

Electronic Supplementary Information

"Solvent effect on a model $S_{N}Ar$ reaction in ionic liquid/water

mixtures at different compositions"

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Table S1. Kinetic data for the reaction between phenyl 2,4,6 trinitrophenyl ether and piperidine at 25°C on a mixture of BMIMBF₄/H₂O at a molar fraction of BMIMBF₄ of 0,030.

Concentration of Piperidine (M)	k_{obs} (s ⁻¹)	$k_{obs}/[Pip]$ (M ⁻¹ s ⁻¹)
0,0030	0,0014	0,4572
0,0051	0,0075	1,4842
0,0096	0,0320	3,3333
0,0116	0,0608	5,2414
0,0137	0,0740	5,4015
0,0162	0,1420	8,7654
0,0192	0,2220	11,5625

Table S2. Kinetic data for the reaction between phenyl 2,4,6 trinitrophenyl ether and piperidine at 25°C on a mixture of BMIMBF₄/H₂O at a molar fraction of BMIMBF₄ of 0,086.

Concentration of Piperidine (M)	k_{obs} (s ⁻¹)	$k_{obs}/[Pip]$ (M ⁻¹ s ⁻¹)
0,0030	0,0036	1,1809
0,0051	0,0128	2,5296
0,0076	0,0364	4,7895
0,0096	0,0597	6,2186
0,0101	0,0743	7,3564
0,0109	0,0701	6,4312
0,0121	0,0949	7,8430

Table S3. Kinetic data for the reaction between 2,4,6 trinitrophenyl phenyl ether and piperidine at 25°C on a mixture of BMIMBF₄/H₂O at a molar fraction of BMIMBF₄ of 0,15.

Concentration of Piperidine (M)	k_{obs} (s ⁻¹)	$k_{obs}/[Pip]$ (M ⁻¹ s ⁻¹)
0,0025	0,0020	0,79
0,0038	0,0065	1,71
0,0051	0,0120	2,37
0,0076	0,0450	5,93
0,0089	0,0610	6,89
0,0102	0,0810	8,02

Table S4. Kinetic data for the reaction between phenyl 2,4,6 trinitrophenyl ether and piperidine at 25°C on a mixture of BMIMBF₄/H₂O at a molar fraction of BMIMBF₄ of 0,220.

Concentration of Piperidine (M)	k_{obs} (s ⁻¹)	$k_{obs}/[Pip]$ (M ⁻¹ s ⁻¹)
0,0030	0,0156	5,1316
0,0051	0,0345	6,8182
0,0063	0,0578	9,219
0,0076	0,0918	12,0790
0,0096	0,1160	12,0833
0,0116	0,1820	15,6897

0,0137	0,2360	17,2263
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Table S5. Kinetic data for the reaction between 2,4,6 trinitrophenyl phenyl ether and piperidine at 25°C on a mixture of BMIMBF₄/H₂O at a molar fraction of BMIMBF₄ of 0,54.

Concentration of Piperidine (M)	k_{obs} (s⁻¹)	$k_{obs}/[Pip]$ (M⁻¹s⁻¹)
0,0025	0,0018	0,71
0,0038	0,0058	1,53
0,0051	0,0150	2,96
0,0076	0,0550	7,25
0,0089	0,0740	8,35
0,0100	0,0880	8,71

Table S6. Kinetic data for the reaction between 2,4,6 trinitrophenyl phenyl ether and piperidine at 25°C on a mixture of BMIMBF₄/H₂O at a molar fraction of BMIMBF₄ of 0,79.

Concentration of Piperidine (M)	k_{obs} (s⁻¹) · 10³	$k_{obs}/[Pip]$ (M⁻¹s⁻¹)
0,0025	1,9	0,75
0,0038	6,2	1,62
0,0051	13,5	2,67
0,0076	54,0	7,11
0,0886	77,5	8,75
0,0102	88,5	8,76

Table S7. Kinetic data for the reaction between phenyl 2,4,6 trinitrophenyl ether and piperidine at 25°C on BMIMBF₄.

