

# What is Better to Enhance the Solubility of Hydrophobic Compounds in Aqueous Solutions: Eutectic Solvents or Ionic Liquids?

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**Table S1** – Solubility in water of the studied solutes.

Solute	Temperature (K)	Solubility in water and standard deviation			
		This work		Literature	
		[g/kg solution]	[g/L]	[g/kg solution]	[g/L]
Benzoic acid	298.2	2.98 ± 0.17	2.97 <sup>a</sup>	-	3.34 ± 0.16 <sup>b</sup>
(S)-Hesperetin	298.2	0.0155 ± 0.0034	0.015 <sup>a</sup>	-	0.00136 <sup>1</sup> 0.001 <sup>2</sup> 0.01572 ± 0.00058 <sup>3</sup>
L-Tryptophan	303.2	-	13.65 ± 0.36	13.6 <sup>4</sup> 17.2 <sup>5</sup>	14.41 <sup>6</sup> 16.54 <sup>7</sup>

<sup>a</sup> The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

<sup>b</sup> Literature average and standard deviation of 26 data points collected from literature.<sup>8</sup>

**Table S2.** Solubility and standard deviation (*s*) of benzoic acid in aqueous solutions of [Ch]Cl:MalA (1:1), and pH of the solutions, at 298.2 K. Standard uncertainties, *u*, are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

ES concentration in solute-free weight fraction ( <i>w</i> )	Solubility (g/kg solution)	± <i>s</i> (g/kg solution)	Solubility (mol/L)*	pH
0.00	2.98	0.17	0.024	2.89
0.25	5.84	0.19	0.050	1.21
0.50	9.68	0.09	0.087	0.75
0.75	14.30	0.21	0.136	0.30
0.95	21.43	0.39	0.214	0.00

\* The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

**Table S3.** Solubility and standard deviation (*s*) of benzoic acid in aqueous solutions of [Ch]Cl:GlyA (1:1), and pH of the solutions, at 298.2 K. Standard uncertainties, *u*, are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

ES concentration in solute-free weight fraction ( <i>w</i> )	Solubility (g/kg solution)	± <i>s</i> (g/kg solution)	Solubility (mol/L)*	pH
0.00	2.98	0.17	0.024	2.89
0.25	5.13	0.21	0.044	1.72
0.50	9.08	0.16	0.081	1.39
0.75	15.76	0.76	0.147	1.09
0.95	34.46	2.06	0.335	0.50

\* The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

**Table S4.** Solubility and standard deviation (*s*) of benzoic acid in aqueous solutions of [Chol][Mal], and pH of the solutions, at 298.2 K. Standard uncertainties, *u*, are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

IL concentration in solute-free weight fraction ( <i>w</i> )	Solubility (g/kg solution)	± <i>s</i> (g/kg solution)	Solubility (mol/L)*	pH
0.00	2.98	0.17	0.024	2.89
0.25	10.6	0.06	0.090	3.99
0.50	27.6	0.14	0.248	4.44
0.75	71.7	2.11	0.679	5.21
0.99	187.2	6.86	1.877	5.52

\* The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

**Table S5.** Solubility and standard deviation ( $s$ ) of benzoic acid in aqueous solutions of [Chol][Gly], and pH of the solutions, at 298.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

IL concentration in solute-free weight fraction ( $w$ )	Solubility (g/kg solution)	$\pm s$ (g/kg solution)	Solubility (mol/L)*	pH
0.00	2.98	0.17	0.024	2.89
0.25	15.8	1.31	0.134	4.56
0.49	43.4	1.84	0.387	5.04
0.75	249.9	3.38	2.405	5.39
0.99	289.3	6.46	2.895	-

\* The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

**Table S6.** Solubility and standard deviation ( $s$ ) of hesperetin in aqueous solutions of [Ch]Cl:MaIA (1:1), and pH of the solutions, at 298.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

ES concentration in solute-free weight fraction ( $w$ )	Solubility (g/kg solution)	$\pm s$ (g/kg solution)	Solubility (mol/L)*	pH
0.00	0.0155	0.0034	5.10E-05	6.05
0.25	0.047	0.006	1.64E-04	1.10
0.50	0.356	0.004	1.29E-03	0.79
0.75	1.424	0.029	5.47E-03	0.29
0.95	5.238	0.226	2.11E-02	0.00

\* The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

**Table S7.** Solubility and standard deviation ( $s$ ) of hesperetin in aqueous solutions of [Ch]Cl:GlyA (1:1), and pH of the solutions, at 298.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

