

## Supporting Information

# Ionic Liquid-Based Green Emulsion Liquid Membrane for the Extraction of the Poorly Soluble Drug Ibuprofen

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**Table S1** ILs used for the removal of Ibf

S. NO.	Removal technique	IL used	Finding	Reference
1.	Adsorption	[TBPPyri][Br]	Misfit, hydrogen bond and vander waal energies are responsible the adsorption of Ibf	[41]
2.	Aqueous biphasic system (ABS)	[EMIm][Trif] [BMIm][Trif] [BMIm][Tos] [TIBMPh][Tos] [TBPh][Cl]	The addition of ILs increases extraction efficiencies	[43]
3.	Solid liquid extraction (SLE)	[TBAm][Cl]	IL results in an improved extraction efficiency of Ibf.	[42]
4.	Adsorption	[VBIm][PF <sub>6</sub> ]	A tremendous increase in Ibf adsorption capacity was observed with the use of IL	[11]
5.	Liquid-liquid microextraction	([BMIm][PF <sub>6</sub> ]) [BMIm][BF <sub>4</sub> ]	The incorporation of IL enhanced the recovery from 89% to 103%	[2]
6.	Dispersive liquid-liquid microextraction	[OMIm][PF <sub>6</sub> ])	Use of IL resulted in enhanced recovery efficiencies with good enrichment factor.	[9]

**Table S2** Chemicals and reagents used

<b>Chemical name</b>	<b>Source</b>	<b>CAS No.</b>	<b>Purity</b>	<b>Impurities</b>
<b>Sodium hydroxide</b>	Sigma Aldrich	1310-73-2	>99	<0.5%
<b>Span 80</b>	Sigma Aldrich	1338-43-8	-	-
<b>Tetramethylammonium acetate</b>	Sigma Aldrich	10581-12-1	>97%	<0.5%
<b>1-butyl-3-methylimidazolium acetate</b>	Sigma Aldrich	254049-75-8	>98.0%	<0.5%
<b>1-butyl-1-methylpyrrolidinium chloride</b>	Sigma Aldrich	479500-35-1	>99.0%	<0.5%
<b>1-butyl-1-methylpyrrolidinium bromide</b>	Sigma Aldrich	93457-69-3 93457-69-3	>98.0%	<0.5%
<b>choline chloride</b>	Sigma Aldrich	67-48-1	>98.0%	<0.5%
<b>tributylmethylammonium chloride</b>	Sigma Aldrich	56375-79-2	>98.0%	<0.5%
<b>Ibuprofen</b>	Sigma Aldrich	15687-27-1	>98%	<0.5%
<b>Sunflower oil</b>		BILLION Seri Iskandar		

**Table S3** AC<sup>id</sup> values predicted using COSMO-RS for ILs

S.N o.	Anions	Cations							
		Ch	TMAm	BMI m	BMP y	BMPy r	BMPi p	TBP h	Gu
1	Sulphate	- 16.64 7	-22.112	- 9.688	- 9.696	- 11.624	- 11.06 2	- 9.493	- 9.066
2	Chloride	- 12.22 2	-17.668	- 5.971	- 6.104	-7.752	-7.286	-6.02	0.7
3	Tetrafluoroborate	4.272	0.431	1.829	0.941	0.706	0.423	-0.74	11.82
4	Butylsulfate	0.973	-0.152	- 1.139	-1.7	-1.975	-2.163	- 2.951	5.415
5	Hexafluoro Phosphate	9.041	9.155	3.503	2.765	3.123	2.681	1.119	- 0.229
6	Acetate	- 8.784	-13.246	- 8.265	- 8.873	- 10.259	-10.18	- 10.30 9	2.988
7	Alaninate	- 6.367	-9.667	- 7.317	- 7.966	-9.033	-9.071	- 9.556	2.484
8	Arginate	- 3.662	-5.475	- 5.568	- 6.182	-6.867	-7.01	- 7.871	1.608
9	Bromide	- 9.071	-14.612	- 3.598	- 3.891	-5.451	-5.102	- 4.359	9.434
10	Decanoate	- 5.881	-7.681	- 7.892	- 8.513	-9.301	-9.438	- 10.35 6	-1.76
11	Perchlorate	5.691	2.347	2.622	1.757	1.611	1.293	0.03	10.60 6
12	Glutamate	- 3.803	-14.79	- 6.842	- 7.342	-8.768	-8.585	- 6.071	6.637
13	Formate	- 9.646	-14.79	- 6.842	- 7.342	-8.768	-8.585	- 8.366	6.637
14	Glycinate	- 5.881	-7.681	- 7.892	- 8.513	-9.301	-9.438	- 10.35 6	-1.76
15	Nitrate	- 2.952	-7.886	- 1.816	- 2.581	-3.478	-3.501	- 3.949	16.76 1

