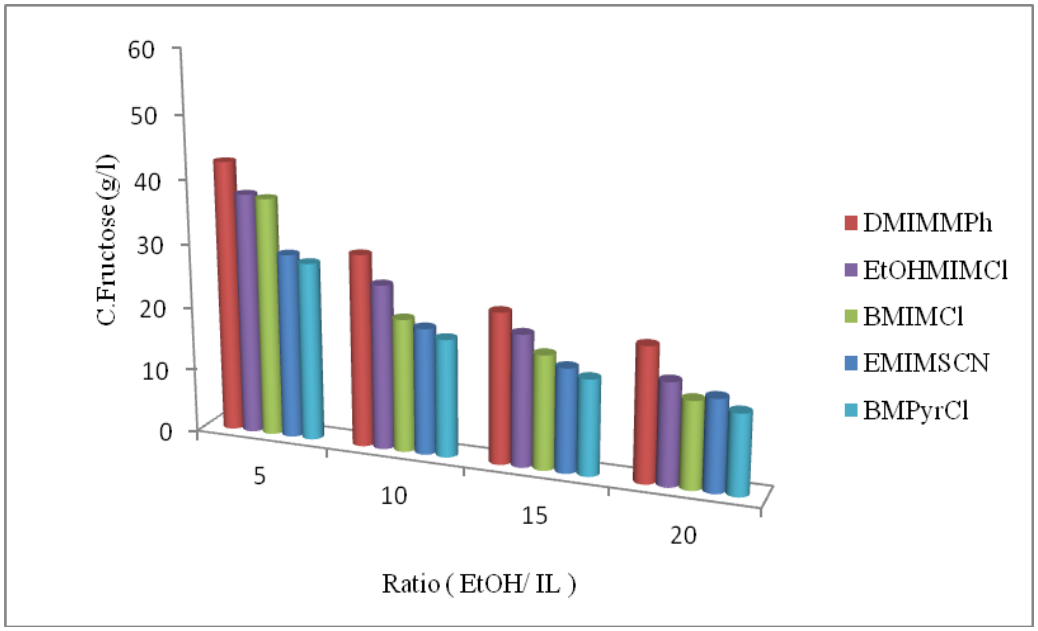
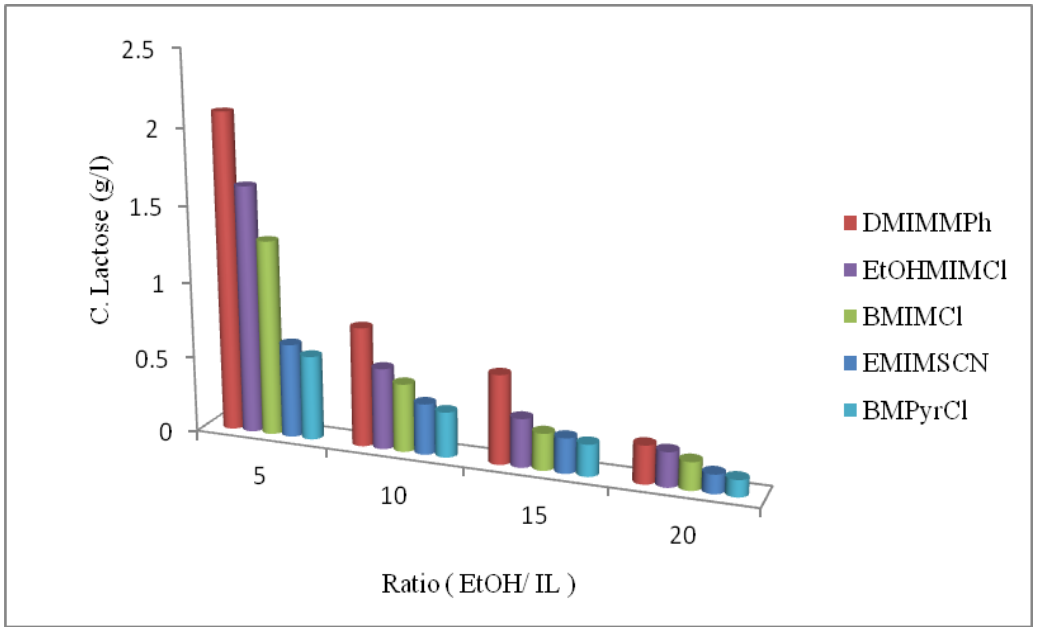
Figure S1: The effect of EtOH / IL ratio by weight on the solubility of (a) fructose and (b) lactose in the mixture at temperature = 298 K, time = 300 min and neglected water content