ES concentration in solute-free weight fraction ( $w$ )	Solubility (g/kg solution)	$\pm s$ (g/kg solution)	Solubility (mol/L)*	pH
0.00	0.0155	0.0034	5.10E-05	6.05
0.25	0.040	0.001	1.37E-04	1.71
0.50	0.270	0.020	9.72E-04	1.37
0.75	1.382	0.080	5.21E-03	1.22
0.94	10.07	1.49	3.94E-02	0.58

\* The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

**Table S8.** Solubility and standard deviation ( $s$ ) of hesperetin in aqueous solutions of [Chol][Mal], and pH of the solutions, at 298.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

IL concentration in solute-free weight fraction ( $w$ )	Solubility (g/kg solution)	$\pm s$ (g/kg solution)	Solubility (mol/L)*	pH
0	0.0155	0.0034	5.10E-05	6.05
0.25	0.059	0.007	2.04E-04	4.07
0.50	0.720	0.015	2.60E-03	4.53
0.75	8.759	0.159	3.33E-02	5.48
0.99	18.10	0.38	7.23E-02	6.86

\* The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

**Table S9.** Solubility and standard deviation ( $s$ ) of hesperetin in aqueous solutions of [Chol][Gly], and pH of the solutions, at 298.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

IL concentration in solute-free weight fraction ( $w$ )	Solubility (g/kg solution)	$\pm s$ (g/kg solution)	Solubility (mol/L)*	pH
0.00	0.0155	0.0034	5.10E-05	6.05
0.25	0.026	0.006	8.93E-05	4.68
0.49	0.289	0.036	1.04E-03	5.32
0.75	1.429	0.022	5.36E-03	6.66
0.99	8.46	0.52	3.33E-02	-

\* The units conversion from [g/kg solution] to [g/L] was calculated considering ideal solution.

**Table S10.** Solubility and standard deviation ( $s$ ) of tryptophan in aqueous solutions of [Ch]Cl:MalA (1:1), and pH of the solutions, at 303.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

ES concentration in solute-free weight fraction ( $w$ )	Solubility (g/L)	$\pm s$ (g/L)	Solubility (mol/L)	pH
0.00	13.65	0.40	0.0668	6.41
0.10	50.6	2.3	0.248	2.16
0.20	77.7	2.8	0.381	2.18
0.30	80.1	4.1	0.392	2.09
0.40	89.4	5.6	0.438	1.97
0.50	93.3	4.9	0.457	1.87
0.60	95.9	3.0	0.470	1.80
0.70	90.4	7.5	0.443	1.73

**Table S11.** Solubility and standard deviation ( $s$ ) of tryptophan in aqueous solutions of [Ch]Cl:GlyA (1:1), and pH of the solutions, at 303.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

ES concentration in solute-free weight fraction ( $w$ )	Solubility (g/L)	$\pm s$ (g/L)	Solubility (mol/L)	pH
0.00	13.65	0.40	0.0668	6.41
0.10	34.6	0.3	0.169	2.40
0.20	55.6	2.9	0.272	2.35
0.30	73.0	9.6	0.357	2.42
0.40	93.1	7.9	0.456	2.59
0.50	94.8	5.1	0.464	2.64
0.60	90.0	3.0	0.441	2.68
0.70	79.0	2.7	0.387	2.53

**Table S12.** Solubility and standard deviation ( $s$ ) of tryptophan in aqueous solutions of [Chol][Mal], and pH of the solutions, at 303.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

