

Mutual Solubility of Water and Structural/Positional Isomers of *N*-Alkylpyridinium-based Ionic Liquids

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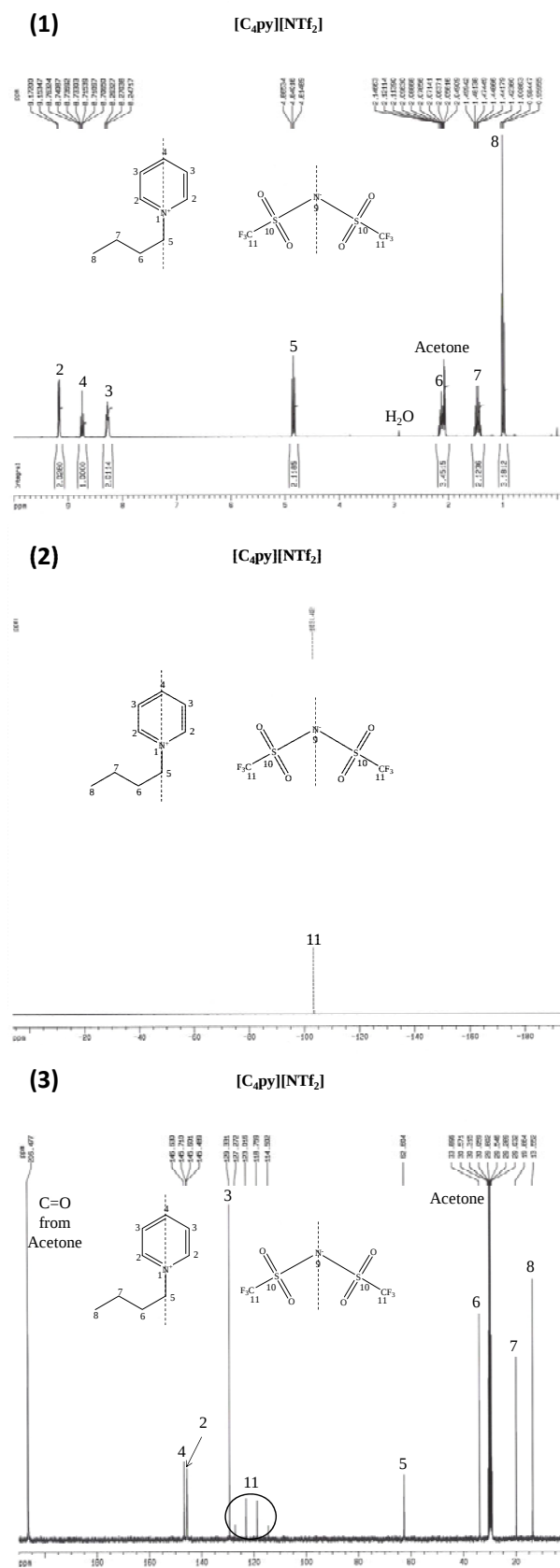


Figure S1. 1H (1), ^{19}F (2), ^{13}C (3) NMR spectra of $[C_4py][NTf_2]$ in CD_3COCD_3 .