Concentration of Piperidine (M)	k_{obs} (s⁻¹)	$k_{obs}/[Pip]$ (M⁻¹s⁻¹)
0,0004	0,0004	0,8950
0,0007	0,0008	1,1571
0,0010	0,0016	1,5900
0,0020	0,0006	3,0800
0,0030	0,0091	3,0167
0,0050	0,0352	7,0400
0,0060	0,0484	8,0667

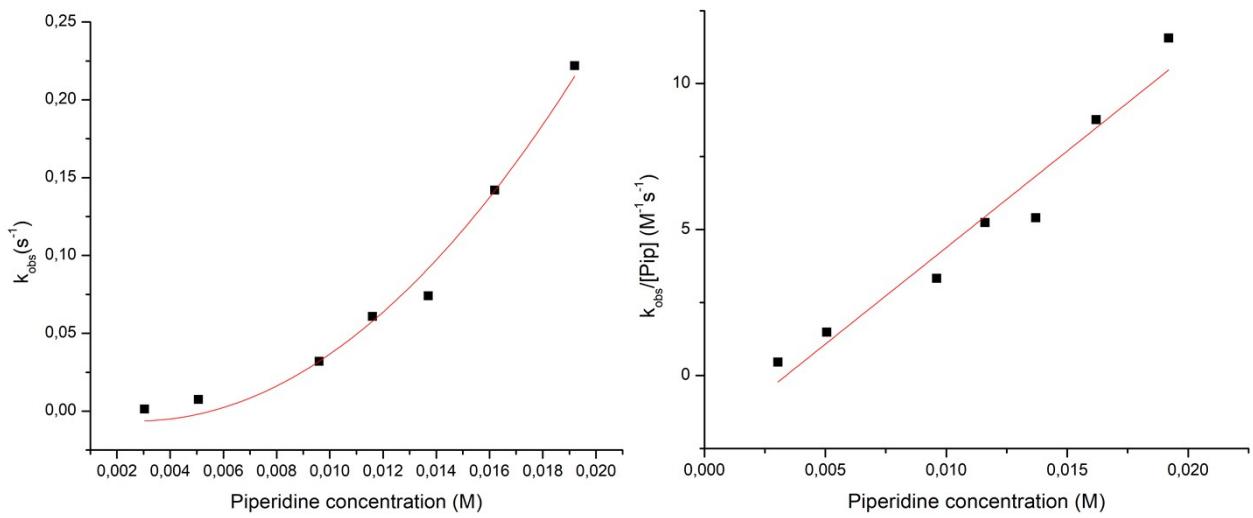


Figure S1. Graph showing the relationship between the concentration of nucleophile and the kinetic rate constant at a molar fraction of BMIMBF_4 of $\chi=0,030$; fitted using the equation 2(left) and the concentration of nucleophile vs the kinetic rate constant over the concentration of nucleophile fitted by a linear regression(right).

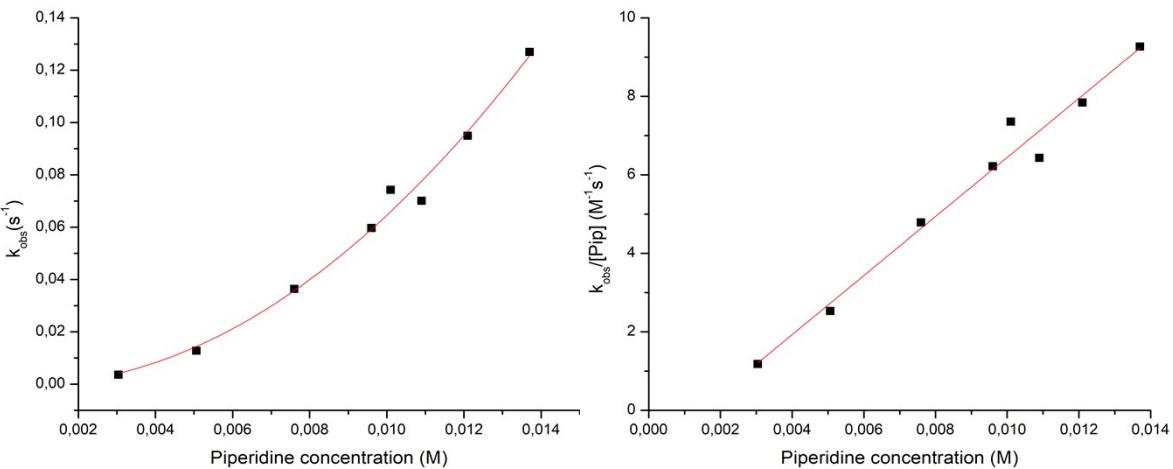


Figure S2. Graph showing the relationship between the concentration of nucleophile and the kinetic rate constant at a molar fraction of BMIMBF_4 of $\chi=0,086$; fitted using the equation 2(left) and the concentration of nucleophile vs the kinetic rate constant over the concentration of nucleophile fitted by a linear regression(right).