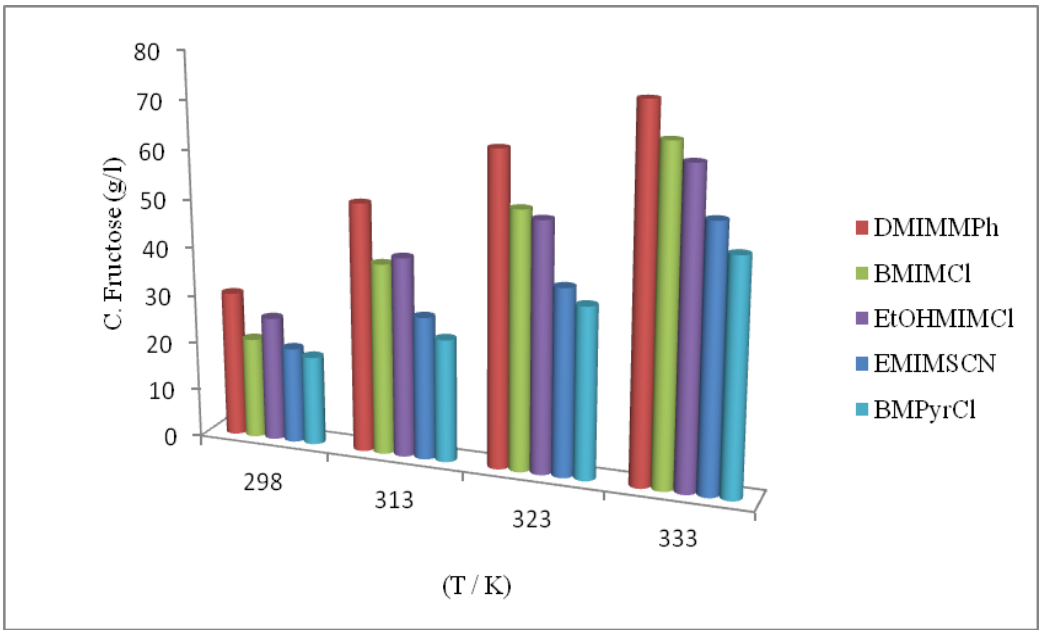


(a)

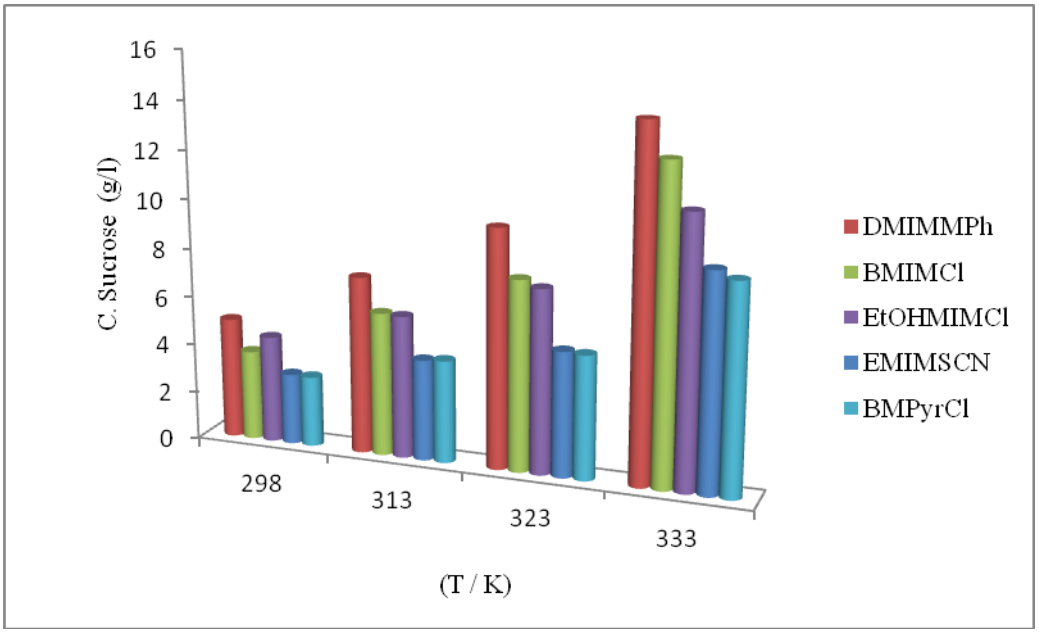


(b)