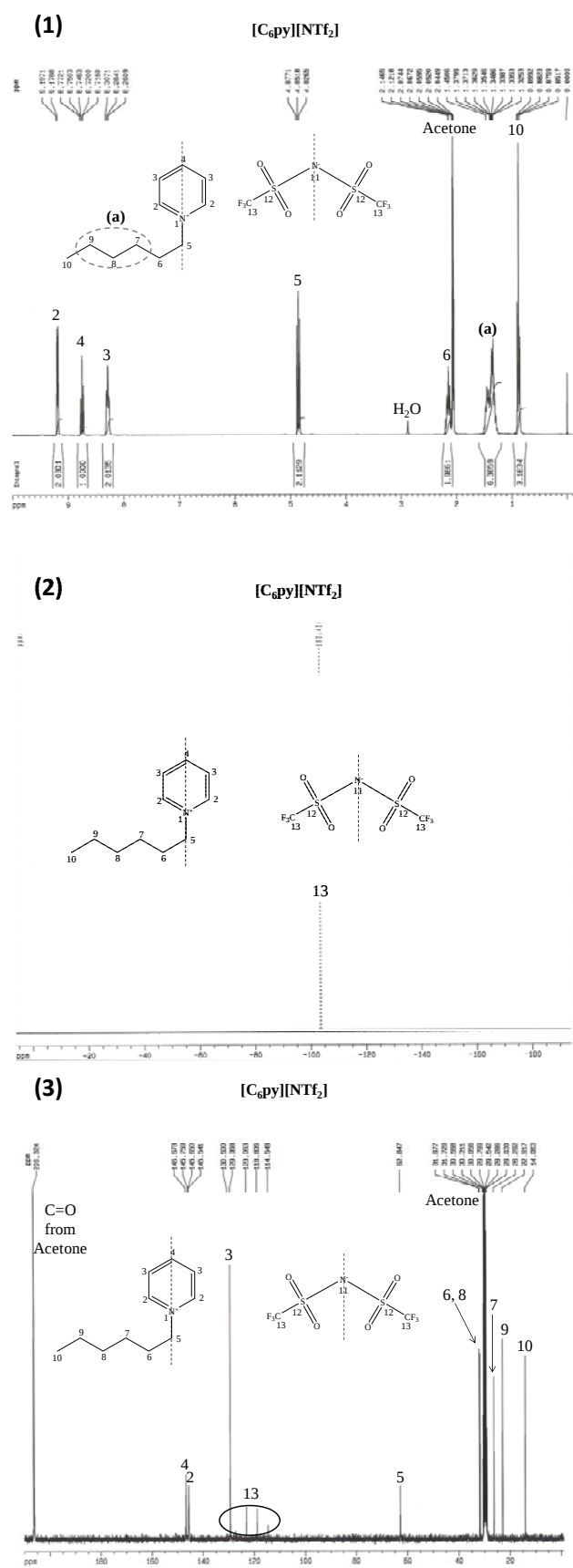


Figure S2. ^1H (1), ^{19}F (2), ^{13}C (3) NMR spectra of $[\text{C}_6\text{py}][\text{NTf}_2]$ in CD_3COCD_3 .