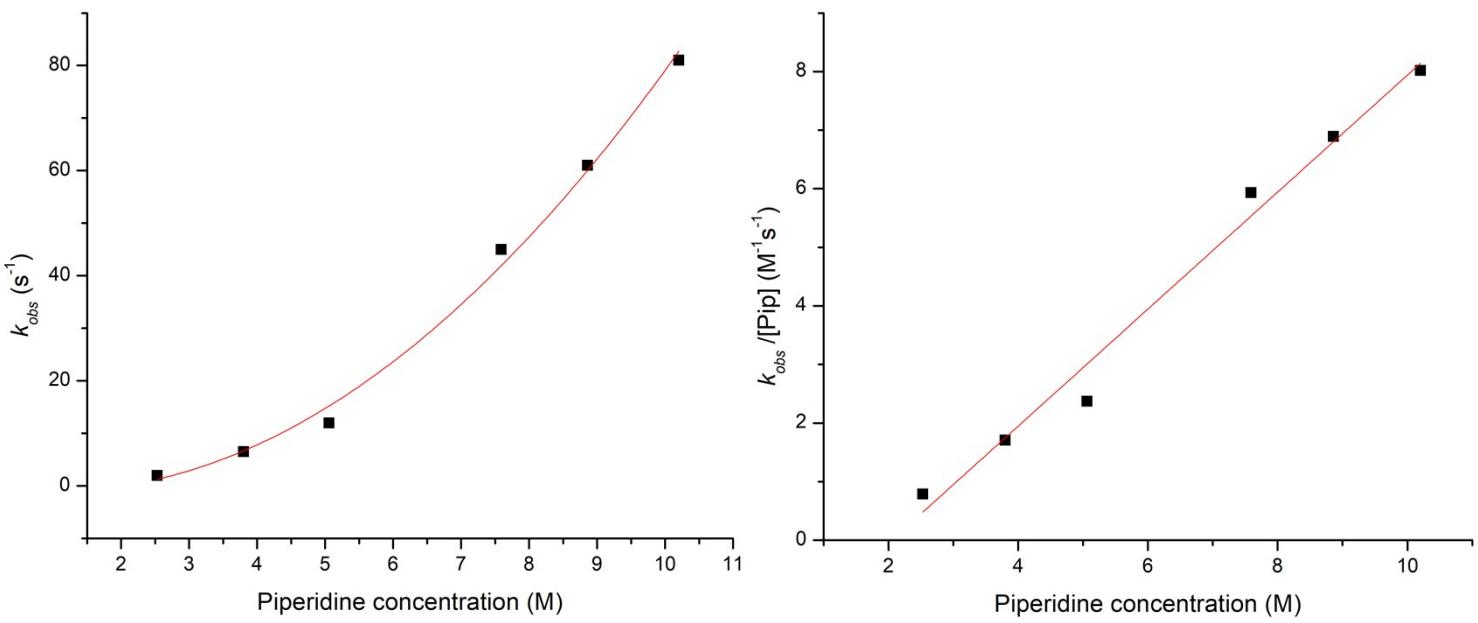


Figure S3. Graph showing the relationship between the concentration of nucleophile and the kinetic rate constant at a molar fraction of BMIMBF₄ of $\chi=0,15$; fitted using the equation 2(left) and the concentration of nucleophile vs the kinetic rate constant over the concentration of nucleophile fitted by a linear regression(right).