Figure S2: The effect of temperature (K) on the solubility of (a) fructose and (b) sucrose in the mixture at EtOH/IL ratio by weight =10, time =300 min and neglected water content

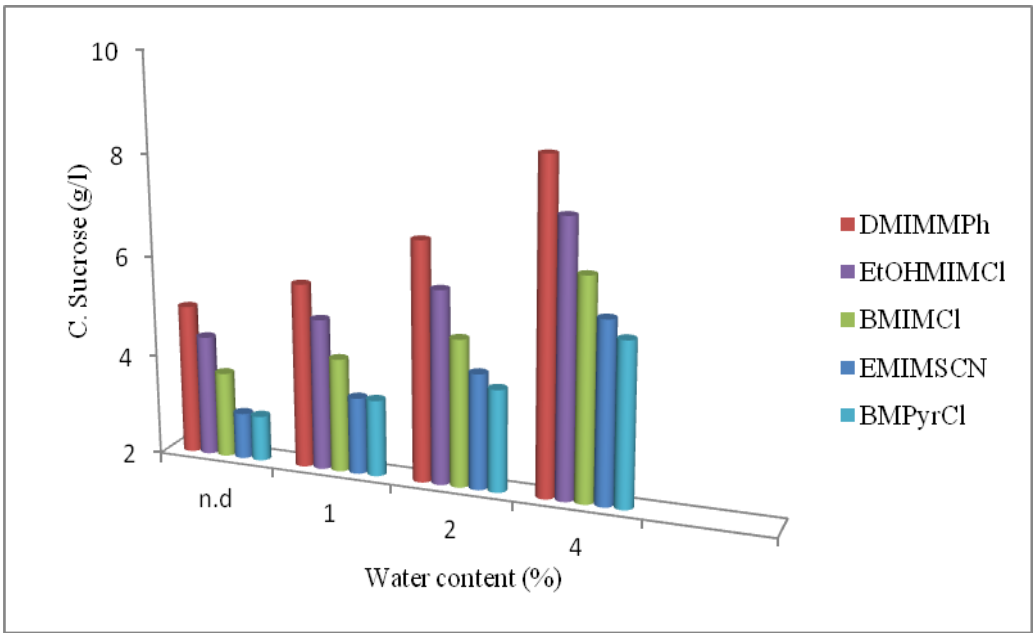


(a)

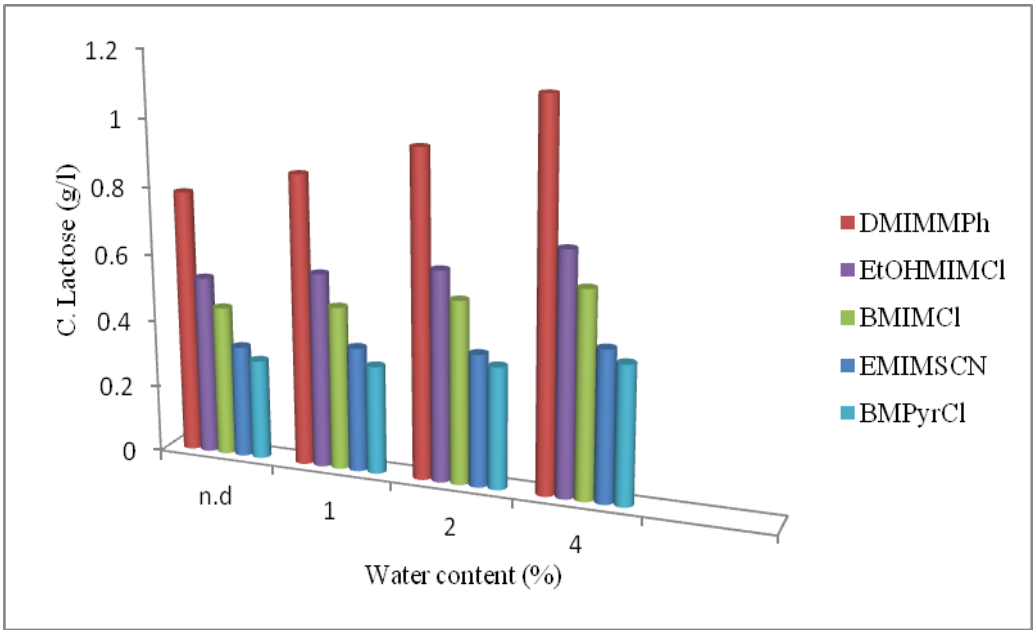


(b)