<b>16</b>	Salicylate	- 0.276	-1.934	- 3.336	- 4.094	-4.725	-4.964	- 6.141	4.538
<b>17</b>	Saccharinate	1.052	-0.419	- 1.322	- 1.972	-2.461	-2.669	- 3.652	6.633
<b>18</b>	bis(trifluorometh yl) sulfonylimide	3.776	3.931	1.726	1.375	1.514	1.298	0.413	4.596
<b>19</b>	Valinate	- 4.939	-7.262	- 6.973	- 7.644	-8.508	-8.634	- 9.448	1.143

**Table S4** Capacity values predicted using COSMO-RS for ILs

S.NO. Anions	Cations							
	Ch	TMAm	BMIIm	BMPy	BMPyr	BMPip	TBPh	Gu
1 Sulphate	5.09E+07	1.28E+10	49201	4958	341619	194652	40448.	2737
2 Chloride	406458.	9.42E+07	783.73	894.84	4653.65	2919.2	822.85	0.993
3 Tetrafluoroborate	0.028	1.307	0.321	0.781	0.987	1.311	4.193	0
4 Butylsulfate	0.756	2.339	6.24	10.944	14.418	17.387	38.255	0.009
5 Hexafluoro Phosphate	0.1	0.15	0.0	0.126	0.088	0.137	0.653	2.514
6 Acetate	13053.56	1.15E+06	7771.0	14267.74	57096.5	52752.4	59984.45	0.101
7 Alaninate	1164.305	32007.2	3009.95	5763.425	16747.2	17391.3	28247.76	0.167
8 Argininate	77.841	477.21	523.9	967.549	1921.02	2214.93	5237.896	0.401
9 Bromide	17398.4	4.44E+06	73.02	97.878	466.06	328.71	156.387	0
10 Decanoate	716.468	4333.646	5349.0	9953.635	21906.1	2510	62865.06	11.625
11 Perchlorate	0.007	0.19	0.14	0.345	0.4	0.54	1.941	0
12 Glutamate	89.707	1288.	129.7	225.13	518.5	535.7	866.30	0.008
13 Formate	30908.	5.30E+	1873	3089.0	12849	10700	8599.8	0.003
14 Glycinate	7912.9	44936	4306	7598.9	26609	24728	27012.	0.105
15 Nitrate	38.28	5363.	12.28	25.502	64.79	66.26	103.71	0
16 Salicylate	2.637	13.82	56.1	119.899	225.37	286.41	929.316	0.021
17 Saccharinate	0.699	3.05	7.5	14.372	23.42	28.84	77.126	0.003
18 bis(trifluoromethyl) sulfonylimide	0.046	0.03	0.346	0.487	0.421	0.52	1.252	0.02
19 Valinate	279.338	2850.4	2134.7	4178.17	9908.2	11237.4	25357.2	0.638