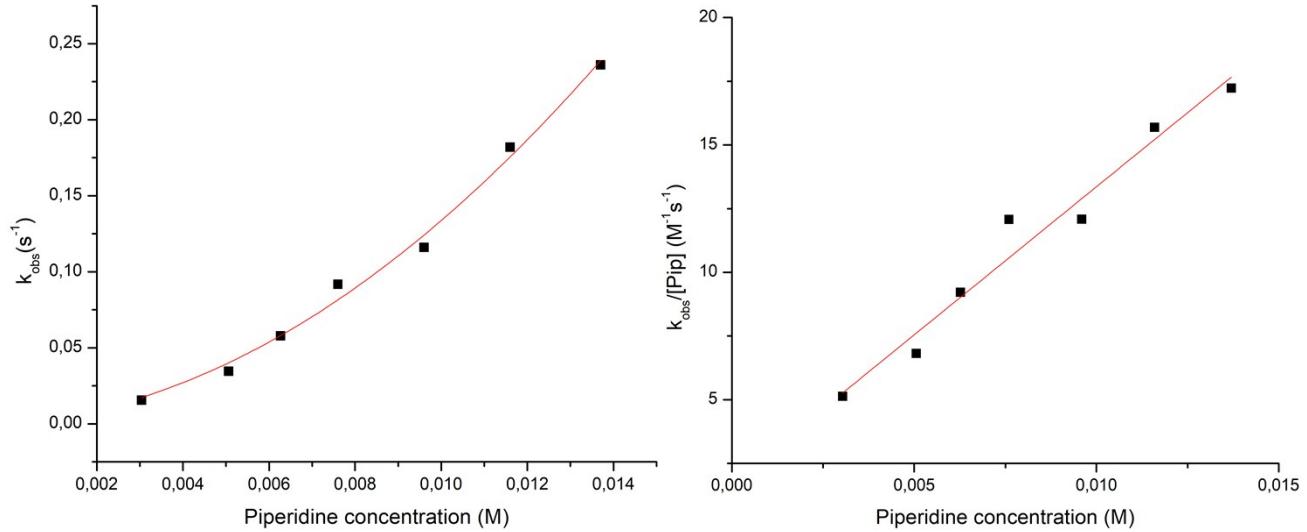


Figure S4. Graph showing the relationship between the concentration of nucleophile and the kinetic rate constant at a molar fraction of BMIMBF₄ of $\chi=0,22$; fitted using the equation 2(left) and the concentration of nucleophile vs the kinetic rate constant over the concentration of nucleophile fitted by a linear regression(right).