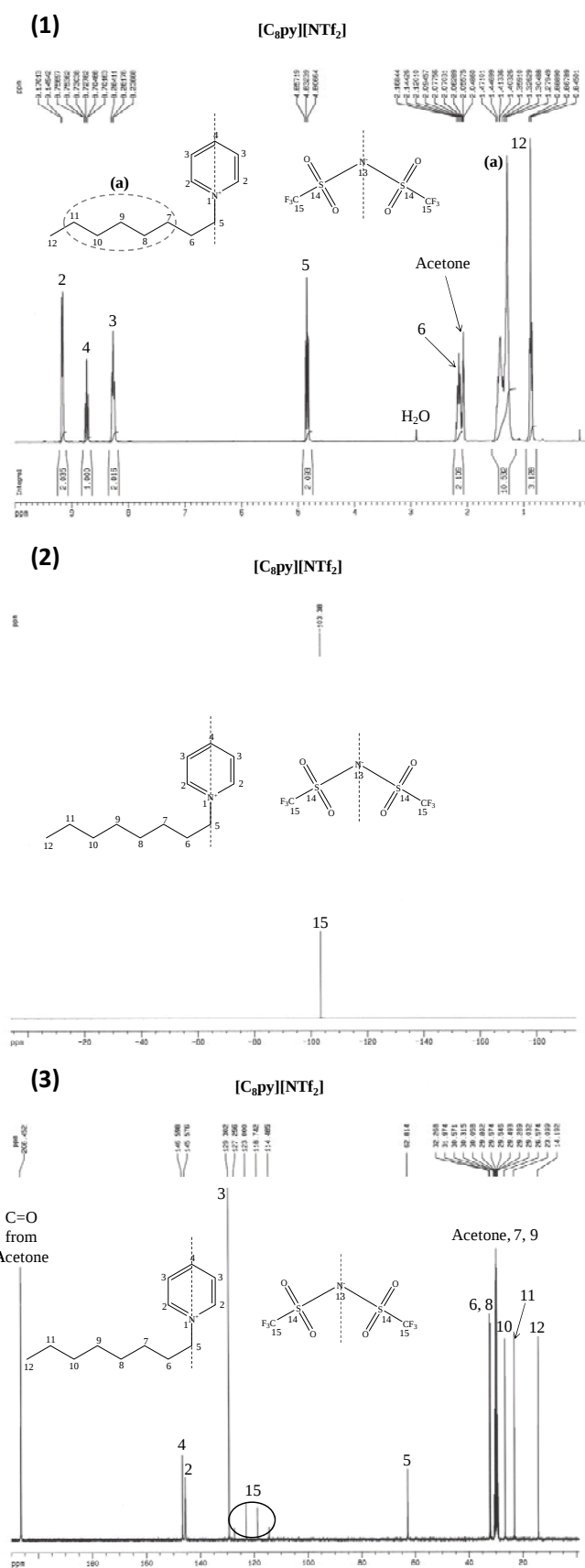


Figure S3. ^1H (1), ^{19}F (2), ^{13}C (3) NMR spectra of $[\text{C}_8\text{py}][\text{NTf}_2]$ in CD_3COCD_3 .