**Table S5** Selectivity values predictive using COSMO-RS for ILs

S.N o.	Anions	Cations							
		Ch	TMAm	BMI m	BMP y	BMP yr	BMPi p	TBP h	Gu
1	Sulphate	23677 8	3.23E+ 07	170.2 18	139.7 7	687.1 44	379.7 32	70.44 5	1219.8 53
2	Chloride	23324	3.77E+ 06	44.19 9	45.69 9	199.7 61	124.3 31	38.02 6	0.185
3	Tetrafluoroborate	0.018	1.495	0.452	1.246	1.721	2.376	12.13 7	0
4	Butylsulfate	0.296	1.015	3.026	5.383	6.947	8.479	23.46 7	0.004
5	Hexafluoro Phosphate	0	1.00E- 03	0.331	0.88	0.75	1.241	10.19	1.562
6	Acetate	178.0 19	5391.72 8	50.62 9	68.02	155.2 8	138.3 58	121.9 2	0.011
7	Alaninate	20.80 1	226.362	27.53 8	40.09	71.19	71.68	95.11	0.017
8	Argininate	2.401	7.35	10.00 2	15.20	20.69	23.53 5	51.1	0.039
9	Bromide	2525. 72	531171	13.28 2	17.12	69.15	49.14 4	27.61	0
10	Decanoate	14.43 6	30.422	45.80 6	60.76	74.51	81.63 3	144.6	1.964
11	Perchlorate	0.006	0.432	0.387	1.07	1.39	1.986	11.07 4	0
12	Glutamate	4.286	38.58	4.639	7.04	12.73	13.01 7	21.02	1.00E- 03
13	Formate	752.1 93	62045.3	30.55 7	40.73	115.6 3	94.14	68.94	0
14	Glycinate	122.2 35	2888.7	36.46 6	49.75	109.8 0	99.09	90.79	0.009
15	Nitrate	8.8	962.1	2.985	5.93	13.37 1	13.81	26.56 5	0
16	Salicylate	0.429	1.17	6.154	10.97	14.46	18.22	57.29 3	0.007
17	Saccharinate	0.243	0.91	2.599	4.81	7.03	8.71	27.1	1.00E- 03
18	bis(trifluoromet hyl)	0.062	0.187	1.804	3.12	3.22	4.16	15.40	0.022

sulfonylimide									
<b>19</b>	Valinate	6.125	24.82	23.61	34.92	49.62	54.58	98.82	0.076



**Table S6** Performance Index for different ILs

S.N o.	Anions	Cations							
		Ch	TMA m	BMI m	BMPy r	BMPy r	BMPi p	TBPh	Gu
1	Sulphate	1.21E+13	4.13E+17	8.38E+06	6.93E+06	2.35E+08	7.39E+07	2.85E+06	3.34E+07
2	Chloride	9.48E+09	3.56E+14	34640.74	40893.49	92961.6	36295.8.6	31290.14	0.1838
3	Tetrafluoroborate	4.94E-04	1.95292	0.14516	0.97266	1.698	3.11382	50.88569	8.24E-11
4	Butylsulfate	0.22378	2.37511	18.90308	58.90791	100.16	147.419	897.7335	3.14E-05
5	Hexafluoro Phosphate	6.38E-08	2.31E-07	0.01992	0.11084	0.0668	0.16993	6.6539	3.92796
6	Acetate	2.32E+06	6.20E+09	39344.1.6	97049.7.8	8.87E+06	7.30E+06	7.31E+06	0.00114
7	Alaninate	24219.19	7.25E+06	82887.99	23109.5.9	1.19E+06	1.25E+06	2.69E+06	0.00282
8	Argininate	186.8633	3507.686	5239.811	14713.5	39753	52128.4	267707	0.01558
9	Bromide	4.39E+07	2.36E+12	969.9269	1676.12	32228	16154	4318.61	7.50E-09
10	Decanoate	10342.77	131839	245020.7	60484	1.63E+06	2.05E+06	9.09E+06	22.83731
11	Perchlorate	4.19E-05	0.08259	0.05625	0.369	0.55563	1.08967	21.4914	1.80E-09
12	Glutamate	384.4966	49711.12	601.9161	1586	6605.931	6973.435	18215	7.88E-06
13	Formate	2.32E+07	3.29E+11	57238.88	125828	1.49E+06	1.01E+06	592878	9.61E-07
14	Glycinate	967241.7	1.30E+09	157036.5	378104	2.92E+06	2.45E+06	2.45E+06	9.90E-04
15	Nitrate	336.8822	5.16E+06	36.68786	151.46	866.4247	915.2552	2755.2	3.77E-15
16	Salicylate	1.13124	16.25055	345.7882	1315.558	3259.764	5220.798	53243	1.56E-04
17	Saccharinate	0.16981	2.80126	19.49564	69.21772	164.7901	251.4512	2090.1	2.68E-06
18	bis(trifluoromethyl)	0.00283	0.00715	0.62352	1.52266	1.35931	2.17617	19.289	4.57E-04

sulfonylimide									
<b>19</b>	Valinate	1711.0	70766.	50420.	14591	49173	61340	2.51E	0.0485
		79	5	43	5.3	1	7.9	+06	8

