Supporting Information

Aqueous two-phase system formed by polyethylene glycol methyl ether 550 and choline-based ionic liquids: from phase diagrams to application in the extraction of proteins

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Table S1. Experimental binodal mass fraction data for the system composed of PEGME 550 (w_1) + [Ch]Cl (w_2) + water (w_3) at 298 K and 0.1 MPa.[a]

100 w_1	**100 w_2**	**100 w_3**
28.63	38.91	32.46
26.79	41.72	31.49
25.05	44.38	30.57
23.75	46.35	29.90
22.51	48.30	29.20
21.42	50.02	28.56
20.37	51.49	28.13
19.53	52.85	27.63
18.71	54.13	27.16
17.76	55.61	26.63
17.08	56.64	26.28
16.30	57.90	25.80
15.57	59.04	25.39
14.97	60.01	25.02
14.33	61.06	24.61
13.79	62.01	24.20
13.20	62.97	23.83
12.66	63.93	23.41
12.48	64.29	23.24
12.05	64.95	23.00
11.65	65.59	22.77
11.19	66.36	22.44
10.81	67.06	22.13
10.42	67.74	21.84
10.08	68.25	21.66
9.76	68.86	21.38
9.47	69.4	21.13
9.14	70.02	20.84

[a]Standard uncertainties u are u (w_1, w_2 or w_3) = 0.01 % (m/m), and expanded uncertainties for 0.98 % confidence are U(T) = 1 K and U(p) = 10 kPa.

Table S2. Experimental binodal mass fraction data for the system composed of PEGME 550 (w_1) + [Ch][DHC] (w_2) + water (w_3) at 298 K and 0.1 MPa.[a]

100 w_1	**100 w_2**	**100 w_3**
60.12	17.86	22.02
50.91	26.41	22.68
43.93	32.99	23.08
40.05	36.85	23.10
34.79	42.01	23.20
31.23	45.50	23.27
29.05	47.72	23.23
26.74	50.04	23.23
23.97	53.34	22.70
21.75	55.64	22.61
19.80	58.06	22.13
17.98	60.17	21.85
16.42	62.10	21.48

[a]Standard uncertainties u are u (w_1, w_2 or w_3) = 0.01 % (m/m), and expanded uncertainties for 0.98 % confidence are U(T) = 1 K and U(p) = 10 kPa.

Table S3. Experimental binodal mass fraction data for the system composed of PEGME 550 (w_1) + [Ch][HEPES] (w_2) + water (w_3) at 298 K and 0.1 MPa.[a]

100 w_1	**100 w_2**	**100 w_3**
46.05	32.89	21.06
35.97	43.65	20.38
29.05	51.20	19.75
23.18	58.57	18.25
20.28	61.22	18.50

[a]Standard uncertainties u are u (w_1, w_2 or w_3) = 0.01 % (m/m), and expanded uncertainties for 0.98 % confidence are U(T) = 1 K and U(p) = 10 kPa.

Table S4. Experimental binodal mass fraction data for the system composed of PEGME 550 (w_1) + [Ch][BIT] (w_2) + water (w_3) at 298.15 K and 0.1 MPa.[a]

100 w_1	**100 w_2**	**100 w_3**
63.49	5.98	30.53
58.49	8.27	33.24
54.55	11.54	33.91
50.34	14.55	35.11
45.23	18.91	35.86
42.61	22.19	35.20
39.25	25.02	35.73
35.41	30.33	34.26
34.07	31.73	34.20
32.35	33.84	33.81
29.81	37.60	32.590

[a]Standard uncertainties u are u (w_1, w_2 or w_3) = 0.01 % (m/m), and expanded uncertainties for 0.98 % confidence are U(T) = 1 K and U(p) = 10 kPa.

Table S5. Partition coefficient (K_{BSA}) and extraction efficiency on bottom phase ($EE\%_{BSA}$) for the overall systems of ATPSs composed of PEGME 550 (45 wt%) and cholinium-based ionic liquids (40 wt%) at 298 K and 0.1 MPa.

Ionic Liquid	K_{BSA}	$EE\%_{BSA}$
[Ch]Cl	0.81 ± 0.04	50.31 ± 1.30
[Ch][DHC]	0.91 ± 0.02	48.71 ± 0.10
[Ch][BIT]	0.85 ± 0.02	45.91 ± 0.60
[Ch][HEPES]	0.950 ± 0.004	42.21 ± 0.51

Table S6. Docking affinity and interacting atoms predicted by AutoDock Vina for BSA + ILs cation and anions

Compound	Affinity (kcal/mol)	Type of interaction	From	To	Distance (Å)
$[Ch]^+$	-3.5	Hydrogen Bond	Threonine44	$[Ch]^+$	2.50
Cl^-	-1.3	-	-	-	-
$[BIT]^-$	-4.8	Hydrogen Bond	AsparticAcid108		2.02
			Tyrosine147	$[BIT]^-$	2.53
					2.73
			Lysine465		2.86
			$[BIT]^-$	Valine461	3.00
				GlutamicAcid 464	2.16
					1.93
				Lysine106	2.48
$[DHC]^-$	-5.2	Electrostatic	Arginine198	$[DHC]^-$	4.14
			Arginine217		5.13
			Arginine256		5.52
		Hydrogen Bond	Arginine198		2.49
			$[DHCit]^-$	Alanine290	2.21
$[HEPES]^-$	-4.9	Electrostatic	Arginine208	$[HEPES]^-$	5.52
		Hydrogen Bond			2.83
			$[HEPES]^-$	Alanine209	3.78