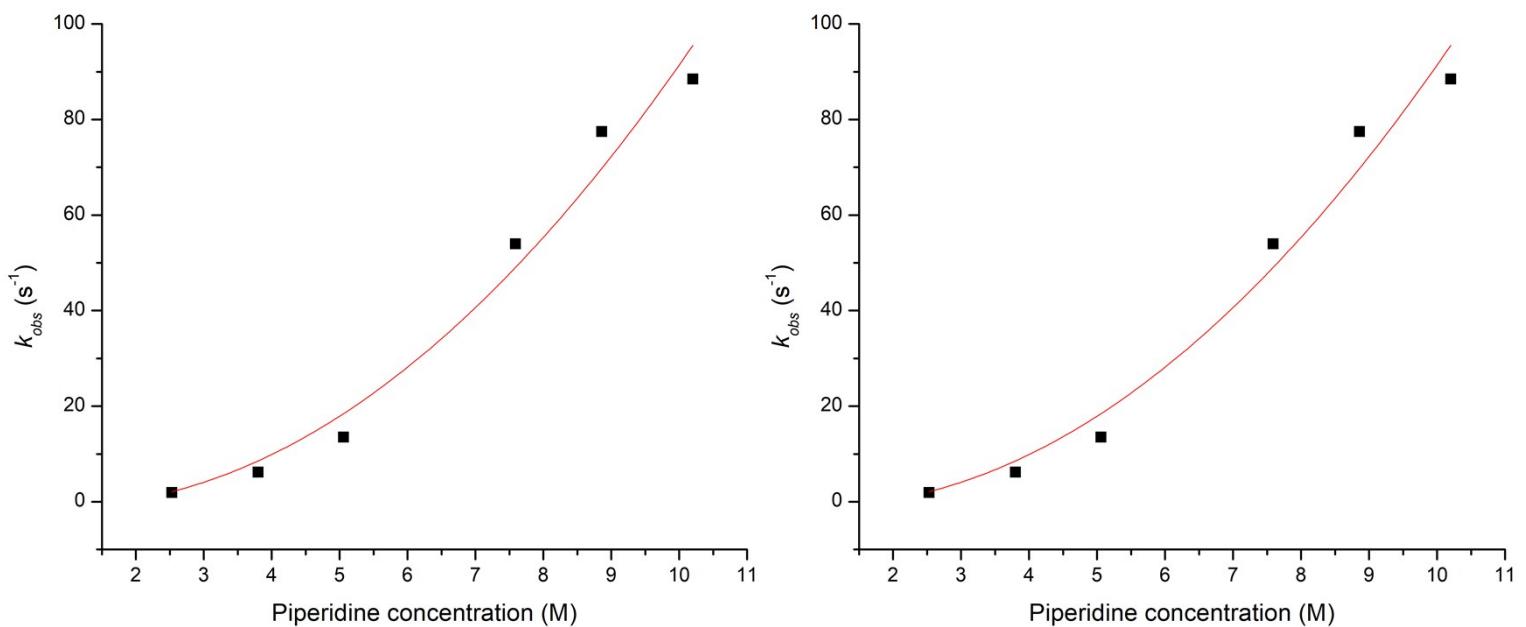
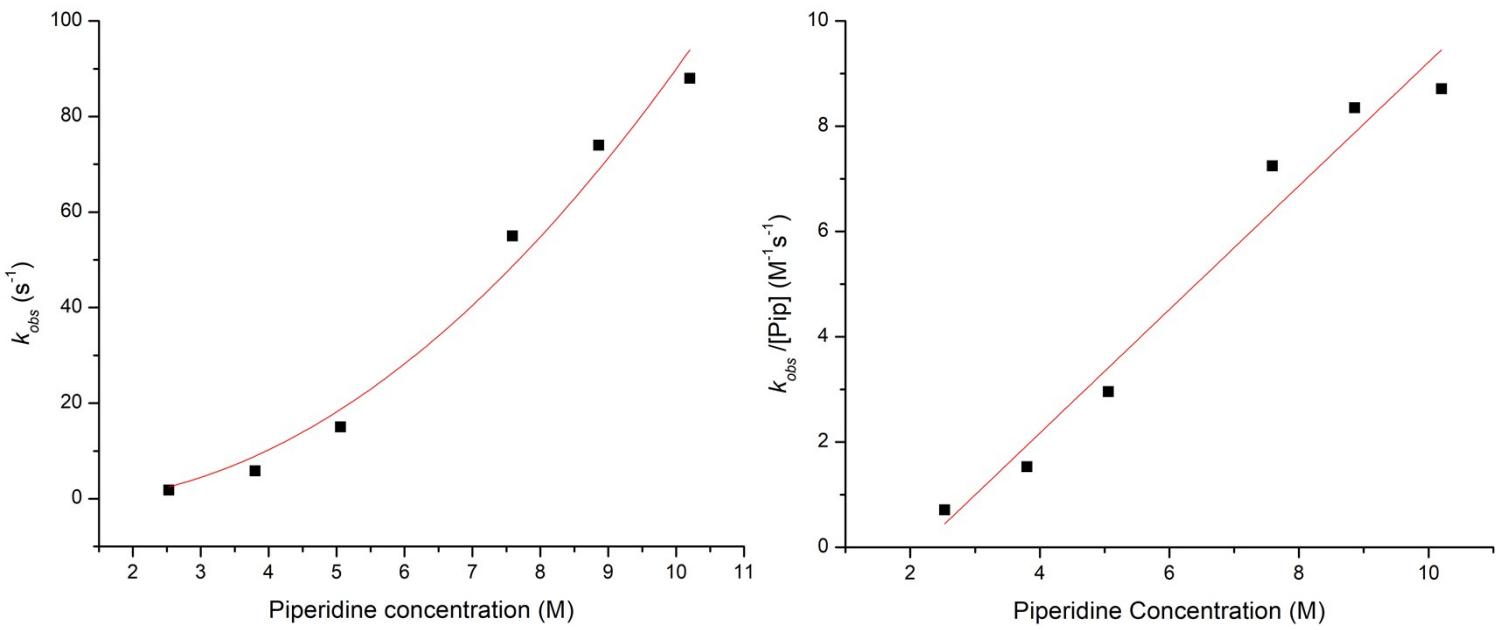


Figure S6. Graph showing the relationship between the concentration of nucleophile and the kinetic rate constant at a molar fraction of BMIMBF₄ of $\chi=0,79$; fitted using the equation 2(left)

and the concentration of nucleophile vs the kinetic rate constant over the concentration of nucleophile fitted by a linear regression(right).

