

EVALUATION OF THE EFFECT OF IONIC LIQUIDS AS ADJUVANTS IN POLYMER-BASED AQUEOUS BIPHASIC SYSTEMS USING BIOMOLECULES AS MOLECULAR PROBES

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Supporting Information

Table S1

Initial mixture compositions and TLL of the quaternary and ternary ABS

ABS	Mass Fraction Composition $\pm \sigma$ / (wt%)			TLL
	PEG	Salt	IL	
PEG400+Salt+Water+[P ₄₄₄₄]Cl	30.31 \pm 0.10	29.48 \pm 0.06	5.04 \pm 0.12	78.36
PEG400+Salt+Water+[N ₄₄₄₄]Cl	30.18 \pm 0.12	29.60 \pm 0.15	5.09 \pm 0.08	77.59
PEG400+Salt+Water+[C ₄ mpip]Cl	29.99 \pm 0.06	30.05 \pm 0.06	5.06 \pm 0.10	69.04
PEG400+Salt+Water+[C ₄ mpyr]Cl	30.10 \pm 0.06	30.02 \pm 0.09	5.06 \pm 0.09	67.85
PEG400+Salt+Water+[C ₄ mim]Cl	30.08 \pm 0.14	29.81 \pm 0.12	5.09 \pm 0.08	67.16
Salt+Water+[P ₄₄₄₄]Cl	30.05 \pm 0.11	29.98 \pm 0.06	0.00	86.89
Salt+Water+[N ₄₄₄₄]Cl	30.08 \pm 0.02	30.07 \pm 0.05	0.00	81.71
Salt+Water+[C ₄ mpip]Cl	30.09 \pm 0.06	29.86 \pm 0.11	0.00	58.84
Salt+Water+[C ₄ mpyr]Cl	30.04 \pm 0.06	30.13 \pm 0.06	0.00	72.58
Salt+Water+[C ₄ mim]Cl	29.98 \pm 0.14	30.08 \pm 0.09	0.00	58.52
Without IL	30.10 \pm 0.06	29.90 \pm 0.09	0.00	60.53

Table S2

Mixture point for a fixed TLL.

ABS	Citrate buffer pH7.0	PEG 400	IL
PEG400+Salt+Water+[P ₄₄₄₄]Cl	20 wt%	36 wt%	5 wt%
PEG400+Salt+Water+[N ₄₄₄₄]Cl	20 wt%	37 wt%	5 wt%
PEG400+Salt+Water+[C ₄ mpip]Cl	20 wt%	42 wt%	5 wt%
PEG400+Salt+Water+[C ₄ mpyr]Cl	20 wt%	42 wt%	5 wt%
PEG400+Salt+Water+[C ₄ mim]Cl	20 wt%	42 wt%	5 wt%
Salt+Water+[P ₄₄₄₄]Cl	28 wt%	26 wt%	-
Salt+Water+[N ₄₄₄₄]Cl	28 wt%	26 wt%	-
Salt+Water+[C ₄ mpip]Cl	20 wt%	31 wt%	-
Salt+Water+[C ₄ mpyr]Cl	28 wt%	32 wt%	-
Salt+Water+[C ₄ mim]Cl	28 wt%	34 wt%	-
Without IL	20 wt%	44 wt%	-

Table S3

Partition coefficient (K) of each antioxidant with the respective standard deviations and mass fraction compositions of the quaternary systems at 298 (± 1) K.

