Electronic Supplementary Information

Recovery of ibuprofen from pharmaceutical wastes using ionic liquids

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Table S.1 Detailed extraction efficiency of ibuprofen data acquired during the initial screening aimed at finding the optimal IL.

IL	100 ω mass fraction composition (wt%)			EE_{IBU} ± σ/ (%)
	IL	Citrate buffer salt	H_2O	
[BzCh]Cl	45	0	55	11.58 ± 0.63
	45	5	50	93.73 ± 1.62
[C_4mim]Cl	45	0	55	17.94 ± 1.20
	45	5	50	90.41 ± 0.50
[N_{4444}]Cl	45	0	55	93.53 ± 0.62
	45	5	50	97.92 ± 2.65

Table S.2 Detailed extraction efficiency of ibuprofen data acquired during the optimization studies aimed at gauging the balance between the $[N_{4444}]Cl$ and citrate buffer salt concentrations.

100 ω mass fraction composition (wt%)			EE_{IBU} ± σ/ (%)
$[N_{4444}]Cl$	Citrate buffer salt	H_2O	
0	0	100	1.69 ± 0.03
15	0	85	2.40 ± 0.02
25	0	75	7.20 ± 0.19
35	0	65	61.12 ± 0.57
45	0	55	93.53 ± 0.62
50	0	50	91.78 ± 3.82
55	0	45	98.49 ± 0.40
0	5	95	16.59 ± 0.57
0	15	85	4.70 ± 0.29
0	25	75	2.51 ± 0.04
0	35	65	0.69 ± 0.11
15	5	80	13.66 ± 0.80
25	5	70	47.55 ± 0.76
35	5	60	88.80 ± 0.45
45	5	50	97.92 ± 2.65
25	10	65	79.52 ± 1.60
10	25	65	12.95 ± 0.76
15	15	70	19.34 ± 1.01
5	15	80	3.53 ± 0.10

Table S.3 Experimental data of recovery efficiency of ibuprofen acquired during the ibuprofen recovery step through precipitation with an anti-solvent.

extract : anti-solvent	**RE_{IBU} ± σ /(%)**	
	45 wt% $[N_{4444}]Cl$ + 5 wt% citrate buffer + 50 wt% H_2O	**45 wt% $[N_{4444}]Cl$ + 55 wt% H_2O**
Anti-solvent: 25 wt% of KCl aqueous solution		
1:1	13.53 ± 0.86	60.94 ± 2.41
1:2	58.40 ± 2.57	85.79 ± 0.29
1:3	75.08 ± 0.53	94.04 ± 0.49
1:4	84.53 ± 1.26	96.00 ± 0.15
1:5	87.97 ± 1.00	97.07 ± 0.14
Anti-solvent: H_2O		
1:1	22.37 ± 2.46	86.11 ± 0.72
1:2	33.71 ± 2.32	90.45 ± 0.13
1:3	34.71 ± 4.00	91.60 ± 0.19
1:4	28.31 ± 0.45	89.17 ± 0.30
1:5	26.72 ± 5.45	88.09 ± 0.17