Figure S3: The effect of water content (%) on the solubility of (a) sucrose and (b) lactose in the mixture at EtOH/IL ratio by weight =10, time =300 min and temperature =298 K

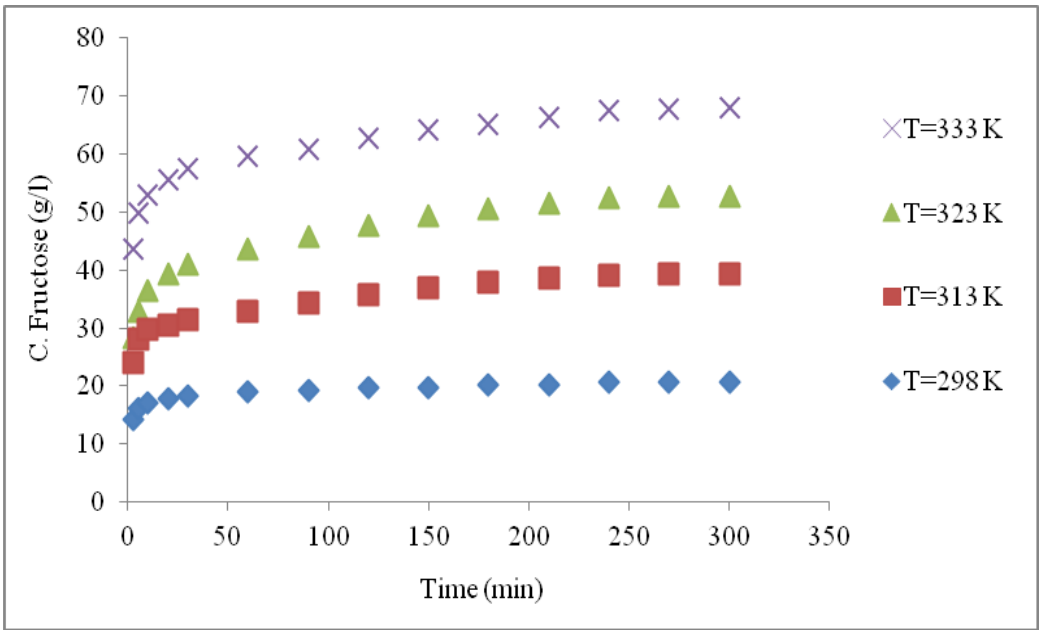


(a)