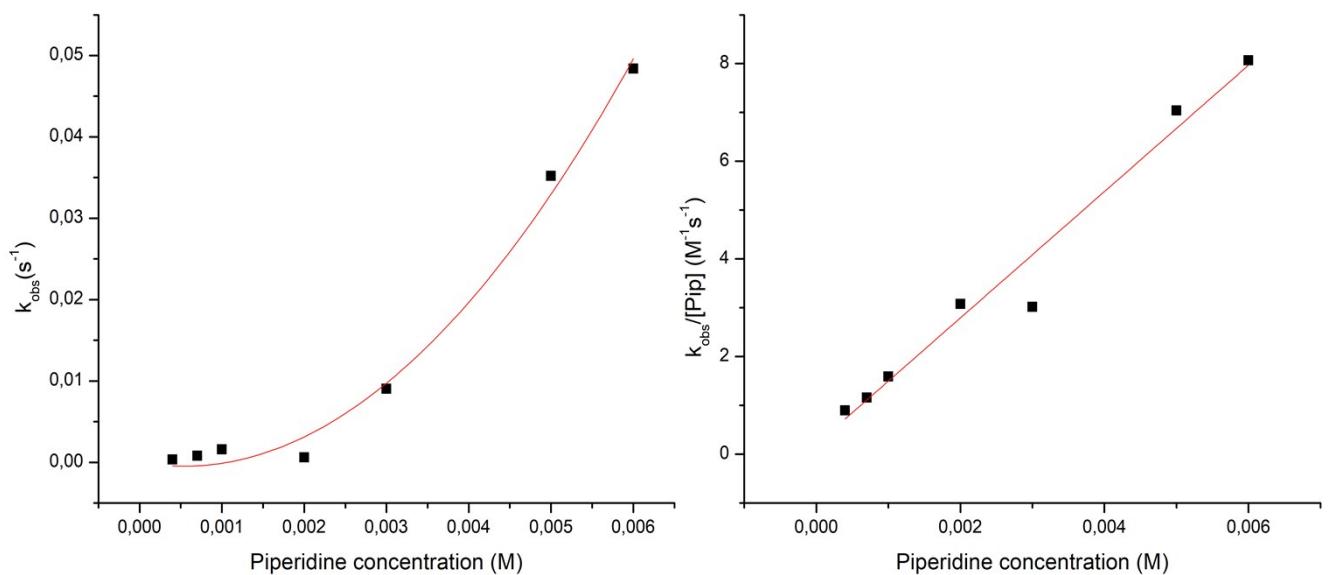


Figure S7. Graph showing the relationship between the concentration of nucleophile and the kinetic rate constant on BMIMBF₄; fitted using the equation 2(left) and the concentration of nucleophile vs the kinetic rate constant over the concentration of nucleophile fitted by a linear regression(right).

Table S8. Weight of water and BMIMBF₄ used for each composition of mixtures and its absorbance value for p-nitroaniline and N,N-diethyl-p-nitroaniline required to determine the KT β parameter.

Masa Agua (g)	Masa BMIMBF ₄ (g)	$\chi_{\text{BMIMBF}4}$	$\lambda_{\text{p-Nitroanilina}}$	$\lambda_{\text{N,N dietil-p-}}\text{nitróanilina}$	β
-	-	0,000	374,0	429,0	0,010
0,573	4,435	0,010	378,5	429,0	0,123
1,013	3,982	0,020	378,5	427,0	0,164
1,405	3,602	0,030	378,5	425,0	0,205
1,716	3,281	0,040	378,0	423,5	0,223
1,991	3,012	0,050	377,5	422,0	0,241
2,421	2,580	0,070	377,0	421,0	0,250
2,646	2,408	0,081	376,5	420,5	0,248
2,766	2,242	0,090	376,5	420,0	0,258
2,915	2,004	0,104	376,5	419,5	0,269
3,448	1,566	0,149	375,5	418,0	0,275
3,803	1,227	0,198	375,0	417,5	0,273
4,046	0,966	0,250	375,5	416,0	0,317
4,238	0,784	0,301	375,5	415,5	0,328
4,383	0,642	0,352	374,0	413,5	0,333
4,460	0,538	0,398	374,0	413,5	0,333
4,626	0,368	0,500	373,0	412,5	0,329
4,775	0,255	0,599	374,0	413,5	0,333
4,836	0,164	0,701	372,5	411,0	0,349
4,873	0,125	0,756	372,0	410,0	0,358
4,947	0,093	0,810	372,0	410,0	0,358
4,955	0,044	0,900	372,0	409,5	0,369
4,980	0,028	0,934	371,5	409,5	0,356
-	-	1,000	370,5	407,0	0,386