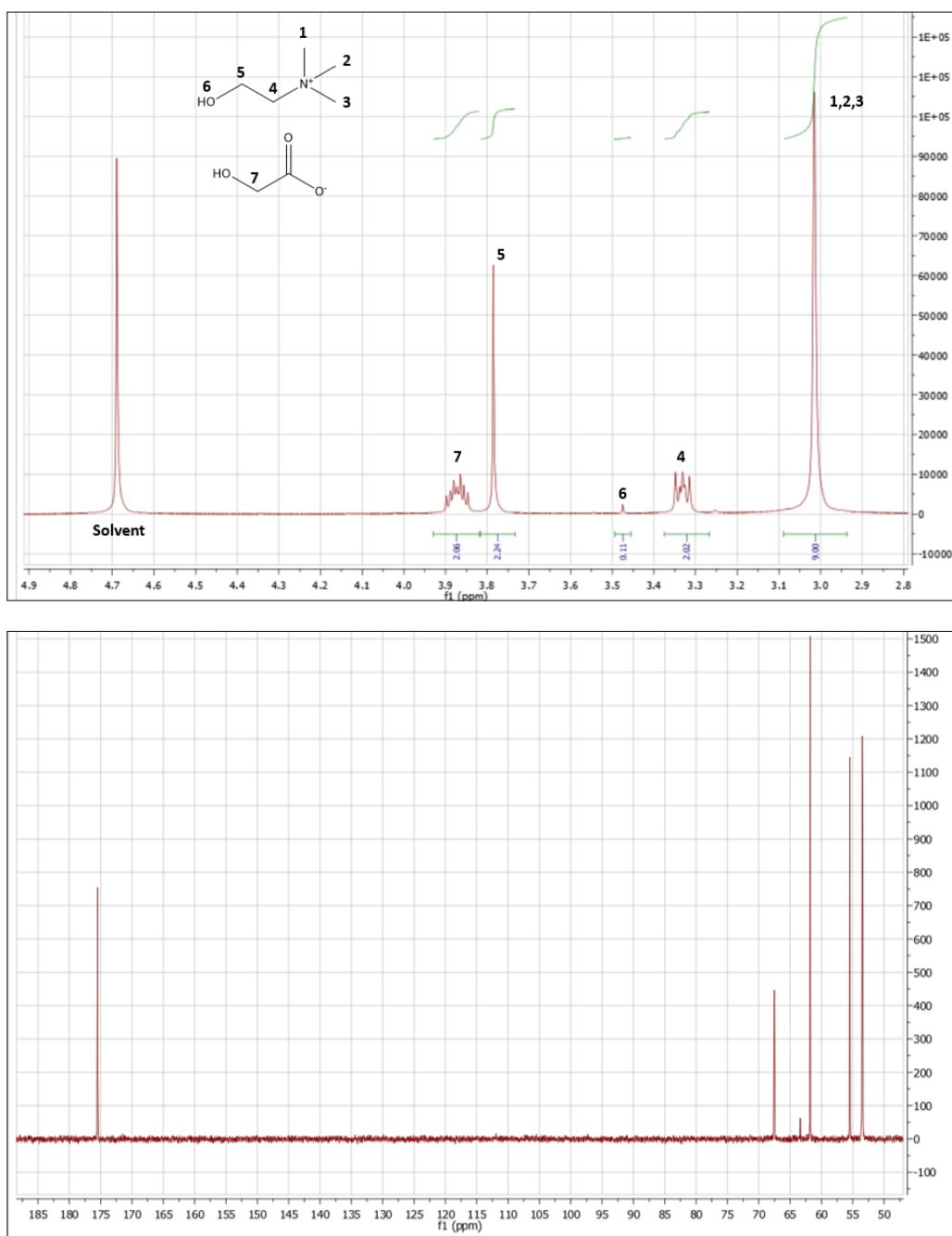
IL concentration in solute-free weight fraction ( $w$ )	Solubility (g/L)	$\pm s$ (g/L)	Solubility (mol/L)	pH
0.00	13.65	0.40	0.0668	6.41
0.10	23.2	0.1	0.113	4.05
0.20	32.8	0.0	0.160	4.15
0.30	43.3	0.1	0.212	4.31
0.40	49.9	0.1	0.244	4.47
0.50	54.8	2.3	0.268	5.10
0.60	54.2	0.1	0.265	4.97
0.70	56.6	1.0	0.277	5.80
0.80	64.9	7.2	0.318	6.32

**Table S13.** Solubility and standard deviation ( $s$ ) of tryptophan in aqueous solutions of [Chol][Gly], and pH of the solutions, at 303.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