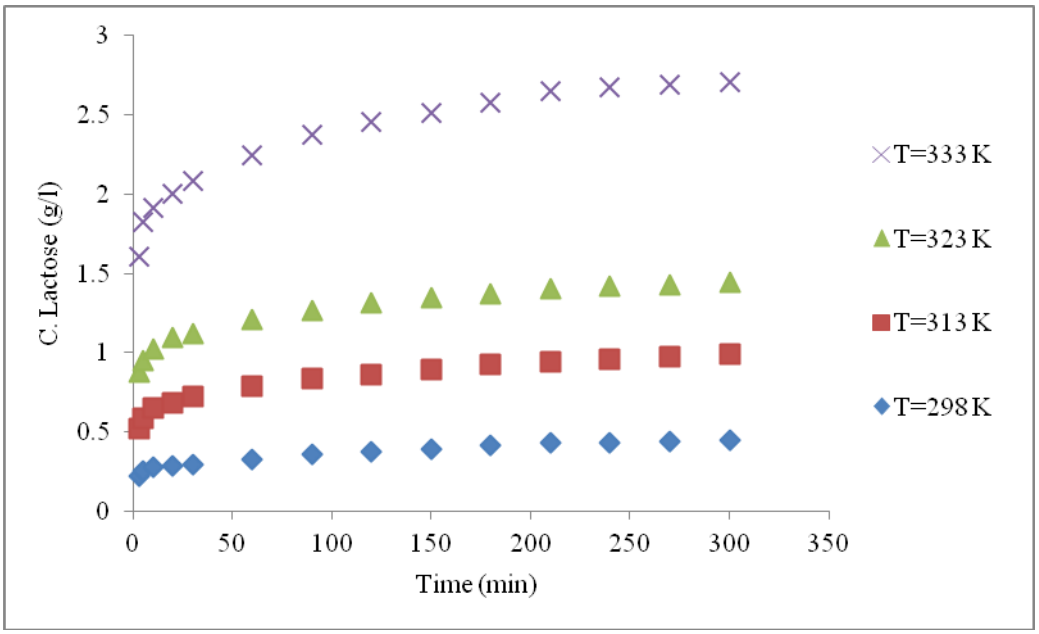


(b)

Figure S4: Dissolution rate of (a) sucrose and (b) lactose in a mixture of (BMIMCl + EtOH) at EtOH/IL ratio by weight =10, neglected water content and temperature =♦298, ■ 313, ▲323, and × 333 K



(a)



(b)

Table S1: Solid-Liquid equilibria (SLE) of the binary system (Sugar+IL), where X_2 is the sugar mass fraction, T_2 is the temperature (K), γ_2 is the activity coefficient calculated with NRTL equation

Fructose											
EMIMSCN			DMIMMPh			BMIMCl			EtOHMIMCl		
X_2	T_2	γ_2	X_2	T_2	γ_2	X_2	T_2	γ_2	X_2	$T_2^{SLE/K}$	γ_2
0.05	281.15	1.00	0.05	284.95	1.32	0.05	343.15	8.30	0.10	355.05	5.13
0.10	288.55	1.00	0.10	296.65	0.87	0.10	345.25	5.33	0.15	356.25	4.29
0.15	293.75	1.00	0.15	302.65	0.75	0.20	348.15	2.98	0.20	357.95	3.47
0.20	300.15	1.00	0.20	307.55	0.69	0.25	350.45	2.34	0.25	358.65	3.14
0.25	311.25	1.00	0.25	310.15	0.68	0.30	351.85	1.97	0.30	360.15	2.67
0.30	322.45	1.00	0.30	313.45	0.67	0.35	354.75	1.66	0.45	365.15	2.12
0.40	332.85	1.00	0.40	323.85	0.64	0.40	356.15	1.48	0.50	366.55	1.69
0.45	358.15	1.00	0.50	336.75	0.63	0.45	357.95	1.34	0.55	367.85	1.52
			0.60	344.15	0.69	0.50	359.25	1.25	0.6	369.15	1.38
Sucrose											
EMIMSCN			DMIMMPh			BMIMCl			EtOHMIMCl		
X_2	T_2	γ_2	X_2	T_2	γ_2	X_2	T_2	γ_2	X_2	$T_2^{SLE/K}$	γ_2
0.025	284.25	0.039	0.05	286.15	0.017	0.05	343.95	0.442	0.05	356.15	0.775
0.05	301.15	0.061	0.10	295.65	0.019	0.10	347.95	0.241	0.10	357.65	0.433
0.08	318.85	0.094	0.15	307.8	0.023	0.15	351.45	0.182	0.15	359.95	0.297
0.10	330.9	0.123	0.20	316.05	0.029	0.20	354.15	0.169	0.20	363.35	0.240
0.15	348.15	0.180	0.25	329.4	0.036	0.22	356.82	0.162	0.25	366.20	0.226
0.20	362.25	0.241	0.30	343.35	0.046	0.25	359.7	0.163	0.28	369.15	0.224
0.25	371.25	0.292	0.40	359.85	0.084	0.30	367.05	0.168	0.30	372.75	0.222
0.30	383.15	0.362	0.50	376.45	0.146	0.35	373.45	0.188	0.35	377.05	0.243
						0.40	380.3	0.219	0.40	384.15	0.271
Lactose											
EMIMSCN			DMIMMPh			BMIMCl			EtOHMIMCl		
X_2	T_2	γ_2	X_2	$T_2^{SLE/}$	γ_2	X_2	$T_2^{SLE/}$	γ_2	X_2	$T_2^{SLE/K}$	γ_2
0.025	288.05	0.0002	0.05	290.55	0.004	0.025	344.15	0.143	0.025	355.75	0.063
0.05	309.65	0.0007	0.10	299.25	0.003	0.05	351.95	0.088	0.05	360.5	0.042
0.08	326.75	0.0022	0.16	308.95	0.003	0.10	359.05	0.067	0.10	366.35	0.032
0.10	339.6	0.0056	0.23	319.05	0.004	0.15	366.85	0.059	0.15	372.55	0.029
0.125	362.25	0.0159	0.30	333.15	0.005	0.20	371.35	0.056	0.20	378.65	0.031
0.155	373.25	0.0320	0.32	338.85	0.006	0.28	381.55	0.058	0.25	384.15	0.039
0.18	382.55	0.0512	0.35	344.45	0.008						
			0.393	356.25	0.011						

