

Supplementary Materials: Recovery and Elimination of Phenolic Pollutants from Water Using [NTf₂] and [Nf₂]-Based Ionic Liquids

Olalla G Sas, Ángeles Domínguez and Begoña González *

Table S1. Cation and anion structure of the studied ionic liquids and their corresponding names.

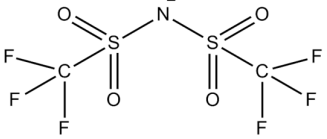
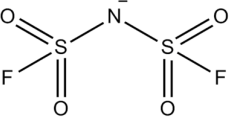
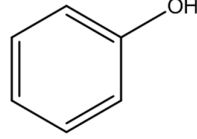
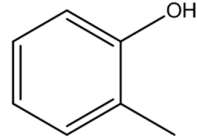
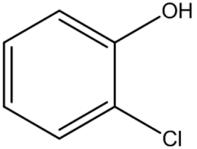
Structure	Name
	1-propyl-1-methylpyrrolidinium
	1-propyl-1-methylpiperidinium
	1-propyl-3-methylpyridinium
	Bis(trifluoromethylsulfonyl)imide
	Bis(fluorosulfonyl)imide
	Phenol
	o-cresol
	2-chlorophenol

Table S2. Initial concentration C_i ($\text{mg}\cdot\text{L}^{-1}$) vs final concentration C_f ($\text{mg}\cdot\text{L}^{-1}$) of phenol o-cresol and 2-chlorophenol after extraction process using $[^1\text{P}^1\text{Mpip}][\text{NTf}_2]$, $[^1\text{P}^3\text{Mpy}][\text{NTf}_2]$, $[^1\text{P}^1\text{Mpyr}][\text{NTf}_2]$ and $[^1\text{P}^1\text{Mpyr}][\text{Nf}_2]$ at $T = 298.15$ K and $P = 101.3$ kPa.

C_i ($\text{mg}\cdot\text{L}^{-1}$)	C_f ($\text{mg}\cdot\text{L}^{-1}$)		
	Phenol	o-cresol	2-chlorophenol
$[^1\text{P}^1\text{Mpip}][\text{NTf}_2]$			
2	0.1602	0.955	0.0912
5	0.2942	1.900	0.1507
50	2.959	20.38	1.268
500	27.40	97.87	13.09
2000	120.5	310.0	52.29
5000	304.4	405.3	148.7
10000	507.8	415.5	277.4
15000	730.5	606.9	472.4
$[^1\text{P}^3\text{Mpy}][\text{NTf}_2]$			
2	0.1856	0.3914	0.0809
5	0.4025	0.4791	0.1322
50	1.207	1.667	0.9708
500	28.23	12.21	10.52
2000	118.9	43.39	31.45
5000	231.0	137.1	99.48
10000	350.2	229.3	218.1
15000	587.2	353.4	323.5
$[^1\text{P}^1\text{Mpyr}][\text{NTf}_2]$			
2	0.2164	0.0214	0.1152
5	0.4443	0.1098	0.1870
50	3.491	1.344	1.297
500	25.29	15.05	15.15
2000	145.8	54.67	58.77
5000	278.3	163.6	158.3
10000	478.4	292.4	313.8
15000	708.0	424.0	481.3
$[^1\text{P}^1\text{Mpyr}][\text{Nf}_2]$			
2	0.1194	0.1257	0.0445
5	0.3092	0.1357	0.1817
50	2.731	1.083	0.9227
500	27.76	11.05	11.84
2000	111.4	42.83	48.12
5000	222.3	109.5	136.0
10000	277.0	177.3	241.5
15000	511.2	348.5	384.9

Table S3. Initial concentration C_i ($\text{mg}\cdot\text{L}^{-1}$) vs extraction efficiency (E%) of phenol o-cresol and 2-chlorophenol after extraction process using $[^1\text{P}^1\text{Mpip}][\text{NTf}_2]$, $[^1\text{P}^3\text{Mpy}][\text{NTf}_2]$, $[^1\text{P}^1\text{Mpyr}][\text{NTf}_2]$ and $[^1\text{P}^1\text{Mpyr}][\text{Nf}_2]$ at $T = 298.15\text{ K}$ and $P = 101.3\text{ kPa}$.

