

## Supporting Information

### **Halogen-free ionic liquids as high performance extractants for phenols separation**

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Conditions: initial phenol content, 103.22 g·dm<sup>-3</sup>; temperature, 298.2 K; separation time, 20 min.

**Table S1** Chemical materials used in this study.

Chemical name	CAS number	Purity <sup>a</sup>	Supplier
phenol	108-95-2	99%	Aladdin Chemical Co., Ltd., Shanghai, China
toluene	108-88-3	98%	Beijing Tongguang Fine Chemicals Co., Ltd., Beijing, China
<i>o</i> -cresol	95-48-7	98%	Aladdin Chemical Co., Ltd., Shanghai, China
<i>m</i> -cresol	108-39-4	98%	Aladdin Chemical Co., Ltd., Shanghai, China
1,3-dihydroxybenzene	108-46-3	99%	Aladdin Chemical Co., Ltd., Shanghai, China
[Emim][LLac]	878132-19-5	98%	Shanghai Cheng Jie Chemical Co., Ltd., Shanghai, China
[Emim][Ac]	143314-17-4	98%	Shanghai Cheng Jie Chemical Co., Ltd., Shanghai, China
[Bmim][DMP]	891772-94-4	98%	Shanghai Cheng Jie Chemical Co., Ltd., Shanghai, China
[Emim][ES]	342573-75-5	98%	Shanghai Cheng Jie Chemical Co., Ltd., Shanghai, China
[Emim][TFMS]	145022-44-2	98%	Shanghai Cheng Jie Chemical Co., Ltd., Shanghai, China
<i>n</i> -hexane	110-54-3	98%	Beijing Tongguang Fine Chemicals Co., Ltd., Beijing, China
diethyl ether	60-29-7	98%	Beijing Tongguang Fine Chemicals Co., Ltd., Beijing, China

<sup>a</sup> The purities of the chemicals are provided by the suppliers.

**Table S2** The amount of phenol dissolved in HFILs during separation.

Mole ratio of [Emim][LLac] to phenol	0.11	0.20	0.30	0.40	0.49	0.61	0.70	0.79	0.95
Amount of phenol dissolved/g	0.434	1.030	1.442	1.760	1.925	1.966	1.987	2.001	2.022
Mole ratio of [Emim][Ac] to phenol	0.11	0.22	0.30	0.43	0.52	0.61	0.70	0.83	1.01
Amount of phenol dissolved/g	0.343	0.863	1.290	1.736	1.930	1.993	2.006	2.018	2.028

**Table S3** Comparison of this method with other methods.

Separation agents	$C_0/\text{g}\cdot\text{dm}^{-3}$	$SE$	$\text{MUCP}/\text{g}\cdot\text{dm}^{-3}$
[Emim][Ac]	103.215	98.6%	1.96
ChCl <sup>a</sup>	97.67	90%	8.89
DIL <sup>b</sup>	100	96.6%	3.90
[Bmim]Cl <sup>c</sup>	100	98.5%	1.2
Amide compounds	200.67	97.0%	-
L-car <sup>d</sup>	105	94.6%	14
Amino acid ILs	100	99.0%	1.40

<sup>a</sup> Choline chloride, a kind of quaternary ammonium salt.

<sup>b</sup> Imidazolium-based dicationic ionic liquids, separating phenol via forming deep eutectic solvents.