Table S9. Fluorescence data of pyrene incorporated in different Bmim⁺ BF₄⁻/water mixtures

Bmim ⁺ BF ₄ ⁻ Molar Fraction	Band I intensity	Band III intensity	I/III
0.000	145.3	96.6	1.50
0.001	186.2	124.0	1.50
0.002	187.5	122.1	1.54
0.003	203.0	130.5	1.56
0.004	203.4	132.3	1.54
0.005	199.5	129.9	1.54
0.006	200.5	130.9	1.53
0.007	208.5	139.7	1.49
0.008	263.4	171.5	1.54
0.009	209.5	135.2	1.55
0.011	202.8	133.5	1.52
0.017	235.5	160.9	1.46
0.023	246.1	166.8	1.48
0.031	321.6	213.5	1.51
0.049	346.4	238.0	1.46
0.060	316.0	237.0	1.33
0.073	349.0	266.0	1.31
0.087	336.0	259.0	1.30
0.125	335.0	267.0	1.26
0.182	383.0	300.0	1.28
0.277	407.0	332.0	1.23
0.462	433.0	373.0	1.16
1.000	471.0	412.0	1.14

Table S10. Coumarin C343 absorption maxima at different probe/ NaBF_4 ratios in aqueous solutions

Coumarin/ NaBF_4	Max. Absorption wavelength (nm)
0.06	457
0.1	456
1.1	458
1.8	454
18.5	449
37	445
184.9	442
Water	441
$\text{Bmim}^+\text{BF}_4^-$	457

Table S11. Coumarin 343 maximum absorption wavelength in water/ BmimBF_4 mixtures

BmimBF_4 (% w/w)	Max. Absorption wavelength (nm)
100	457
90	455
80	455
70	456
60	456
50	456
40	456
30	456
20	457
10	456
5	455
2	454

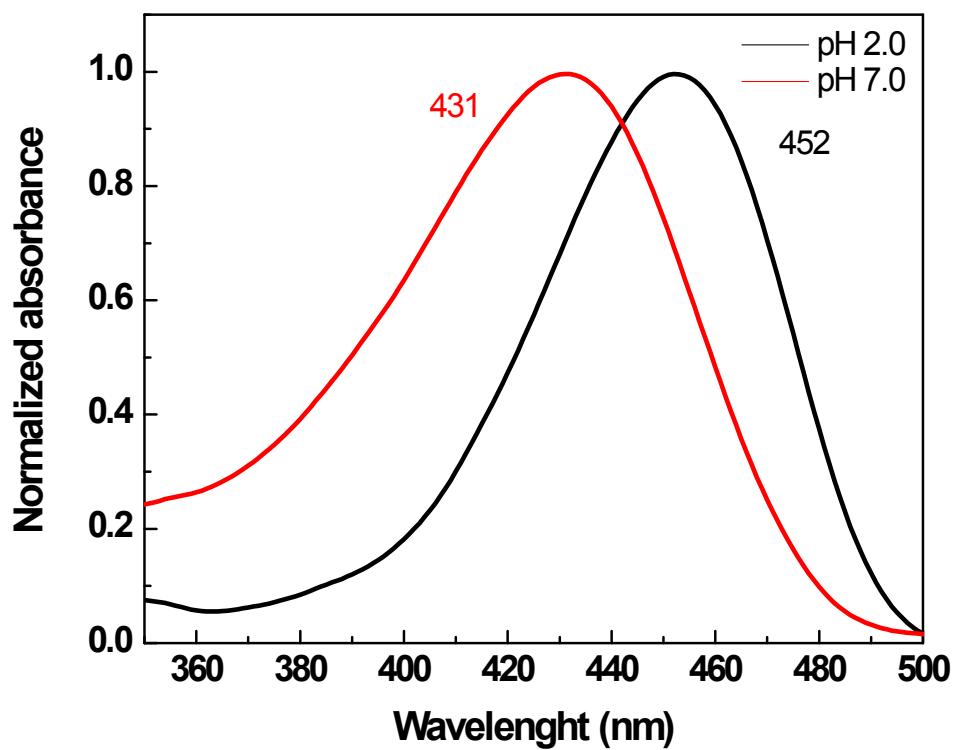


Figure S8. Coumarin 343 absorption spectra in acidic and neutral conditions