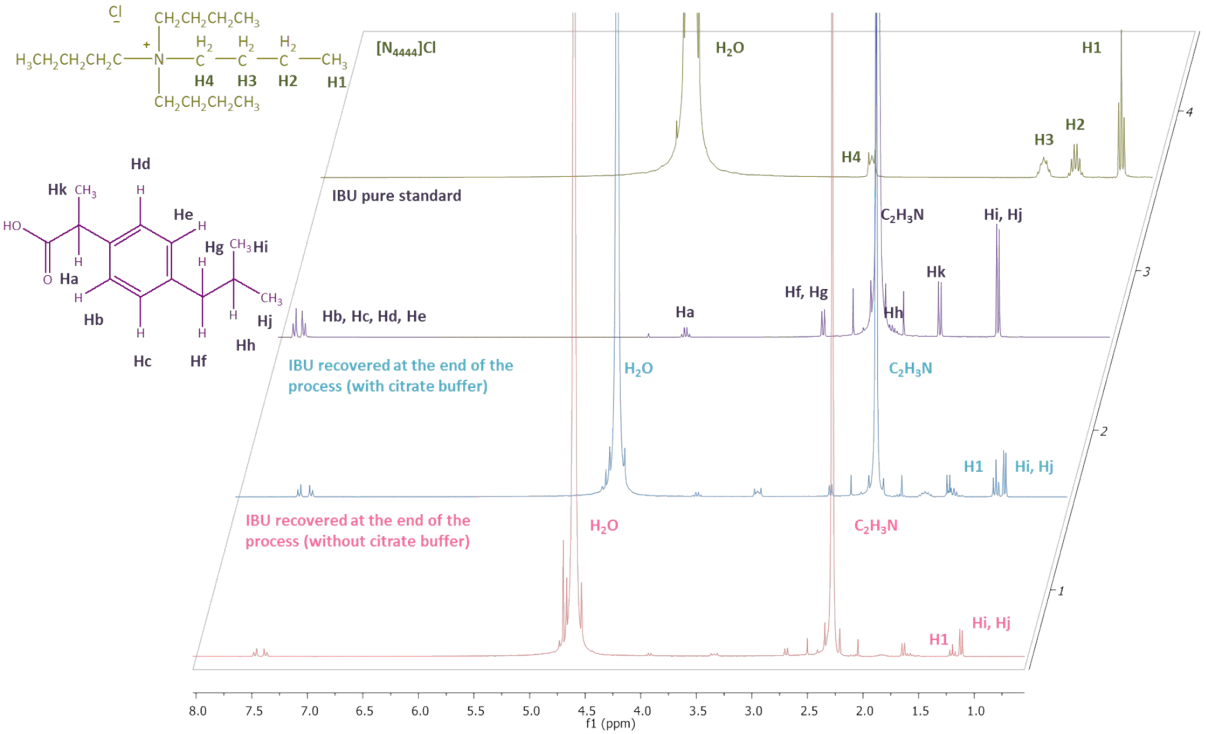

Fig. S.1 ^{1}H NMR spectra for ibuprofen recovered from the 45 wt% $[N_{4444}]Cl$ aqueous solution after the addition of water in a ratio of 1:3 in a 50:50 H_2O:C_2H_3N mixture (1), 45 wt% $[N_{4444}]Cl$ + 5 wt% citrate buffer aqueous solution after the addition of KCl aqueous solution in a ratio of 1:4 in a 50:50 H_2O:C_2H_3N mixture (2), ibuprofen pure standard from Sigma in C_2H_3N (3) and $[N_{4444}]Cl$ in H_2O (4). A Bruker Avance 300 spectrometer operating at 300.13 MHz was used for this purpose, utilizing appropriate tubes containing closed reference capillaries with D_2O and TSP as the internal reference. Ibuprofen and $[N_{4444}]Cl$ atom labelling are also provided.

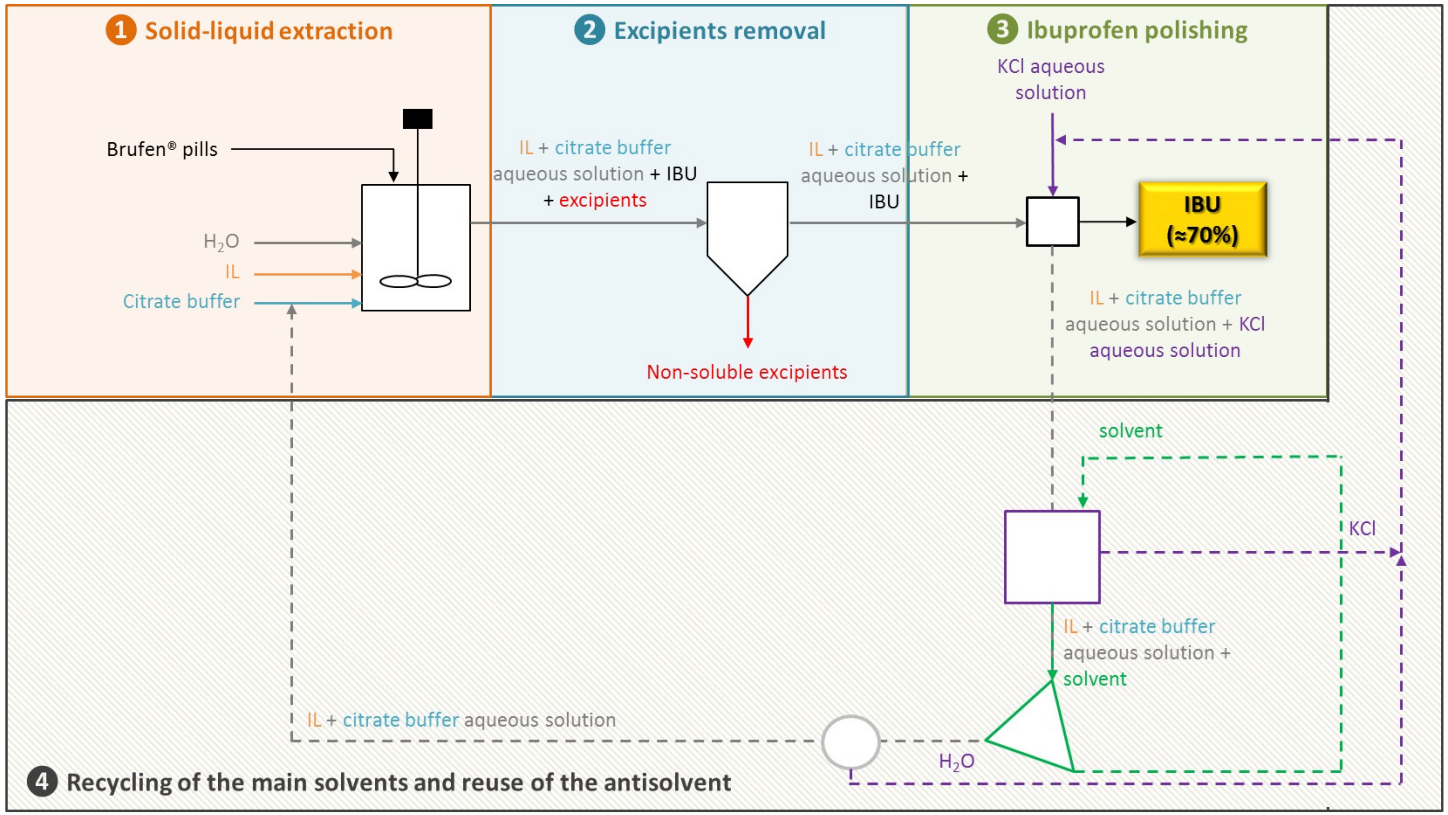

Fig. S.2 Schematic representation of the integrated process of extraction, purification, ibuprofen recovery and recycling of the main solvents based on the use of $[N_{4444}]Cl$ + citrate buffer aqueous solution and KCl as the solvent and anti-solvent, respectively. The purple square represents the removal of KCl in solution, the green square consists on the separation of the solvent used in the KCl removal and the grey circle is the evaporation of the extra amount of water added together with KCl as anti-solvent.