**Table S7** Effect of alkyl chain length on the capacity of ILs

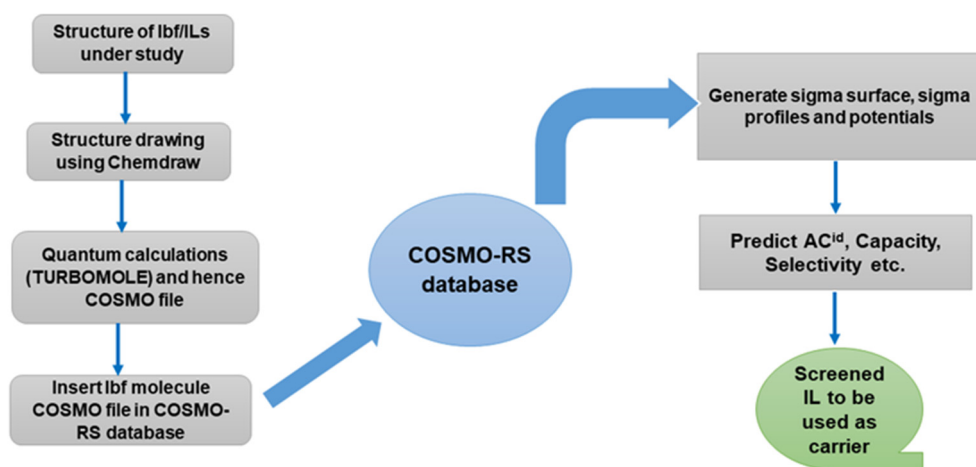
<b>Cations with varying alkyl chain</b>	<b>SO<sub>4</sub><sup>2-</sup></b>	<b>BF<sub>4</sub><sup>-</sup></b>	<b>Cl<sup>-</sup></b>	<b>PF<sub>6</sub><sup>-</sup></b>	<b>CH<sub>3</sub>COO<sup>-</sup></b>
Butyltrimethylammonium	623831	0.251795	7035.61	0.022432	26876.85
Tetra-Methylammonium	1.28E+10	1.306643	94200000	2.11E-04	1150711
Tetra-Ethylammonium	2361269	2.455515	29307.39	0.104792	215443.4
Tetra-N-Butylammonium	46169.69	4.356306	924.9798	0.660108	65562.94
Tetrapropylammonium	122488	3.579502	2127.145	0.427954	93126.82
Octyltrimethylammonium	13518.56	0.626098	251.9838	0.163583	8391.253
Methyl-Trioctyl-Ammonium	17416.07	4.409811	417.8525	0.789394	31363.8
Tetradecyltrimethylammonium	5707.758	1.821895	145.8008	0.489927	8074.289
Hexyl-Dimethyl-Isopropylammonium	51818.58	1.241607	889.0637	0.201463	27604.16
1-Hexyl-3-methyl-imidazolium	12877.04	0.555179	253.5241	0.150625	5454.082
1-Butyl-3-ethylimidazolium	26283.51	0.625398	500.0794	0.126039	8217.749
1-Butyl-1-methylpiperidinium	194652.4	1.310575	2919.298	0.136944	52752.43
1-Hexyl-1-methylpiperidinium	51786.71	1.498975	906.2461	0.235345	32065.02
1-Methyl-1-propylpiperidinium	620058.5	1.394286	8408.815	0.095941	85157.97
1-Pentyl-1-methylpiperidinium	94048.66	1.374526	1520.235	0.181949	40616.06
1-Hexadecyl-1-methyl-Piperidinium[2]	12640.47	3.406373	306.7085	0.689067	20992.9
1-Ethyl-1-methyl-Pyrrolidinium	13883000	1.649153	147727.1	0.030103	270434.1
1-Hexyl-1-methyl-Pyrrolidinium	62358.15	1.129228	1019.11	0.173879	30607.61
1-Methyl-1-pentylpyrrolidinium	126886.7	1.005834	1895.63	0.125882	39066.52
1-Methyl-1-propylpyrrolidinium	1494319	1.141635	18337.28	0.056765	105417.2
1-Octyl-1-methyl-pyrrolidinium	26465.07	1.488233	497.9222	0.281652	23241.9
1-Butyl-1-ethyl-pyrrolidinium	325703.6	1.914692	4667.77	0.171112	94258.02
Butyl-trihexyl-phosphonium	33814.22	5.184436	717.5374	0.804386	64042.84
Decyl-trihexyl-phosphonium	31695.48	5.22572	671.4244	0.804366	62390.03
Tetrabutyl-phosphonium	40448.12	4.192579	822.8536	0.652953	59984.45
Tetrahexyl-phosphonium	32616.22	5.24789	695.1285	0.813184	63002.88
Tributyl-ethyl-phosphonium	57649.8	3.924964	1090.038	0.570416	73102.75
Di[N-Dimethyl]-N(butyl,tetradecyl)guanidinium	110507.2	7.01794	1715.96	0.878806	244127