Biomolecule	IL in Quaternary System	Mass Fraction			K $\pm \sigma$
		Composition $\pm \sigma$ / (wt%)			
		PEG	Salt	IL	
Gallic acid	[P ₄₄₄₄]Cl	30.01 \pm 0.10	30.98 \pm 0.06	5.04 \pm 0.12	6.55 \pm 0.93
	[N ₄₄₄₄]Cl	30.02 \pm 0.12	29.97 \pm 0.15	5.09 \pm 0.08	7.78 \pm 0.36
	[C ₄ mpyr]Cl	30.10 \pm 0.06	30.05 \pm 0.06	5.06 \pm 0.10	12.16 \pm 0.58
	[C ₄ mpip]Cl	30.10 \pm 0.06	30.10 \pm 0.09	5.06 \pm 0.09	12.72 \pm 1.47
	[C ₄ mim]Cl	30.04 \pm 0.14	30.08 \pm 0.02	5.09 \pm 0.08	12.81 \pm 1.53
Vanillic acid	[P ₄₄₄₄]Cl	30.03 \pm 0.05	29.99 \pm 0.05	5.10 \pm 0.06	7.25 \pm 0.98
	[N ₄₄₄₄]Cl	30.00 \pm 0.13	30.11 \pm 0.03	5.14 \pm 0.31	8.06 \pm 0.58
	[C ₄ mpyr]Cl	30.09 \pm 0.05	30.07 \pm 0.02	5.12 \pm 0.09	11.02 \pm 1.01
	[C ₄ mpip]Cl	29.99 \pm 0.08	30.12 \pm 0.06	5.01 \pm 0.07	10.76 \pm 0.69
	[C ₄ mim]Cl	30.13 \pm 0.09	30.05 \pm 0.06	5.05 \pm 0.03	10.97 \pm 0.24
Eugenol	[P ₄₄₄₄]Cl	30.03 \pm 0.05	29.98 \pm 0.09	5.11 \pm 0.03	9.76 \pm 1.22
	[N ₄₄₄₄]Cl	30.01 \pm 0.03	30.11 \pm 0.03	5.04 \pm 0.11	8.35 \pm 0.70
	[C ₄ mpyr]Cl	30.06 \pm 0.08	30.09 \pm 0.09	5.09 \pm 0.11	11.83 \pm 0.36
	[C ₄ mpip]Cl	30.11 \pm 0.11	30.01 \pm 0.06	5.04 \pm 0.09	13.28 \pm 0.84
	[C ₄ mim]Cl	30.03 \pm 0.09	29.99 \pm 0.06	5.12 \pm 0.06	12.76 \pm 0.70

Table S4

Partition coefficient (K) of each antioxidant with the respective standard deviations and mass fraction compositions of the ternary systems at 298 (± 1) K.

Biomolecule	Ternary System	Mass Fraction		K $\pm \sigma$
		Composition $\pm \sigma$ / (wt%)		
		PEG	Salt	
Gallic acid	Without IL	30.10 \pm 0.06	30.10 \pm 0.03	9.56 \pm 1.20
	[P ₄₄₄₄]Cl	30.05 \pm 0.11	29.98 \pm 0.06	4.06 \pm 0.06
	[N ₄₄₄₄]Cl	30.08 \pm 0.12	30.07 \pm 0.05	4.92 \pm 0.09
	[C ₄ mpyr]Cl	30.10 \pm 0.06	30.05 \pm 0.11	12.03 \pm 0.76
	[C ₄ mpip]Cl	30.04 \pm 0.06	30.13 \pm 0.06	10.2 \pm 0.94
	[C ₄ mim]Cl	29.98 \pm 0.14	30.08 \pm 0.09	10.05 \pm 0.73
Vanillic acid	Without IL	30.12 \pm 0.02	30.14 \pm 0.01	10.72 \pm 1.17
	[P ₄₄₄₄]Cl	30.03 \pm 0.05	30.12 \pm 0.05	6.78 \pm 0.46
	[N ₄₄₄₄]Cl	30.01 \pm 0.03	30.11 \pm 0.03	5.76 \pm 0.39
	[C ₄ mpyr]Cl	30.06 \pm 0.05	30.07 \pm 0.02	8.98 \pm 0.66
	[C ₄ mpip]Cl	30.10 \pm 0.06	30.10 \pm 0.02	8.69 \pm 1.07
	[C ₄ mim]Cl	30.03 \pm 0.02	30.04 \pm 0.02	8.89 \pm 0.31
Eugenol	Without IL	30.10 \pm 0.09	30.09 \pm 0.06	12.75 \pm 0.88
	[P ₄₄₄₄]Cl	30.09 \pm 0.04	30.11 \pm 0.05	8.51 \pm 0.24
	[N ₄₄₄₄]Cl	30.08 \pm 0.09	29.99 \pm 0.03	6.76 \pm 1.19
	[C ₄ mpyr]Cl	30.12 \pm 0.05	30.09 \pm 0.09	9.91 \pm 0.60
	[C ₄ mpip]Cl	30.11 \pm 0.01	29.98 \pm 0.09	6.55 \pm 0.64
	[C ₄ mim]Cl	30.00 \pm 0.09	30.05 \pm 0.10	8.92 \pm 2.01

Table S5

Partition coefficient (K) of each amino acid with the respective standard deviations and mass fraction compositions of the quaternary systems at 298 (± 1) K.

