

Supporting Information

Optimization of the Gallic Acid Extraction using Ionic-Liquid-Based Aqueous Two- Phase Systems

*Ana Filipa M. Cláudio, Ana M. Ferreira, Carmen S. R. Freire, Armando J. D. Silvestre,
Mara G. Freire* and João A. P. Coutinho*

Departamento de Química, CICECO, Universidade de Aveiro, 3810-193 Aveiro,
Portugal

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*Corresponding author

Tel: +351-234-370200; Fax: +351-234-370084; E-mail address: maragfreire@ua.pt

Table S 1

Experimental weight fraction composition and partition coefficients of gallic acid in ILs + Na₂SO₄ ATPS at 298.15 K.

IL + Na ₂ SO ₄ + water system	Weight fraction composition / wt %		$K_{GA} \pm \sigma^a$	%EE _{GA} $\pm \sigma^a$
	IL	Na ₂ SO ₄		
[C ₂ mim][CF ₃ SO ₃]	24.88	15.28	9.76 \pm 0.56	81.23 \pm 2.31
[C ₄ mim][CF ₃ SO ₃]	24.95	14.97	21.98 \pm 2.25	88.90 \pm 0.60
[C ₄ mim][CH ₃ SO ₄]	24.69	14.52	26.46 \pm 0.53	97.05 \pm 0.06
[C ₄ mim][C ₂ H ₅ SO ₄]	25.71	15.36	29.58 \pm 0.79	98.53 \pm 0.04
[C ₄ mim][OctylSO ₄]	24.98	14.95	2.04 \pm 0.41	58.36 \pm 3.36
[C ₄ mim][N(CN) ₂]	25.00	15.00	20.45 \pm 2.08	93.37 \pm 0.74
[C ₄ mim]Br	24.96	15.22	23.68 \pm 1.51	96.84 \pm 0.15
[C ₇ mim]Cl	25.05	15.00	21.94 \pm 1.57	98.80 \pm 0.08
[C ₈ mim]Cl	25.92	15.23	3.28 \pm 0.59	96.45 \pm 1.79

^astandard deviation

Table S 2

Experimental weight fraction composition and partition coefficients of gallic acid in ILs + K₂HPO₄/KH₂PO₄ ATPS at 298.15 K.

IL + K ₂ HPO ₄ /KH ₂ PO ₄ + water system	Weight fraction composition / wt %		$K_{GA} \pm \sigma^a$	%EE _{GA} $\pm \sigma^a$
	IL	K ₂ HPO ₄ /KH ₂ PO ₄		
[C ₂ mim][CF ₃ SO ₃]	25.06	14.99	0.90 \pm 0.06	33.32 \pm 1.27
	30.05	14.97	0.84 \pm 0.04	40.05 \pm 2.01
[C ₄ mim][CF ₃ SO ₃]	25.89	14.85	0.76 \pm 0.03	26.30 \pm 0.50
	29.93	15.09	1.70 \pm 0.07	51.60 \pm 1.01
[C ₄ mim][CH ₃ SO ₄]	29.10	16.59	6.43 \pm 0.44	94.75 \pm 0.35
[C ₄ mim][OctylSO ₄]	25.04	15.01	1.18 \pm 0.01	44.57 \pm 0.19
[C ₄ mim][N(CN) ₂]	25.01	15.00	3.19 \pm 0.12	72.53 \pm 0.65
	29.96	15.03	3.87 \pm 0.09	81.20 \pm 1.64
[C ₄ mim]Br	29.94	15.41	11.35 \pm 0.65	96.93 \pm 0.37
[C ₇ mim]Cl	30.00	15.40	5.02 \pm 0.40	96.06 \pm 0.30
[C ₈ mim]Cl	30.90	15.05	6.98 \pm 0.48	96.97 \pm 0.60

^astandard deviation

Table S 3

Experimental weight fraction composition and partition coefficients of gallic acid in ILs + K₃PO₄ ATPS at 298.15 K.

IL + K ₃ PO ₄ + water system	Weight fraction composition / wt %		$K_{GA} \pm \sigma^a$	%EE _{GA} ± σ ^a
	IL	K ₃ PO ₄		
[C ₂ mim][CF ₃ SO ₃]	25.07	14.93	0.58 ± 0.19	14.70 ± 4.19
[C ₄ mim][CF ₃ SO ₃]	25.08	14.96	0.18 ± 0.03	34.66 ± 1.39
[C ₄ mim][CH ₃ SO ₄]	24.97	15.29	1.03 ± 0.09	52.81 ± 0.93
[C ₄ mim][OctylSO ₄]	24.98	15.02	0.38 ± 0.09	18.53 ± 3.63
[C ₄ mim][N(CN) ₂]	25.02	15.02	0.51 ± 0.08	26.02 ± 1.43
[C ₄ mim]Br	24.82	15.09	0.97 ± 0.20	56.17 ± 0.47
[C ₇ mim]Cl	25.01	15.26	8.16 ± 0.36	89.86 ± 2.76
[C ₈ mim]Cl	25.01	15.08	2.52 ± 0.53	74.22 ± 4.09

^astandard deviation

Table S 4

Weight fraction compositions (wt %) of the top (T) phase, the initial mixture (M), and the bottom (B) phase of the ternary systems composed of ionic liquid + K₃PO₄ + H₂O systems at 298 K.