1-Butyl-3-ethyl-pyridinium	26372.66	1.071053	539.1929	0.202725	12307.15
1-Butyl-3-methyl-pyridinium	49589.57	0.780658	894.8488	0.125964	14267.74
1-Hexadecylpyridinium	3991.602	2.519436	123.1845	0.718999	5188.235
1-Hexyl-4-methyl-pyridinium	16446.33	1.148992	354.3297	0.252073	10155.16
4-Methyl-1-octyl-pyridinium	10296.15	1.591048	245.7814	0.388041	9045.078
Guanidinium	27377.82	1.47E-05	0.992824	2.514337	0.10076
Hexamethylguanidinium	15421000	15.00865	155608.2	0.428502	2425178
Di[N-Dimethyl]-N-[butyl,octyl]-guanidinium	98852.36	6.692637	1534.847	0.848473	230458.1
Di[N-Di(2-methoxyethyl)]-N-dimethyl-guanidinium	210354	5.830743	2937.677	0.953614	250311.2

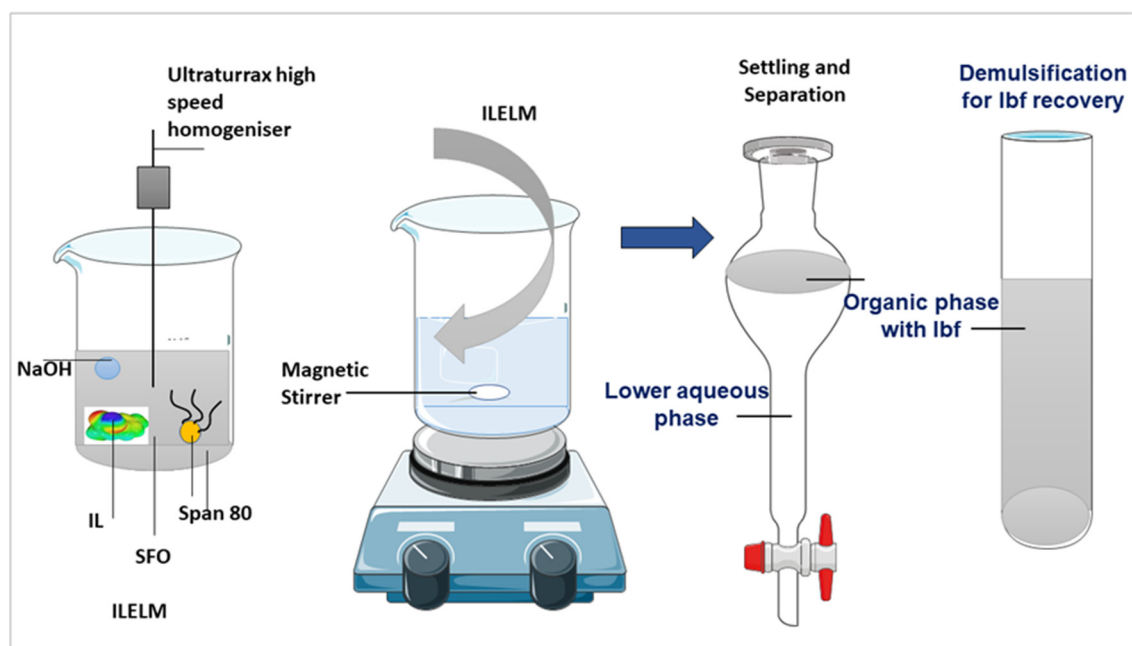
**Table S8** Effect of alkyl chain length on the selectivity of ILs