Table S7. Docking affinity and interacting atoms predicted by AutoDock Vina for IgG + [Ch]Cl (cation and anion)

Compound	Affinity (kcal/mol)	Type of interaction	From	To	Distance (Å)
$[Ch]^+$	-3.5	Electrostatic	$[Ch]^+$	Aspartic Acid220	5.50
		Hydrogen Bond	Valine210	$[Ch]^+$	2.66
Cl^-	-1.1	-	-	-	-

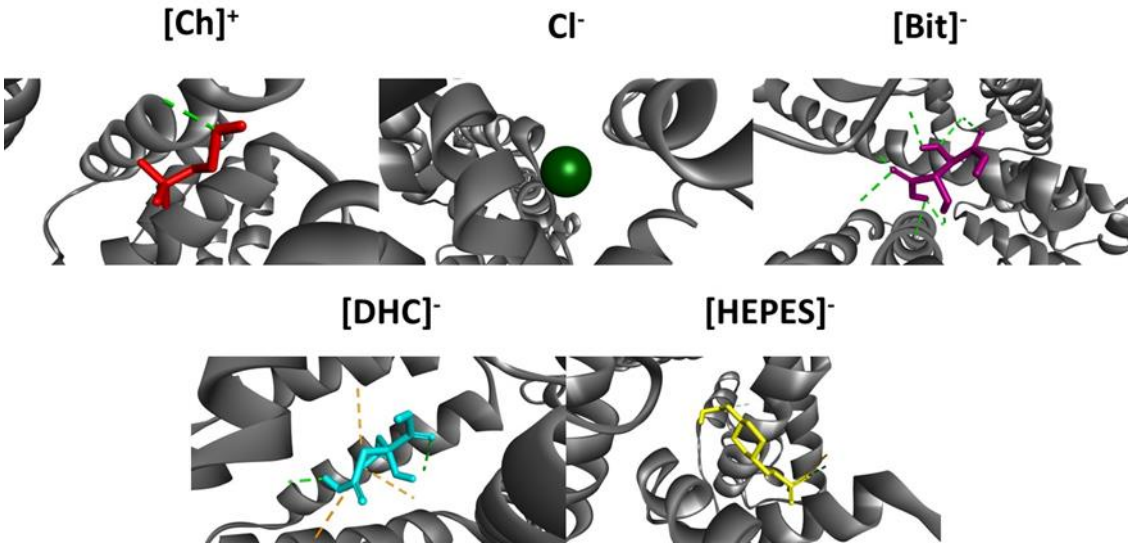

Figure S1. Docking pose with the lowest absolute value of affinity (kcal mol^{-1}) for BSA with: $[Ch]^+$ (■), Cl^- (■), $[BIT]^-$ (■), $[DHC]^-$ (■), and $[HEPES]^-$ (■).

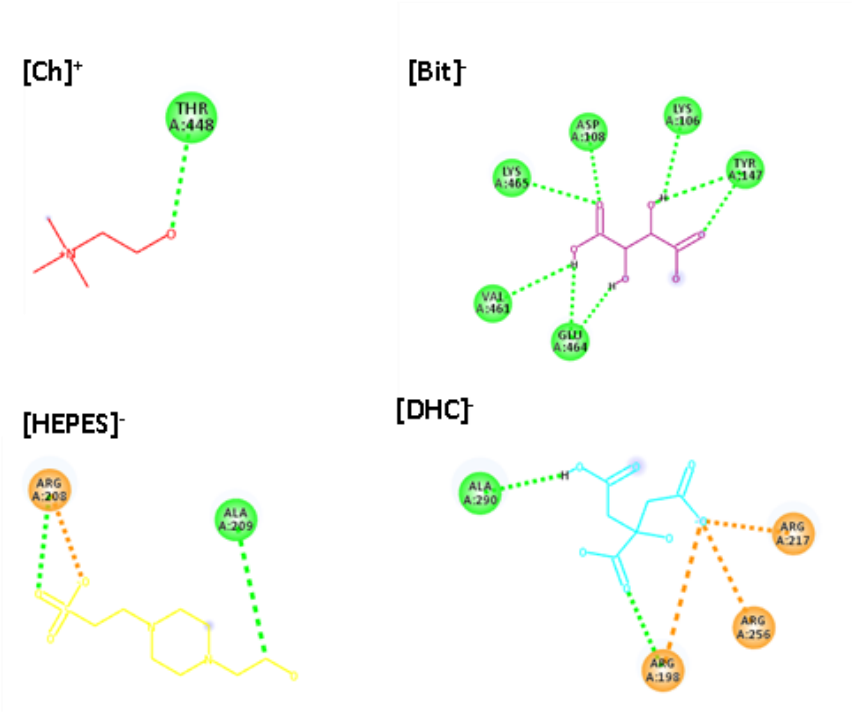

Figure S2. 3D molecular interaction diagrams of BSA with IL ions: ■ – hydrogen bond interactions; ■ – electrostatic interactions.