Extraction efficiency (E%)			
C_i ($\text{mg}\cdot\text{L}^{-1}$)	Phenol	o-cresol	2-chlorophenol
$[^1\text{P}^1\text{Mpip}][\text{NTf}_2]$			
2	91.74	53.52	95.63
5	93.66	58.59	96.97
50	93.60	55.90	97.49
500	93.83	78.09	97.39
2000	93.75	83.38	97.60
5000	93.71	91.71	97.15
10000	94.74	95.76	97.32
15000	94.97	95.88	96.98
$[^1\text{P}^3\text{Mpy}][\text{NTf}_2]$			
2	91.38	81.15	96.18
5	92.15	90.59	97.45
50	97.68	96.75	98.09
500	94.44	97.66	97.90
2000	94.54	98.07	98.52
5000	95.79	97.52	98.11
10000	96.78	97.92	97.91
15000	96.41	97.85	97.93
$[^1\text{P}^1\text{Mpyr}][\text{NTf}_2]$			
2	90.81	99.04	94.86
5	91.60	98.02	96.43
50	93.35	97.48	97.44
500	95.04	97.12	96.97
2000	93.51	97.44	97.20
5000	94.93	97.00	96.91
10000	95.61	97.34	96.98
15000	95.68	97.42	96.93
$[^1\text{P}^1\text{Mpyr}][\text{Nf}_2]$			
2	93.97	95.92	97.90
5	93.62	97.43	96.29
50	94.24	97.82	98.06
500	94.08	97.68	97.56
2000	94.43	97.94	97.63
5000	95.55	97.87	97.35
10000	97.22	98.26	97.65
15000	96.57	97.72	97.49

Table S4. Initial concentration C_i ($\text{mg}\cdot\text{L}^{-1}$) vs extraction efficiency (E%) of a mixture of phenolic compounds (PCM) after extraction process using $[^1\text{P}^1\text{Mpip}][\text{NTf}_2]$, $[^1\text{P}^3\text{Mpy}][\text{NTf}_2]$, $[^1\text{P}^1\text{Mpyr}][\text{NTf}_2]$ and $[^1\text{P}^1\text{Mpyr}][\text{Nf}_2]$ at $T = 298.15$ K and $P = 101.3$ kPa.

C_i ($\text{mg}\cdot\text{L}^{-1}$)	Extraction efficiency (E%)			
	$[^1\text{P}^1\text{Mpip}][\text{NTf}_2]$	$[^1\text{P}^3\text{Mpy}][\text{NTf}_2]$	$[^1\text{P}^1\text{Mpyr}][\text{NTf}_2]$	$[^1\text{P}^1\text{Mpyr}][\text{Nf}_2]$
2	95.73	96.25	92.60	80.92
5	95.74	96.16	93.96	90.17
50	95.72	96.36	94.33	95.46
500	95.59	96.20	95.17	95.91
2000	95.34	95.93	94.85	96.38
5000	95.36	96.20	96.48	96.50
10000	96.02	96.50	97.40	96.79
15000	96.25	96.42	96.88	96.82

Table S5. Initial concentration C_i ($\text{mg}\cdot\text{L}^{-1}$) vs final concentration C_f ($\text{mg}\cdot\text{L}^{-1}$) of a mixture of phenolic compounds (PCM) after extraction process using $[^1\text{P}^1\text{Mpip}][\text{NTf}_2]$, $[^1\text{P}^3\text{Mpy}][\text{NTf}_2]$, $[^1\text{P}^1\text{Mpyr}][\text{NTf}_2]$ and $[^1\text{P}^1\text{Mpyr}][\text{Nf}_2]$ at $T = 298.15$ K and $P = 101.3$ kPa.

C_i ($\text{mg}\cdot\text{L}^{-1}$)	C_f ($\text{mg}\cdot\text{L}^{-1}$)			
	$[^1\text{P}^1\text{Mpip}][\text{NTf}_2]$	$[^1\text{P}^3\text{Mpy}][\text{NTf}_2]$	$[^1\text{P}^1\text{Mpyr}][\text{NTf}_2]$	$[^1\text{P}^1\text{Mpyr}][\text{Nf}_2]$
2	0.0890	0.0716	0.1356	0.3837
5	0.2047	0.1850	0.2477	0.4912
50	2.009	1.709	2.335	2.198
500	20.76	17.89	19.69	19.55
2000	87.85	80.55	96.73	74.95
5000	218.8	179.1	165.8	182.3
10000	375.5	328.6	243.5	335.3
15000	529.8	505.9	441.6	499.5