Table S2: Kamlet-Taft parameters of some ionic liquids and organic compounds, where α the hydrogen bond acidity, β is the hydrogen bond basicity and π* is the dipolarity[41-46].

ILs and organic compounds	α	β	π*
H_2O	1.17	0.47	1.09
EtOH	0.86	0.75	0.51
MeOH	0.98	0.66	0.60
1-propanol	0.84	0.85	0.53
2-propanol	0.76	0.93	0.48
Acetonitrile	0.19	0.40	0.66
DMSO	0	0.76	1
$BMPyTf_2N$	0.52	0.37	0.93
$BMIMPF_4$	0.63	0.38	1.05
$BMIMC(CN)_3$	0.51	0.54	0.94
$BMIMN(CN)_2$	0.54	0.71	1.05
EMIM $N(CN)_2$	0.54	0.64	1.07
$HOMMIMN(CN)_2$	0.80	0.51	1.11
$BMIMHSO_4$	-	0.67	1.09
$EMIMMSO_4$	0.57	0.61	1.09
$BMIMMSO_3$	0.44	0.77	1.02
$EMIMEtSO_4$	n.a.	0.710	n.a.
$BMIMCF_3SO_3$	0.50	0.57	0.90
BMIMSCN	-	0.71	1.06
EtOHMIMCl	0.73	0.68	1.16
BMIMCl	0.48 0.47	0.94 0.87	1.03 1.10
EMIMMPh	0.51	1	1.06

Table S3: Solubility of carbohydrates in ILs in the literature[29-31, 37, 47]

Sucrose					
BMIMSCN		$BMIMHSO_4$		$BMIMC(CN)_3$	
S. (Wt%)	T/K	S. (Wt%)	T/K	S. (Wt%)	T/K
2	315.2	2.0	358.74	1.0	381.2
5.2	325.01	5.0	363.05	2.1	391.38
10.0	339.78	10.1	368.27	5.3	406.64
20.0	369.2	15.1	372.45	$BMIMCF_3SO_3$	
30.0	399.92	25.9	380.13	S. (g/l)	T/K
35.3	411.67	35.0	388.5	2.0	298.15
$BMIMBF_4$		$EMIMBF_4$		5.3	333.15
S. (g/l)	T/K	S. (g/l)	T/K	$EMIMCH_3SO_3$	
0.5	298.15	0.6	298.15	S. (g/l)	T/K
0.6	333.15	0.6	333.15	12.4	298.15
				80	348.15
Fructose					
$EMIMEtSO_4$		$BMIMCF_3SO_3$		$EMIMCF_3SO_3$	
S. (Wt%)	T/K	S. (g/l)	T/K	S. (g/l)	T/K
25.7	288.2	27.0	298.15	32.8	298.15
29	298.2	87.5	333.15	123.9	333.15
37.4	318.4				
Lactose					
$Bt_{14}CH_3SO_3$		$Bt_{14}N(CN)_2$		MOEOEMIMCl	
S. (Wt%)	T/K	S. (Wt%)	T/K	S. (Wt%)	T/K
8	348.15	8	348.15	10.69	308.15

Table S4: Van der waals volume and surface parameters for UNIQUAC model.