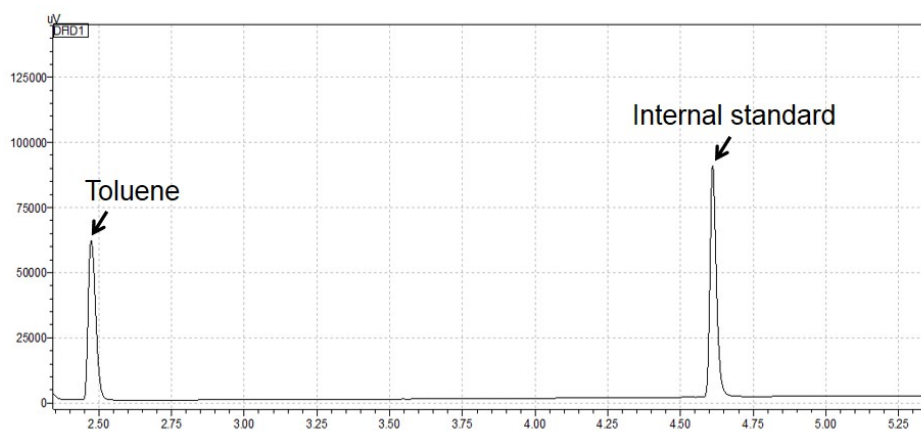
<sup>c</sup> 1-Butyl-3-methylimidazolium chloride.

<sup>d</sup> L-carnitine, a kind of inner salt.

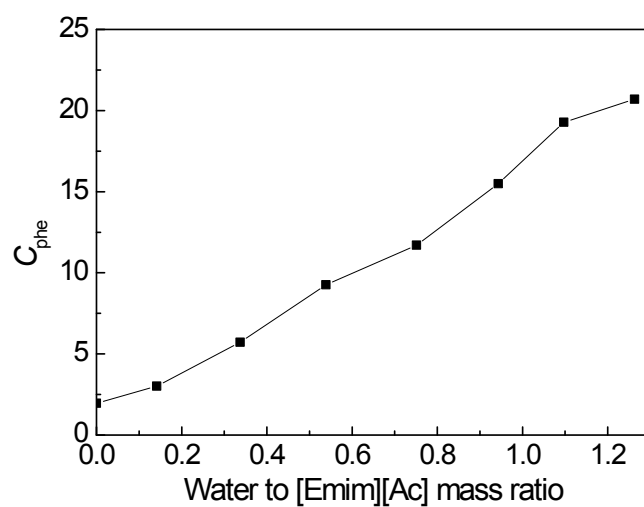
**Table S4** Comparison of this method with other methods.

Chemicals	Frequency/cm <sup>-1</sup>	Functional group	Assignment
Phenol	3322	-OH	stretching vibration
	3021	C-H in benzene ring	stretching vibration
	1335	-OH	bending vibration
	1234	C-O	stretching vibration
[Emim][LLac]	3452	C=O	stretching vibration
	3412 (overlapping peak)	-OH	stretching vibration
	3111	C-H in imidazole ring	stretching vibration
	2700-3000	C-H in CH <sub>3</sub> and CH <sub>2</sub>	stretching vibration
	1643 (overlapping peak) and 1416	-COO-	stretching vibration
	1589	imidazole ring	skeleton vibration
	1456	C-H in CH <sub>3</sub>	bending vibration
	1172	imidazole ring	stretching vibration
500-1000	C-H	in-plane bending vibration	
[Emim][Ac]	3437	C=O	stretching vibration
	3111	C-H in imidazole ring	stretching vibration
	2700-3000	C-H in CH <sub>3</sub> and CH <sub>2</sub>	stretching vibration
	1654 (overlapping)	-COO-	stretching vibration

	peak) and 1402		
	1572	imidazole ring	skeleton vibration
	1452	C-H in CH <sub>3</sub>	bending vibration
	1169	imidazole ring	stretching vibration
	500-1000	C-H	in-plane bending vibration
[Emim][LLac] +phenol	about 3200	-OH in phenol	stretching vibration
[Emim][Ac] +phenol	3111	-OH in phenol	stretching vibration



**Fig. S1** Results of *n*-hexane phase analysis by GC.



**Fig. S2** Phenol content in oil as a function of water to [Emim][Ac] mass ratio. Conditions: initial phenol content,  $103.22 \text{ g}\cdot\text{dm}^{-3}$ ; temperature,  $298.2 \text{ K}$ ; separation time,  $20 \text{ min}$ .