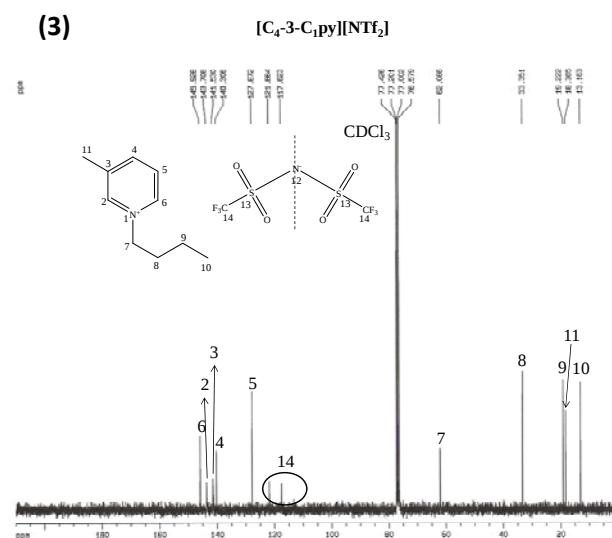
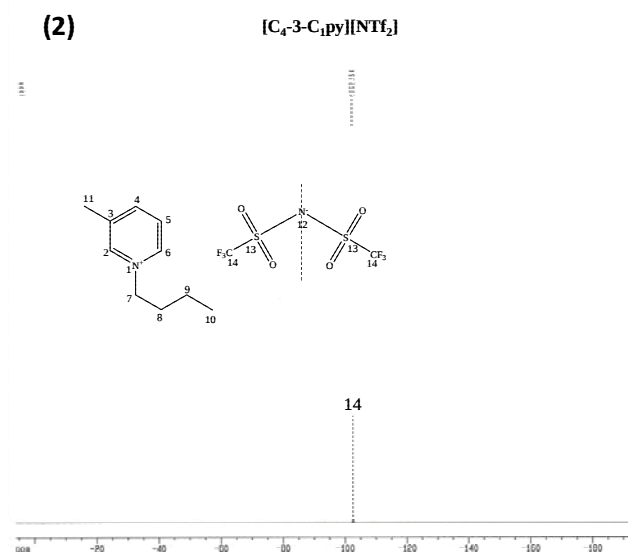
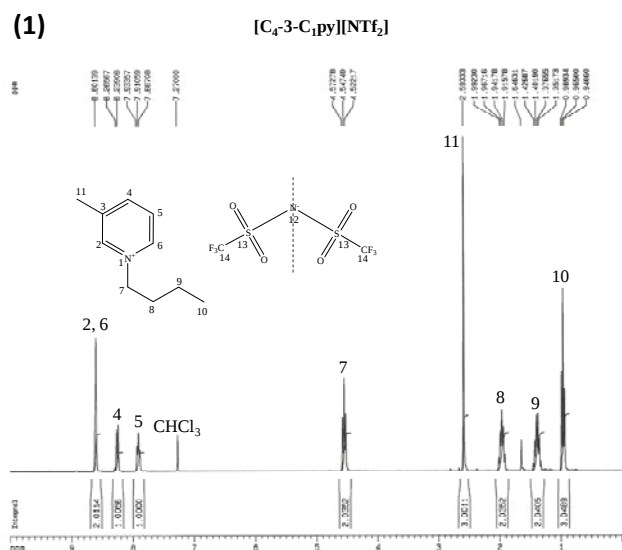
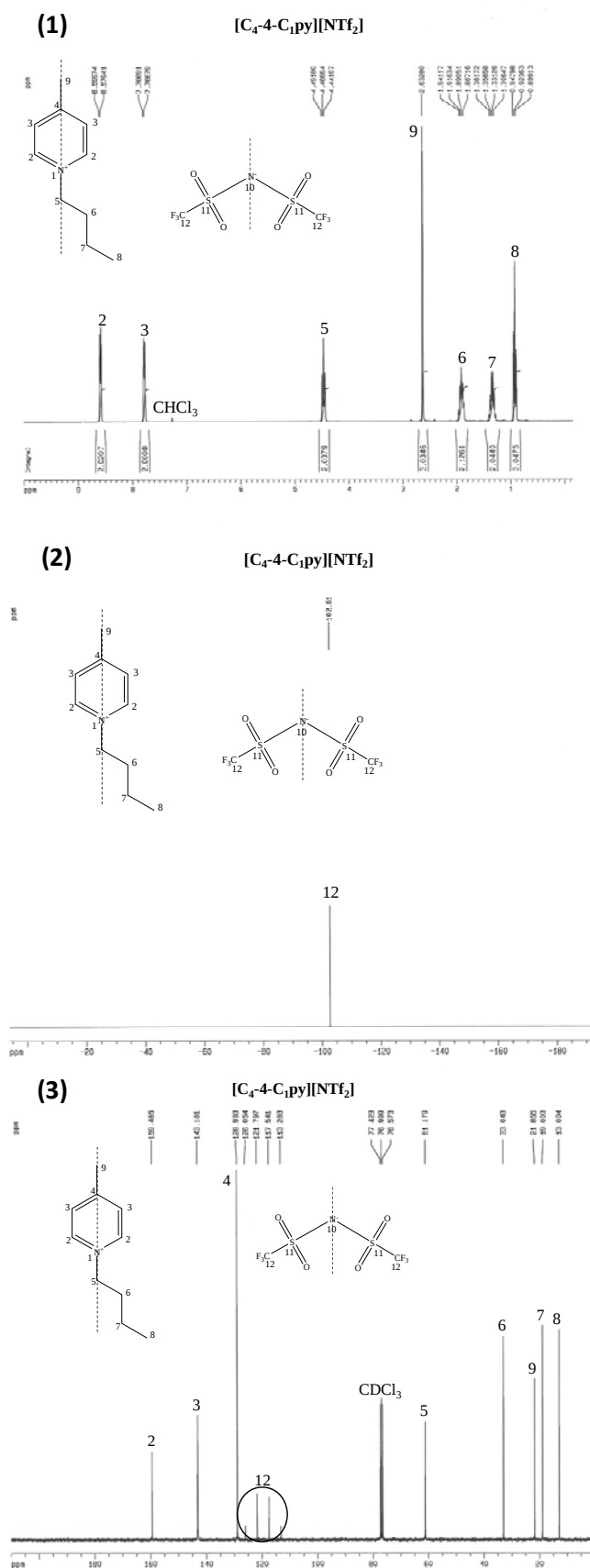


Figure S4. ^1H (1), ^{19}F (2), ^{13}C (3) NMR spectra of $[\text{C}_4\text{-3-C}_1\text{py}][\text{NTf}_2]$ in CD_3COCD_3 .