Ionic liquid	Weight fraction composition / wt %					
	[IL] _T	[K ₃ PO ₄] _T	[IL] _M	[K ₃ PO ₄] _M	[IL] _B	[K ₃ PO ₄] _B
[C ₂ mim][CF ₃ SO ₃]	0.52	29.92	25.07	14.93	74.85	1.47
[C ₄ mim][CF ₃ SO ₃]	1.59	14.96	25.08	1.09	66.42	22.83
[C ₄ mim][N(CN) ₂]	59.21	1.96	25.02	15.02	2.95	23.45
[C ₄ mim]Br	45.96	3.51	24.82	15.09	5.48	25.67
[C ₇ mim]Cl	42.33	4.57	25.01	15.26	4.21	28.11
[C ₈ mim]Cl	38.96	6.95	25.01	15.08	7.34	25.37

Table S 5

Weight fraction compositions (wt %) of the top (T) phase, the initial mixture (M), and the bottom (B) phase of the ternary systems composed of ionic liquid + $\text{K}_2\text{HPO}_4/\text{KH}_2\text{PO}_4 + \text{H}_2\text{O}$ systems at 298 K.

Ionic liquid	Weight fraction composition / wt %					
	[IL] _T	[K ₂ HPO ₄ / KH ₂ PO ₄] _T	[IL] _M	[K ₂ HPO ₄ / KH ₂ PO ₄] _M	[IL] _B	[K ₂ HPO ₄ / KH ₂ PO ₄] _B
[C ₄ mim][CF ₃ SO ₃]	74.59	1.20	25.89	14.85	0.80	21.88
	80.09	1.00	29.93	15.09	0.47	23.36
[C ₄ mim][N(CN) ₂]	49.79	2.10	25.01	15.00	3.75	26.10
	56.86	1.17	29.96	15.03	1.91	29.48
[C ₇ mim]Cl	33.72	11.54	30.00	15.40	11.88	34.18
[C ₈ mim]Cl	47.56	6.09	31.90	15.05	26.66	18.04

Table S 6

Weight fraction compositions (wt %) of the top (T) phase, the initial mixture (M), and the bottom (B) phase of the ternary systems composed of ionic liquid + Na₂SO₄ + H₂O systems at 298 K.

Ionic liquid	Weight fraction composition / wt %					
	[IL] _T	[Na ₂ SO ₄] _T	[IL] _M	[Na ₂ SO ₄] _M	[IL] _B	[Na ₂ SO ₄] _B
[C ₂ mim][CF ₃ SO ₃]	71.67	0.80	24.88	15.28	2.22	22.30
[C ₄ mim][CF ₃ SO ₃]	2.15	20.00	24.95	14.97	90.03	0.60
[C ₄ mim][CH ₃ SO ₄]	45.93	4.36	24.69	14.52	11.88	20.64
[C ₄ mim][OctylSO ₄]	73.70	1.75	24.98	14.95	0.14	21.68
[C ₄ mim][N(CN) ₂]	60.82	0.56	25.00	15.00	0.40	24.92
[C ₄ mim]Br	39.71	5.21	24.96	15.22	12.73	23.52
[C ₇ mim]Cl	63.27	1.66	25.05	15.00	12.88	19.25
[C ₈ mim]Cl	72.69	0.38	25.92	15.23	7.64	21.03

Table S 7

Experimental weight fraction composition and partition coefficients of vanillin in ILs + K_3PO_4 ATPS at 298.15 K.

IL + K_3PO_4 + water system	Weight fraction composition / wt %		$K_{Van} \pm \sigma^a$
	IL	K_3PO_4	
[C ₄ mim]Cl	25.00	15.02	44.98 ± 0.10
[C ₇ mim]Cl	24.61	14.88	42.39 ± 1.35
[C ₄ mim]Br	24.74	15.55	25.66 ± 0.40
[C ₄ mim][CF ₃ SO ₃]	24.67	15.16	9.75 ± 1.34
[C ₄ mim][CH ₃ SO ₄]	25.05	15.16	22.74 ± 0.55
[C ₄ mim][N(CN) ₂]	24.63	14.77	31.87 ± 3.97