<b>Cations with varying alkyl chain</b>	<b>SO<sub>4</sub><sup>2-</sup></b>	<b>BF<sub>4</sub><sup>-</sup></b>	<b>Cl<sup>-</sup></b>	<b>PF<sub>6</sub><sup>-</sup></b>	<b>CH<sub>3</sub>COO<sup>-</sup></b>
Butyltrimethylammonium	1821.1	0.3	357.89	0.14	119.4
Tetra-Methylammonium	32253000.0	1.4	3774875.8	0.0010	5391.7
Tetra-Ethylammonium	3567.6	4.11	1033.6	0.91	430.9
Tetra-N-Butylammonium	78.1	12.4	41.8	10.2	130.6
Tetrapropylammonium	180.03	8.01	81.0	5.2	167.0
Octyltrimethylammonium	49.2	1.2	16.3	1.3	43.0
Methyl-Trioctyl-Ammonium	49.2	17.66	29.2	15.5	108.9
Tetradecyltrimethylammonium	25.2	4.7	11.7	5.60	48.7
Hexyl-Dimethyl-Isopropylammonium	120.3	2.4	43.8	1.9	85.5
1-Hexyl-3-methyl-imidazolium	49.0	0.8	15.9	0.9	38.0
1-Butyl-3-ethylimidazolium	83.5	0.94	27.3	0.7	49.3
1-Butyl-1-methylpiperidinium	379.7	2.37	124.3	1.2	138.3
1-Hexyl-1-methylpiperidinium	111.8	3.08	43.1	2.4	90.3
1-Methyl-1-propylpiperidinium	1132.3	2.3	333.6	0.8	213.6
1-Pentyl-1-methylpiperidinium	192.3	2.6	68.5	1.7	109.1
1-Hexadecyl-1-methyl-Piperidinium	38.6	11.0	21.1	10.7	81.9
1-Ethyl-1-methyl-Pyrrolidinium	24030.9	2.4	5385.4	0.2	675.6
1-Hexyl-1-methyl-Pyrrolidinium	140.2919479	2.248682	49.5	1.06	89.2
1-Methyl-1-pentylpyrrolidinium	271.584757	1.876005	87.02	1.15	110.3
1-Methyl-1-propylpyrrolidinium	2800.053031	1.8	727.9	0.45	274.6
1-Octyl-1-methyl-pyrrolidinium	65.1	3.3	26.6	3.07	72.7
1-Butyl-1-ethyl-pyrrolidinium	531.6	3.6	181.7	1.6	194.1

Butyl-trihexyl-phosphonium	66.1	20.1	39.4	16.7	139.1
Decyl-trihexyl-phosphonium	70.93	25.1	43.2	20.1	154.0
Tetrabutyl-phosphonium	70.4	12.1	38.0	10.1	121.9
Tetrahexyl-phosphonium	67.02394	22.0280	40.42 4808	18.130	143.64
Tributyl-ethyl-phosphonium	92.8467869	10.4715 3	46.943426	8.28944 2	134.88157 3
Di[N-Dimethyl]- N(butyl,tetradecyl)guanidini um	139.6	31.7	78.2	22.9	268.3
1-Butyl-3-ethyl-pyridinium	74.9	1.8	28.1	1.5	59.2
1-Butyl-3-methyl-pyridinium	139.7	1.2	45.6	0.8	68.0
1-Hexadecylpyridinium	22.8	6.60	11.5	7.5	49.0
1-Hexyl-4-methyl- Pyridinium	50.6	2.089	20.05	1.98	52.2
4-Methyl-1-octyl-Pyridinium	34.38	3.2	15.2	3.3	50.2
Guanidinium	1219.85	0.001	0.18	1.5	0.01
Hexamethylguanidinium	11302.1515	28.9706 8	3731.613243	5.01703	1868.3
Di[N-Dimethyl]-N- [butyl,octyl]-Guanidinium	136.5	34.8	77.8	25.0	272.5
Di[N-Di(2-Methoxyethyl)]- N-dimethyl-guanidinium	243.9	15.5	112.51	10.7	274.9