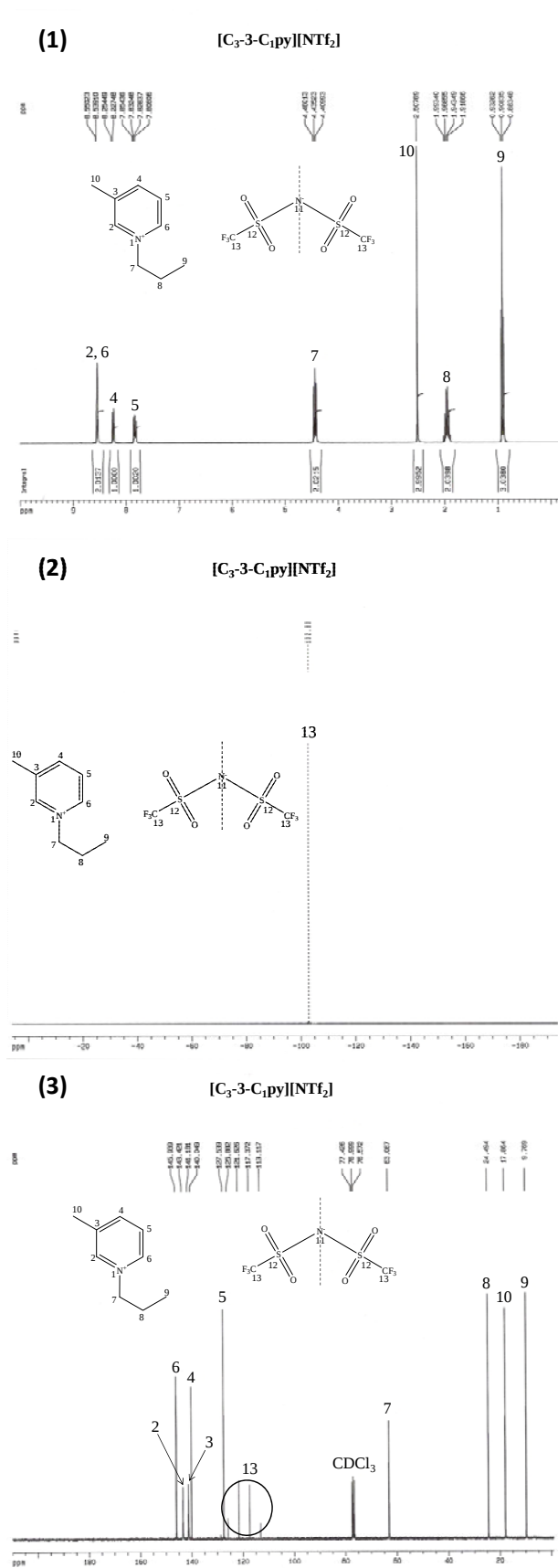


Figure S6. ^1H (1), ^{19}F (2), ^{13}C (3) NMR spectra of $[\text{C}_3\text{-3-C}_1\text{py}][\text{NTf}_2]$ in CD_3COCD_3 .

TABLE S1: Weight Fraction Solubility of Water in the IL-rich Phase (w_w) and Weigh Fraction Solubility of IL in the Water-rich Phase (w_{IL}) at Different Temperatures