^astandard deviation

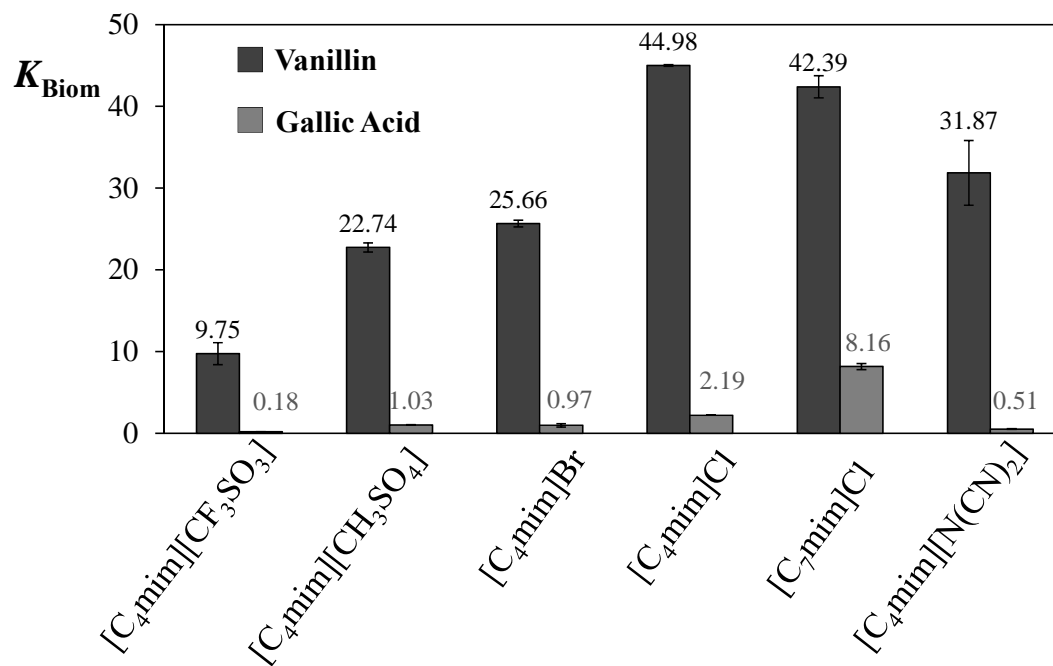


Fig. S1: Partition coefficients of vanillin and gallic acid in different ATPS composed of 25 wt % of IL + 15 wt % of K_3PO_4 at 298.15 K.

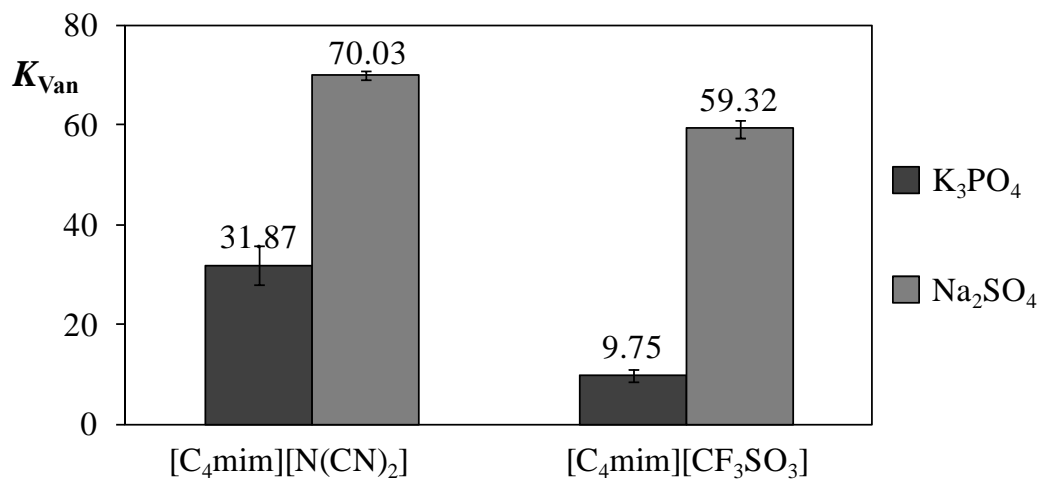


Fig. S2: Partition coefficients of vanillin for different ATPS composed of 25 wt % of IL + 15 wt % of inorganic salt at 298.15 K.

Table S 8

Experimental weight fraction composition and partition coefficients of vanillin in ILs + Na₂SO₄ ATPS at 298.15 K.

IL + Na ₂ SO ₄ + water system	Weight fraction composition / wt %		$K_{\text{Van}} \pm \sigma^a$
	IL	Na ₂ SO ₄	
[C ₄ mim][CF ₃ SO ₃]	24.71	14.89	70.03 ± 0.77
[C ₄ mim][N(CN) ₂]	24.93	14.97	59.32 ± 1.75

^astandard deviation