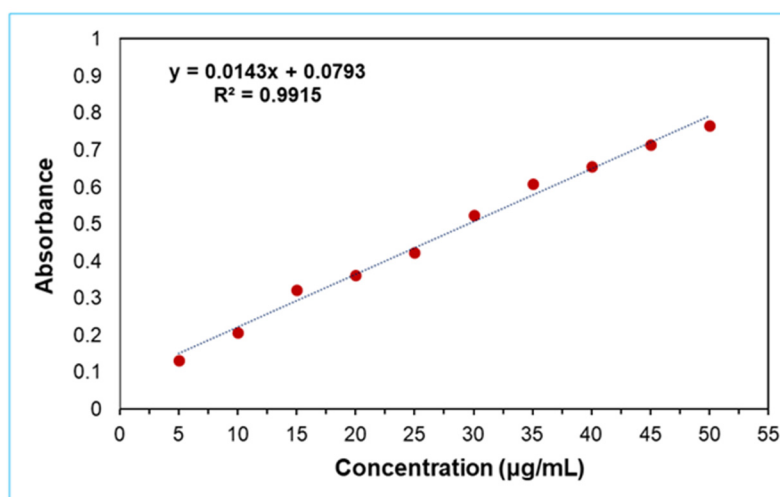


**Figure S1** Step by step COSMO-RS methodology to screen ILs for Ibuprofen (Ibf)

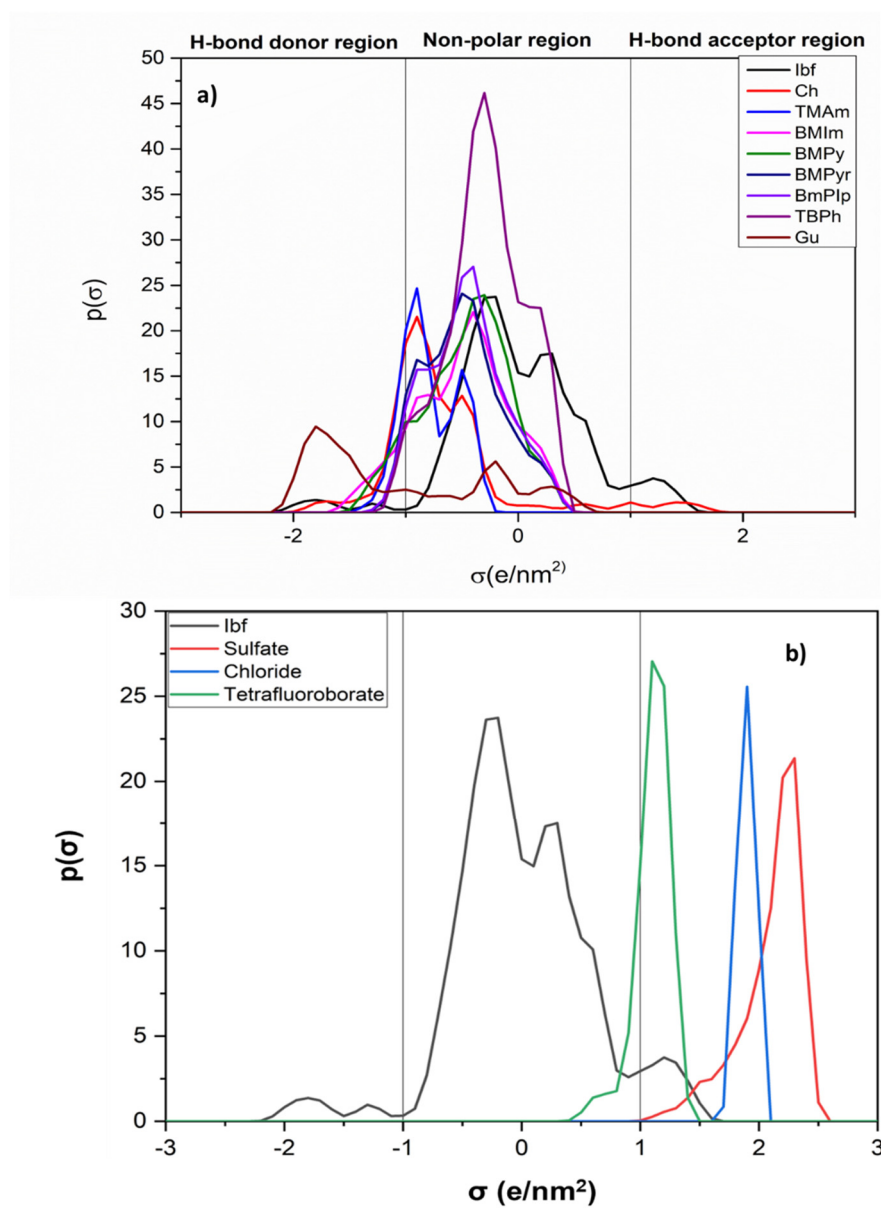


**Figure S2** Schematic representation of ionic liquid based green emulsion liquid membrane