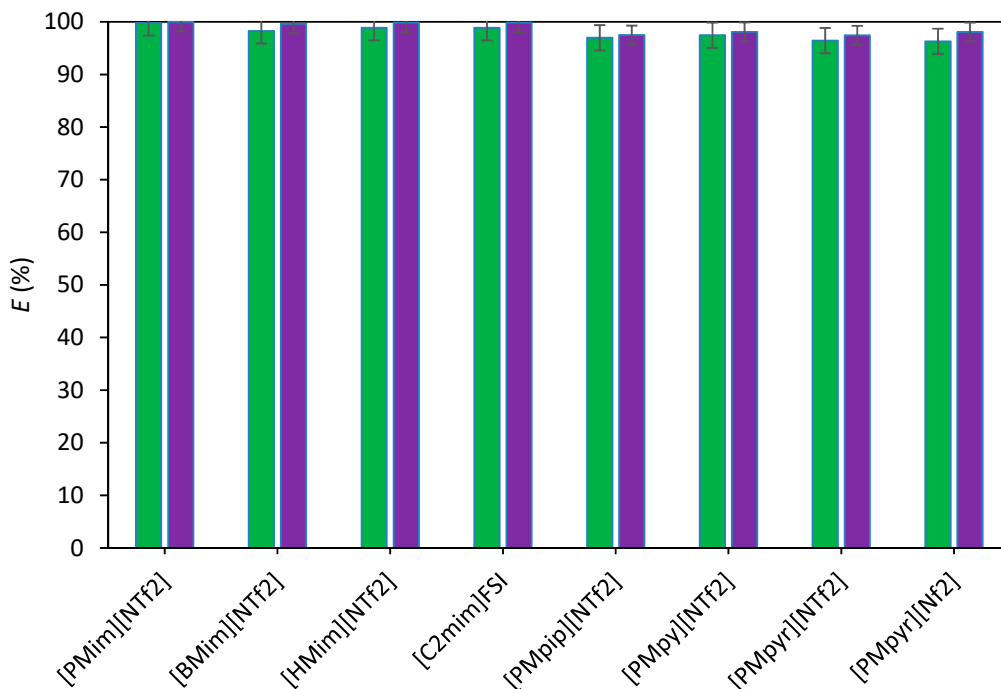


Figure S1. Extraction efficiencies (E%) of 2-chlorophenol using [PMim][NTf₂], [BMim][NTf₂], [HMim][NTf₂], [C₂mim]FSI, [PMpip][NTf₂], [PMpy][NTf₂], [PMpyr][NTf₂] and [PMpyr][Nf₂]. Initial concentrations (—) 5 mg·L⁻¹ and (—) 50 mg·L⁻¹.