Biomolecule	IL in Quaternary System	Mass Fraction Composition $\pm \sigma$ / (wt%)			K $\pm \sigma$
		PEG	Salt	IL	
L-tryptophan	[P ₄₄₄₄]Cl	30.01 \pm 0.10	30.98 \pm 0.06	5.04 \pm 0.12	16.58 \pm 1.30
	[N ₄₄₄₄]Cl	30.02 \pm 0.12	29.97 \pm 0.15	5.09 \pm 0.08	21.1 \pm 1.10
	[C _{4mpyr}]Cl	30.10 \pm 0.06	30.05 \pm 0.06	5.06 \pm 0.10	18.25 \pm 0.91
	[C _{4mpip}]Cl	30.10 \pm 0.06	30.10 \pm 0.09	5.06 \pm 0.09	14.96 \pm 1.49
	[C _{4mim}]Cl	30.04 \pm 0.14	30.08 \pm 0.02	5.09 \pm 0.08	13.98 \pm 0.5
L-phenylalanine	[P ₄₄₄₄]Cl	30.03 \pm 0.05	29.99 \pm 0.05	5.10 \pm 0.06	8.57 \pm 1.13
	[N ₄₄₄₄]Cl	30.01 \pm 0.03	30.11 \pm 0.03	5.14 \pm 0.31	8.89 \pm 0.60
	[C _{4mpyr}]Cl	30.06 \pm 0.05	30.07 \pm 0.02	5.12 \pm 0.09	7.84 \pm 0.89
	[C _{4mpip}]Cl	30.10 \pm 0.06	30.10 \pm 0.06	5.06 \pm 0.09	8.91 \pm 0.76
	[C _{4mim}]Cl	30.13 \pm 0.09	30.05 \pm 0.06	5.05 \pm 0.03	9.19 \pm 0.88
L-tyrosine	[P ₄₄₄₄]Cl	30.03 \pm 0.05	29.98 \pm 0.05	5.10 \pm 0.06	5.52 \pm 0.16
	[N ₄₄₄₄]Cl	30.01 \pm 0.03	30.11 \pm 0.03	5.04 \pm 0.11	4.27 \pm 0.51
	[C _{4mpyr}]Cl	30.06 \pm 0.08	30.07 \pm 0.09	5.09 \pm 0.11	4.55 \pm 0.52
	[C _{4mpip}]Cl	30.10 \pm 0.16	30.10 \pm 0.06	5.06 \pm 0.09	4.16 \pm 0.74
	[C _{4mim}]Cl	30.03 \pm 0.09	29.99 \pm 0.06	5.09 \pm 0.06	4.67 \pm 0.01

Table S6

Partition coefficient (K) of each amino acid with the respective standard deviations and mass fraction compositions of the ternary systems at 298 (± 1) K.

Biomolecule	Ternary System	Mass Fraction		K $\pm \sigma$	
		Composition $\pm \sigma$ / (wt%)			
		PEG	Salt		
L-tryptophan	Without IL	30.10 \pm 0.06	30.10 \pm 0.06	13.48 \pm 0.33	
	[P ₄₄₄₄]Cl	30.05 \pm 0.11	29.98 \pm 0.06	15.4 \pm 0.61	
	[N ₄₄₄₄]Cl	30.08 \pm 0.12	30.07 \pm 0.05	24.39 \pm 2.07	
	[C ₄ mpyr]Cl	30.10 \pm 0.06	30.05 \pm 0.11	6.96 \pm 0.71	
	[C ₄ mpip]Cl	30.10 \pm 0.06	30.10 \pm 0.06	6.73 \pm 0.61	
	[C ₄ mim]Cl	29.98 \pm 0.14	30.08 \pm 0.09	5.66 \pm 0.84	
L-phenylalanine	Without IL	30.10 \pm 0.06	30.10 \pm 0.06	7.58 \pm 0.95	
	[P ₄₄₄₄]Cl	30.03 \pm 0.05	30.12 \pm 0.05	7.92 \pm 0.35	
	[N ₄₄₄₄]Cl	30.01 \pm 0.03	30.11 \pm 0.03	13.39 \pm 0.70	
	[C ₄ mpyr]Cl	30.06 \pm 0.05	30.07 \pm 0.02	4.57 \pm 0.88	
	[C ₄ mpip]Cl	30.10 \pm 0.06	30.10 \pm 0.06	5.76 \pm 0.28	
	[C ₄ mim]Cl	30.03 \pm 0.09	30.05 \pm 0.02	5.12 \pm 1.06	
L-tyrosine	Without IL	30.10 \pm 0.06	30.10 \pm 0.06	4.85 \pm 0.35	
	[P ₄₄₄₄]Cl	30.03 \pm 0.05	30.12 \pm 0.05	7.23 \pm 0.09	
	[N ₄₄₄₄]Cl	30.01 \pm 0.03	29.99 \pm 0.03	6.99 \pm 0.36	
	[C ₄ mpyr]Cl	30.06 \pm 0.05	30.07 \pm 0.09	4.13 \pm 0.19	
	[C ₄ mpip]Cl	30.10 \pm 0.06	30.10 \pm 0.06	4.40 \pm 0.02	
	[C ₄ mim]Cl	30.03 \pm 0.09	30.05 \pm 0.10	5.12 \pm 0.36	