	[C ₄ py][NTf ₂]	[C ₆ py][NTf ₂]	[C ₈ py][NTf ₂]	[C ₄ -3-C ₁ py][NTf ₂]	[C ₄ -4-C ₁ py][NTf ₂]
T / K	$100(w_w \pm \sigma^a)$				
288.15	1.212 ± 0.014	1.029 ± 0.007	0.804 ± 0.012	0.970 ± 0.009	1.159 ± 0.004
293.15	1.334 ± 0.004	1.107 ± 0.004	0.873 ± 0.005	1.049 ± 0.004	1.262 ± 0.013
298.15	1.435 ± 0.005	1.165 ± 0.007	0.927 ± 0.003	1.119 ± 0.006	1.353 ± 0.014
303.15	1.571 ± 0.015	1.307 ± 0.011	1.037 ± 0.022	1.248 ± 0.009	1.479 ± 0.010
308.15	1.741 ± 0.005	1.408 ± 0.003	1.153 ± 0.010	1.362 ± 0.005	1.643 ± 0.011
313.15	1.896 ± 0.011	1.528 ± 0.020	1.252 ± 0.003	1.460 ± 0.014	1.776 ± 0.010
318.15	2.056 ± 0.011	1.659 ± 0.004	1.369 ± 0.008	1.579 ± 0.001	1.919 ± 0.005
T / K	$100(w_{IL} \pm \sigma^a)$				
288.15	0.760 ± 0.004	0.454 ± 0.001	0.0810 ± 0.0026	0.473 ± 0.002	0.490 ± 0.006
293.15	0.778 ± 0.006	0.481 ± 0.005	0.0883 ± 0.0007	0.489 ± 0.003	0.505 ± 0.008
298.15	0.815 ± 0.011	0.491 ± 0.001	0.0917 ± 0.0008	0.500 ± 0.010	0.526 ± 0.015
303.15	0.855 ± 0.004	0.508 ± 0.012	0.1018 ± 0.0010	0.518 ± 0.009	0.565 ± 0.008
308.15	0.911 ± 0.004	0.554 ± 0.019	0.1102 ± 0.0005	0.546 ± 0.012	0.598 ± 0.016
313.15	0.942 ± 0.002	0.596 ± 0.022	0.1168 ± 0.0019	0.579 ± 0.004	0.623 ± 0.018
318.15	1.036 ± 0.006	0.628 ± 0.015	0.1328 ± 0.0046	0.604 ± 0.006	0.670 ± 0.018

^aStandard Deviation

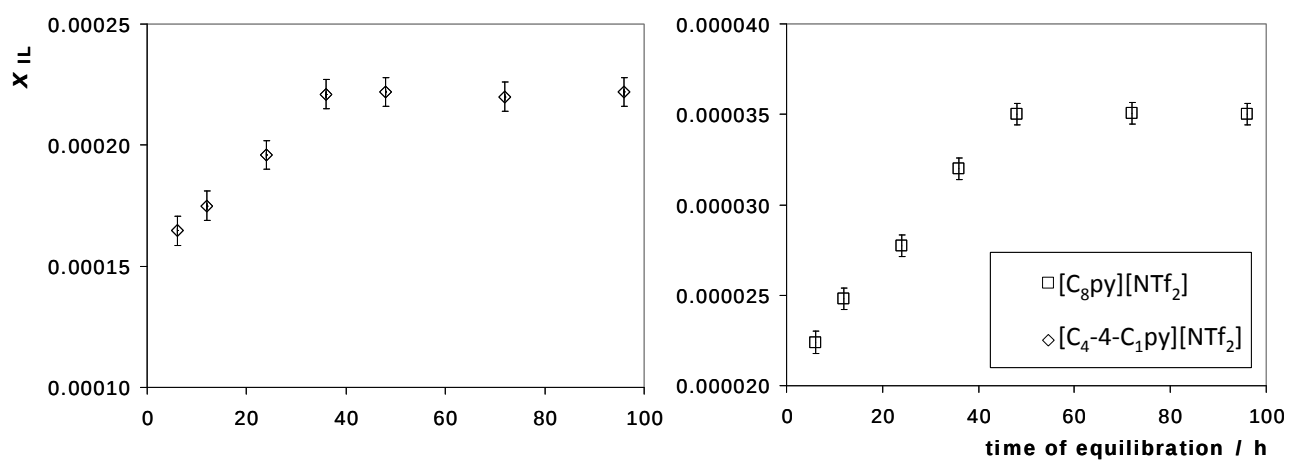


Figure S7. Solubility of $[C_4-4-C_1py][NTf_2]$ and $[C_8py][NTf_2]$ *versus* time of equilibration at 298.15 K.