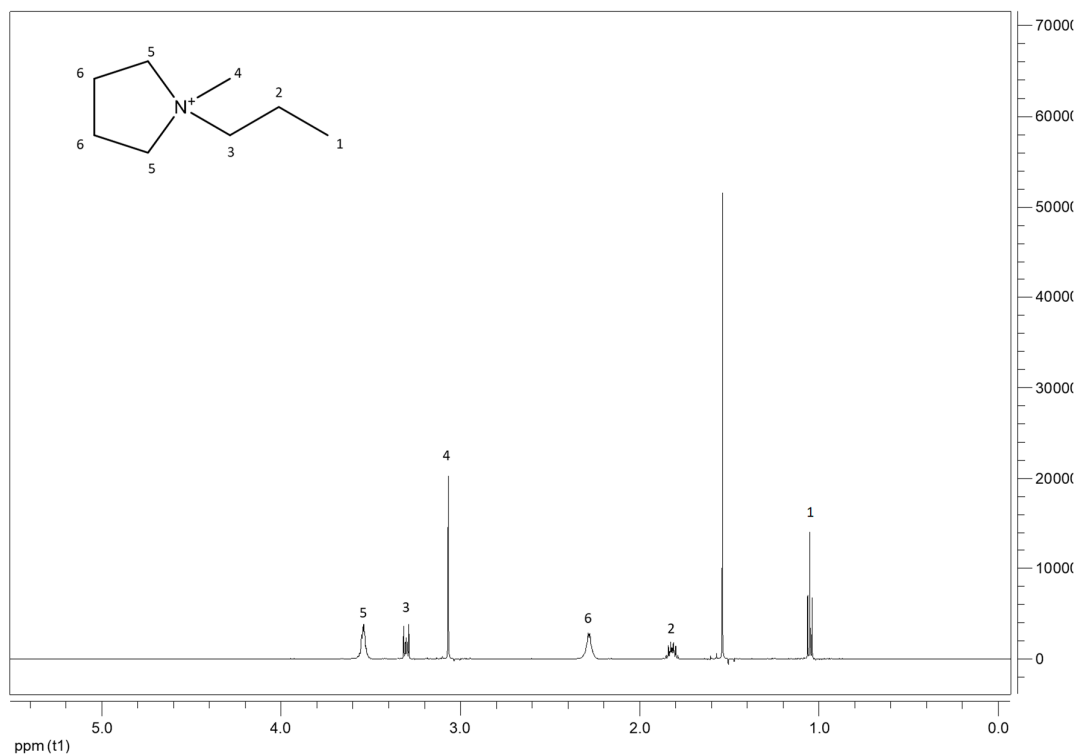


Figure S2. ¹H NMR spectrum for the pure IL 1-methyl-1-propylpyrrolidinium bis(trifluoromethylsulfonyl)imide.

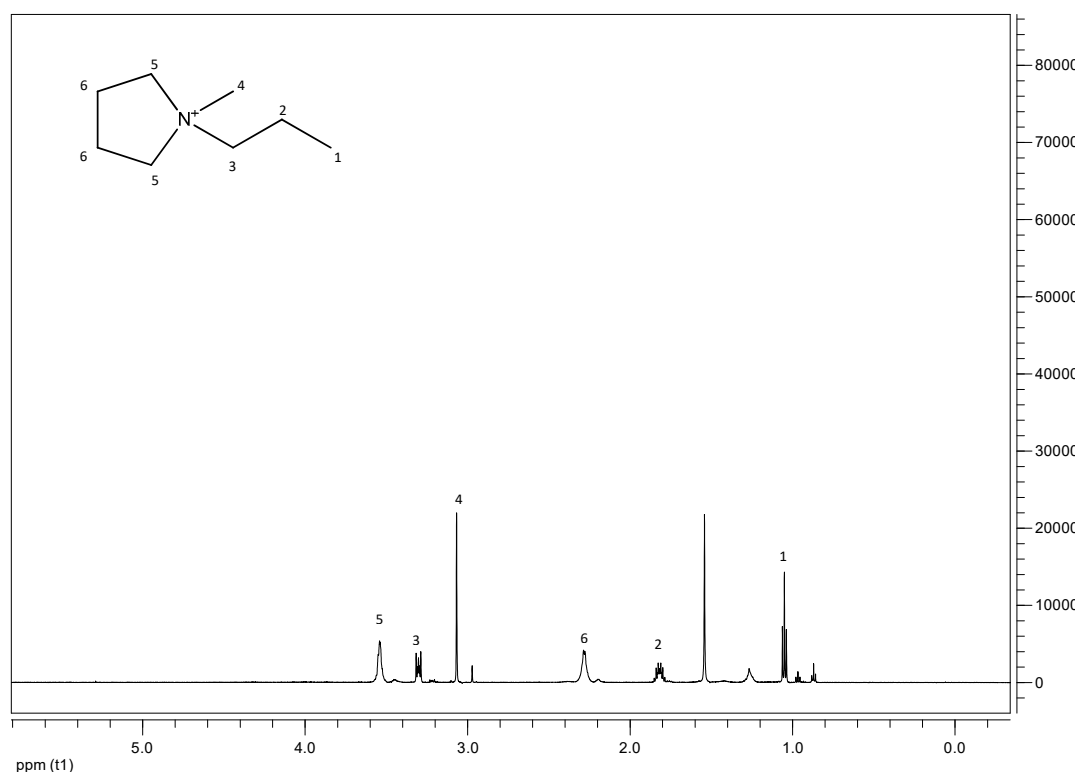


Figure S3. ^1H NMR spectrum for the IL 1-methyl-1-propylpyrrolidinium bis(trifluoromethylsulfonyl)imide after the recovery process using 0.5 M NaOH.