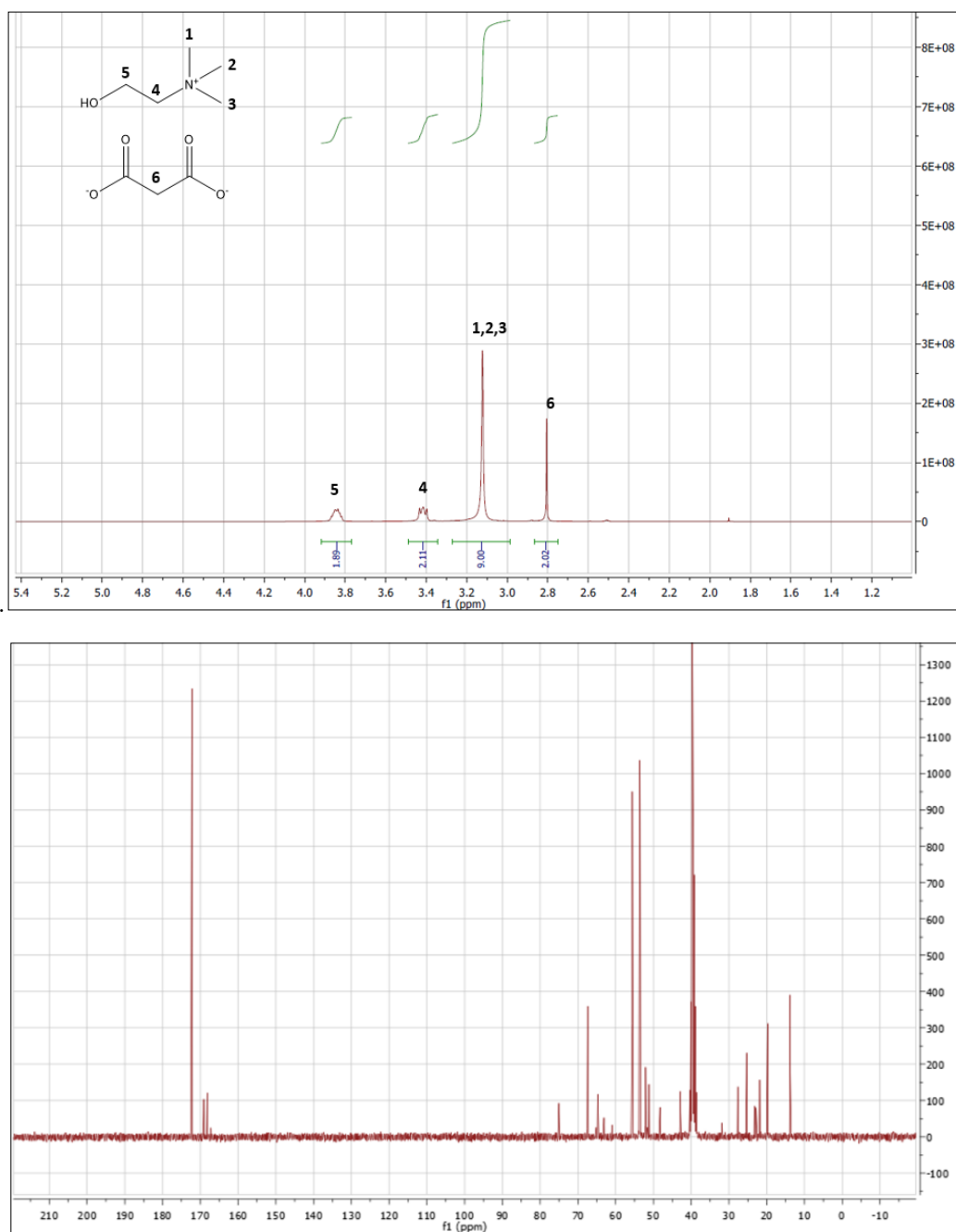
IL concentration in solute-free weight fraction ( $w$ )	Solubility (g/L)	$\pm s$ (g/L)	Solubility (mol/L)	pH
0.00	13.65	0.40	0.0668	6.41
0.10	20.4	0.03	0.100	4.44
0.20	25.1	0.02	0.123	4.56
0.30	30.6	0.2	0.150	4.73
0.40	35.4	0.1	0.173	4.93
0.50	39.6	0.1	0.194	5.26
0.60	44.9	3.7	0.220	5.63
0.70	56.3	4.7	0.276	6.04

**Table S14.** pH of the aqueous solutions of the ES and IL studied in this work, measured at 303.2 K. Standard uncertainties,  $u$ , are  $u_r(p) = 0.05$ ,  $u(w) = 0.01$  and  $u(\text{pH}) = 0.05$ .

[Chol][Gly]		[Chol][Mal]		[Ch]Cl:GlyA		[Ch]Cl:MalA	
$w_{\text{IL}}$	pH	$w_{\text{IL}}$	pH	$w_{\text{ES}}$	pH	$w_{\text{ES}}$	pH
0.10	4.51	0.10	4.07	0.11	1.74	0.10	1.47
0.20	4.60	0.21	4.16	0.20	1.51	0.21	1.23
0.30	4.79	0.31	4.24	0.32	1.39	0.31	1.01
0.40	5.01	0.41	4.47	0.41	1.28	0.41	0.86
0.50	5.26	0.50	4.69	0.51	1.19	0.50	0.71
0.60	5.69	0.60	4.96	0.59	0.97	0.60	0.45
0.70	6.26	0.70	5.27	0.71	0.89	0.70	0.27
0.80	6.85	0.80	5.89	0.81	0.75	0.80	0.06
0.89	7.51	0.90	6.46	0.90	0.69	0.90	-0.34



**Figure S1.** <sup>1</sup>H and <sup>13</sup>C-NMR spectra of choline glycolate in D<sub>2</sub>O as solvent.



**Figure S2.** <sup>1</sup>H and <sup>13</sup>C-NMR spectra of choline malonate in DMSO as solvent.

## References

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