Table S7

Partition coefficient (K) of each alkaloid with the respective standard deviations and mass fraction compositions of the quaternary systems at 298 (± 1) K.

Biomolecule	IL in Quaternary System	Mass Fraction			K $\pm \sigma$
		Composition $\pm \sigma$ / (wt%)			
		PEG	Salt	IL	
Nicotine	[P ₄₄₄₄]Cl	30.01 \pm 0.10	30.98 \pm 0.06	5.04 \pm 0.12	7.61 \pm 1.46
	[N ₄₄₄₄]Cl	30.02 \pm 0.12	29.97 \pm 0.15	5.09 \pm 0.08	7.97 \pm 0.13
	[C ₄ mpyr]Cl	30.10 \pm 0.06	30.05 \pm 0.06	5.06 \pm 0.10	10.03 \pm 0.71
	[C ₄ mpip]Cl	30.10 \pm 0.06	30.10 \pm 0.09	5.06 \pm 0.09	9.02 \pm 1.97
	[C ₄ mim]Cl	30.04 \pm 0.14	30.08 \pm 0.02	5.09 \pm 0.08	7.16 \pm 0.52

	[P ₄₄₄₄]Cl	30.03 ± 0.05	29.99 ± 0.05	5.10 ± 0.06	8.99±0.95
	[N ₄₄₄₄]Cl	30.01 ± 0.03	30.11 ± 0.03	5.14 ± 0.31	8.28±0.77
Caffeine	[C _{4mpyr}]Cl	30.06 ± 0.05	30.07 ± 0.02	5.12 ± 0.09	11.94±0.56
	[C _{4mpip}]Cl	30.10 ± 0.06	30.10 ± 0.06	5.06 ± 0.09	10.57±1.12
	[C _{4mim}]Cl	30.13 ± 0.09	30.05 ± 0.06	5.05 ± 0.03	5.22±0.32

Table S8

Partition coefficient (K) of each alkaloid with the respective standard deviations and mass fraction compositions of the ternary systems at 298 (± 1) K.

Biomolecule	Ternary System	Mass Fraction		K ± σ
		Composition ± σ / (wt%)		
		PEG	Salt	
	Without IL	30.10 ± 0.06	30.10 ± 0.06	10.86±0.05
	[P ₄₄₄₄]Cl	30.05 ± 0.11	29.98 ± 0.06	11.67±0.36
	[N ₄₄₄₄]Cl	30.08 ± 0.12	30.07 ± 0.05	9.25±0.24
Nicotine	[C _{4mpyr}]Cl	30.10 ± 0.06	30.05 ± 0.11	8.11±0.84
	[C _{4mpip}]Cl	30.10 ± 0.06	30.10 ± 0.06	7.38±0.13
	[C _{4mim}]Cl	29.98 ± 0.14	30.08 ± 0.09	10.65±0.83
	Without IL	30.10 ± 0.06	30.10 ± 0.06	10.13±0.97
	[P ₄₄₄₄]Cl	30.03 ± 0.05	30.12 ± 0.05	13.01±1.30
	[N ₄₄₄₄]Cl	30.01 ± 0.03	30.11 ± 0.03	7.53±0.34
Caffeine	[C _{4mpyr}]Cl	30.06 ± 0.05	30.07 ± 0.02	15.41±1.84
	[C _{4mpip}]Cl	30.10 ± 0.06	30.10 ± 0.06	15.03±0.72
	[C _{4mim}]Cl	30.03 ± 0.09	30.05 ± 0.02	7.29±1.12

Table S9

Partition coefficients of each IL.

IL	K_{IL}
[P4444]Cl	4.67 ± 0.20
[N4444]Cl	5.43 ± 0.01
[C4mpyr]Cl	4.68 ± 0.16
[C4mpip]Cl	5.25 ± 0.05
[C4mim]Cl	4.01 ± 0.20