ILs/ Sugar	r_i	q_i
BMIMCl	4.709	3.967
EtOHMIMCl	4.487	3.790
DMIMMPh	6.017	4.756
EMIMSCN	4.437	3.75
Fructose	5.8	4.92
Sucrose	14.5496	13.764
Lactose	12.5265	12.228

Table S5: Correlation of the solid-liquid equilibria data by means of the NRTL and UNIQUAC equations, σ_T the temperature deviation

	Fructose				
Solvent	NRTL parameters				rmsd
Ionic liquid	a_{12}/(J.mol^{-1})	a_{21}/(J.mol^{-1})	b_{12}/(J.mol^{-1}.K^{-1})	b_{21}/(J.mol^{-1}.K^{-1})	σ_T
BMIMCl	89998.38	9998.16	-241.59	-1226.26	1.65
DMIMMPh	28596.29	524.41	-96.48	-3.09	2.54
EMIMSCN	100001.28	5002.78	151.19	856.42	6.08
EtOHMIMCl	147201.97	90547.33	-415.29	-206.45	1.17
Solvent	UNIQUAC parameters				rmsd
Ionic liquid	a_{12}/(J.mol^{-1})	a_{21}/(J.mol^{-1})	b_{12}/(J.mol^{-1}.K^{-1})	b_{21}/(J.mol^{-1}.K^{-1})	σ_T
BMIMCl	-4296.64	13303.32	17.67	-39.54	2.64
DMIMMPh	-4296.65	13303.31	13.67	-43.35	1.43
EMIMSCN	4009.51	10979.11	-21.81	111.23	5.39
EtOHMIMCl	9.98	9.97	3.17	0.83	3.40
	Sucrose				
Solvent	NRTL parameters				rmsd
Ionic liquid	a_{12}/(J.mol^{-1})	a_{21}/(J.mol^{-1})	b_{12}/(J.mol^{-1}.K^{-1})	b_{21}/(J.mol^{-1}.K^{-1})	σ_T
BMIMCl	93902.37	10365.21	-215.09	-59.64	0.65
DMIMMPh	-1993.92	5922.61	-9.37	-34.90	2.84
EMIMSCN	-18249.49	16869.27	36.39	4925.43	2.34
EtOHMIMCl	93902.41	10364.49	-202.85	-57.62	0.62
Solvent	UNIQUAC parameters				rmsd
Ionic liquid	a_{12}/(J.mol^{-1})	a_{21}/(J.mol^{-1})	b_{12}/(J.mol^{-1}.K^{-1})	b_{21}/(J.mol^{-1}.K^{-1})	σ_T
BMIMCl	-19791.44	17061.38	66.95	-55.81	0.89
DMIMMPh	912.18	322.39	-10.56	5.07	2.76
EMIMSCN	0.86	0.82	4.76	-4.79	2.25
EtOHMIMCl	18108.31	11535.19	-41.56	-38.23	0.99
	Lactose				
Solvent	NRTL parameters				rmsd
Ionic liquid	a_{12}/(J.mol^{-1})	a_{21}/(J.mol^{-1})	b_{12}/(J.mol^{-1}.K^{-1})	b_{21}/(J.mol^{-1}.K^{-1})	σ_T
BMIMCl	16672.21	30671.24	-44.28	-103.84	0.60
DMIMMPh	18055.20	26076.84	-59.27	-117.40	0.58
EMIMSCN	-58208.87	-32291.41	118.89	212.59	3.59
EtOHMIMCl	21787.11	21399.52	-10.25	-93.37	0.48
Solvent	UNIQUAC parameters				rmsd
Ionic liquid	a_{12}/(J.mol^{-1})	a_{21}/(J.mol^{-1})	b_{12}/(J.mol^{-1}.K^{-1})	b_{21}/(J.mol^{-1}.K^{-1})	σ_T
BMIMCl	-1550.39	14159.91	-0.63	-36.09	0.54
DMIMMPh	-3377.67	12309.61	4.55	-39.55	0.61
EMIMSCN	0.00	0.00	6.71	-6.71	3.78
EtOHMIMCl	-19451.16	30000.08	52.87	-83.45	0.92

Table S6: Solubility of sugars in water and ethanol

Solvent	T /K	Solubility (g/l)			
		Glucose	Fructose	Sucrose	Lactose
Water	293.15	900	3750	2000	
	298.15	1100		2074.1	233.12
	313.15			2345	235.97
	333.15			2885.7	592.73
Ethanol	293.15	1.29	11.597	0.414	0.02
	298.15	1.31	18.20	0.599	0.11
	313.15		23.897	0.761	0.19
	333.15		30.547	0.987	0.27