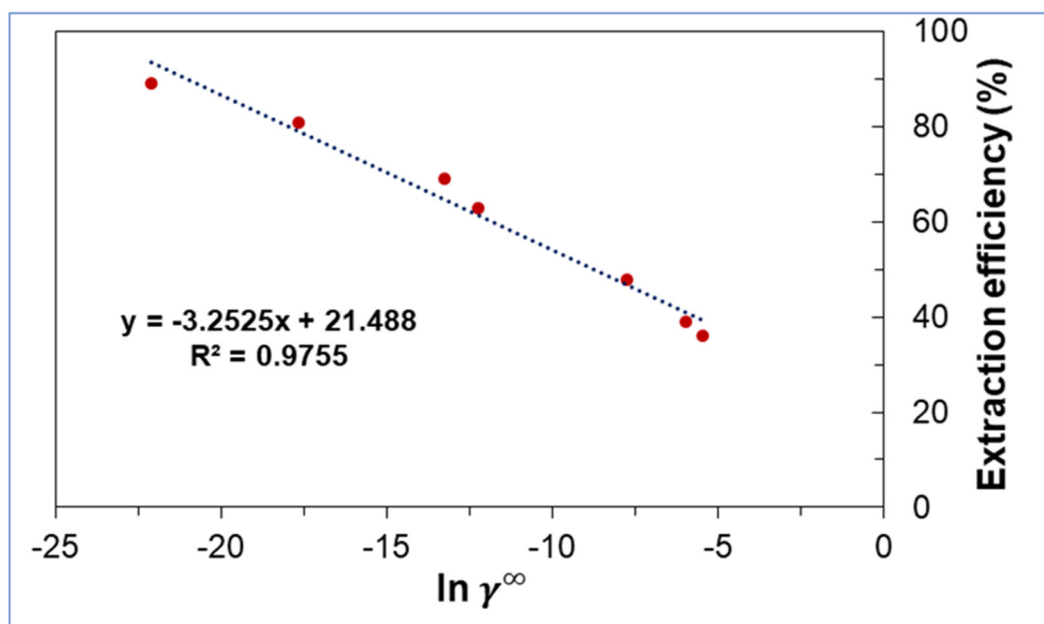




**Figure S3** Calibration curve for Ibf using UV-vis



**Figure S4**  $\sigma$ -profiles a) for cations and b) for anions under study



**Figure S5** Regression curve for  $AC^{id}$  and experimental extraction efficiency