Electronic Supporting Information (ESI)

Lipase Dissolution and Stabilization in Ether-Functionalized Ionic Liquids

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NMR Characterization of Three New Ionic Liquids

Triethyl (2-(2-methoxyethoxy)ethoxy)ethylammonium formate (**12**, [Me(OEt)$_3$-Et$_3$N][HCOO]): ^{1}H NMR (300 MHz, $CDCl_3$, [ppm]): δ = 1.37 (t, 9H, $N(CH_2CH_3)_3$, *J* = 7.2 Hz), 3.36 (s, 3H, $NCH_2CH_2OCH_2CH_2OCH_3$), 3.51 (m, 8H, $(CH_3CH_2)_3N$ and $NCH_2CH_2OCH_2CH_2OCH_3$), 3.61 (m, 4H, $NCH_2CH_2OCH_2CH_2OCH_3$), 3.68 (m, 2H, $NCH_2CH_2OCH_2CH_2OCH_3$), 8.85 (s, 1H, *H*COO). ^{13}C-NMR (DMSO-d$_6$, [ppm]) *δ* = 7.78, 53.3, 56.2, 58.6, 64.1, 70.0, 70.3, 71.8, 165.6.

1-ethyl-3-(2-(2-methoxyethoxy)ethoxy)ethyl)-2-methylimidazolium acetate (**18**, [Me(OEt)$_3$-Me-Et-Im][OAc]). ^{1}H-NMR (400 MHz, DMSO-d$_6$, [ppm]) *δ* = 1.30 (3H, t, CH_3CH_2N, *J* = 3.8 Hz), 1.49 (3H, s, CH_3CN), 2.62 (3H, s, CH_3COO^-), 3.20 (3H, s, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$), 3.34-3.49 (8H, m, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$), 3.70 (2H, t, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$, *J* = 5.2 Hz), 4.19 (2H, q, CH_3CH_2N, *J* = 7.2 Hz), 4.36 (2H, t, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$, *J* = 4.8 Hz), 7.86 (1H, d, NC*H*CHN, *J* = 2.1), 7.92 (1H, d, NCHC*H*N, *J* = 2.1). ^{13}C-NMR (DMSO-d$_6$, [ppm]) *δ* = 9.70, 15.4, 26.7, 43.2, 47.9, 58.6, 69.2, 70.0, 70.1, 70.2, 70.3, 71.8, 121.4, 122.4, 144.7, 173.1.

1-ethyl-3-(2-(2-methoxyethoxy)ethoxy)ethyl)imidazolium dicyanamide (**19**, [Me(OEt)$_3$-Et-Im][dca]). ^{1}H-NMR (400 MHz, DMSO-d$_6$, [ppm]) *δ* = 1.41 (3H, t, CH_3CH_2N, *J* = 4.1 Hz), 3.20 (3H, s, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$), 3.39 (2H, m, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$), 3.43-3.54 (6H, m, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$), 3.75 (2H, t, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$, *J* = 4.8 Hz), 4.20 (2H, q, CH_3CH_2N, *J* = 7.2 Hz), 4.31 (2H, t, $NCH_2CH_2OCH_2CH_2OCH_2CH_2OCH_3$, *J* = 6.0 Hz), 7.71 (1H, m, NC*H*CHN), 7.76 (1H, m, NCHC*H*N), 9.10 (1H, s, NC*H*N). ^{13}C-NMR (DMSO-d$_6$, [ppm]) *δ* = 15.6, 44.7, 49.3, 58.6, 68.6, 70.1, 70.3, 71.8, 122.4, 123.3, 136.5.

NMR Characterization of Glucose Laurate

^{1}H NMR (300 MHz, $CDCl_3$, [ppm]) δ = 0.87 (3 H, t, -CH_3), 1.25 (16 H, m, aliphatic CH_2), 1.62 (2 H, m, -$O_2CCH_2CH_2$-), 2.32 (2 H, t, -O_2CCH_2-), 3.5-5.0 (7H, m, glucose H2-H6), 5.50 (1H, d, glucose H1). The glucose hydrogen signals have been assigned by a literature.[1]

^{13}C NMR (75.6 MHz, $CDCl_3$, [ppm]) δ(C-1) = 90.8, δ(C-2) = 70.7, δ(C-3) = 72.0, δ(C-4) = 69.4, δ(C-5) = 63.7, δ(C-6) = 59.1, δ(C-1') = 178, δ(C-2') = 33.8, δ(C-3') = 32.0, δ(C-4' – C-9') = 29.5, δ(C-10') = 24.8, δ(C-11') = 22.8, δ(C-12') = 14.2 (chloroform 77.1 ppm). Glucose-$^{13}C_6$ laurate was used for ^{13}C NMR spectrum.

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Table S.1 Assignments of infrared amide I band components of proteins

Wavenumber (cm^{-1})	Assignment	Reference
1623, 1628, 1636, 1640, 1647	β-sheets	[2-6]
1654	α-helix	[2, 4, 5, 7]
1663, 1669, 1676, 1684	β-turns	[4, 5, 7]
1689	β-sheets or β-turns	[4, 5]

References

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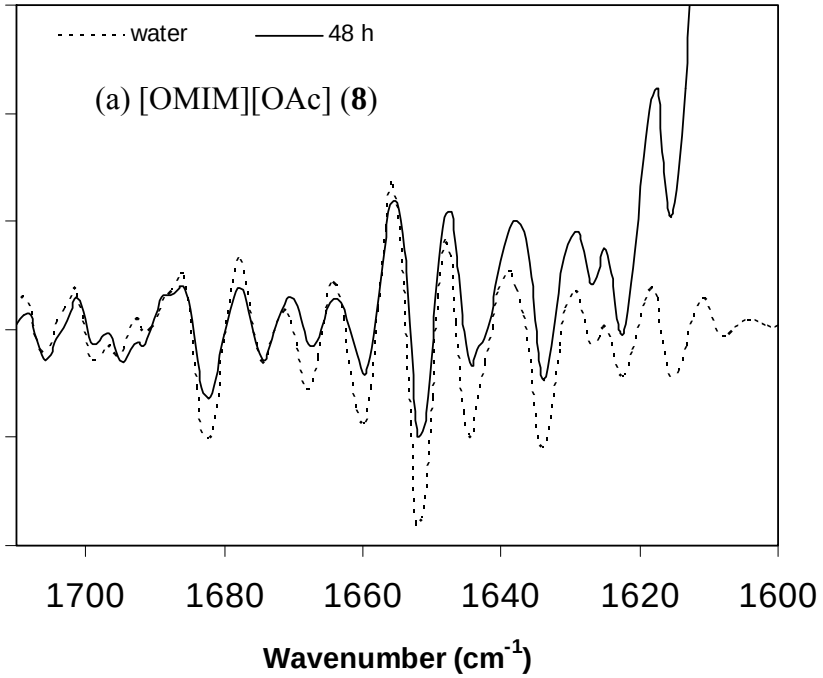
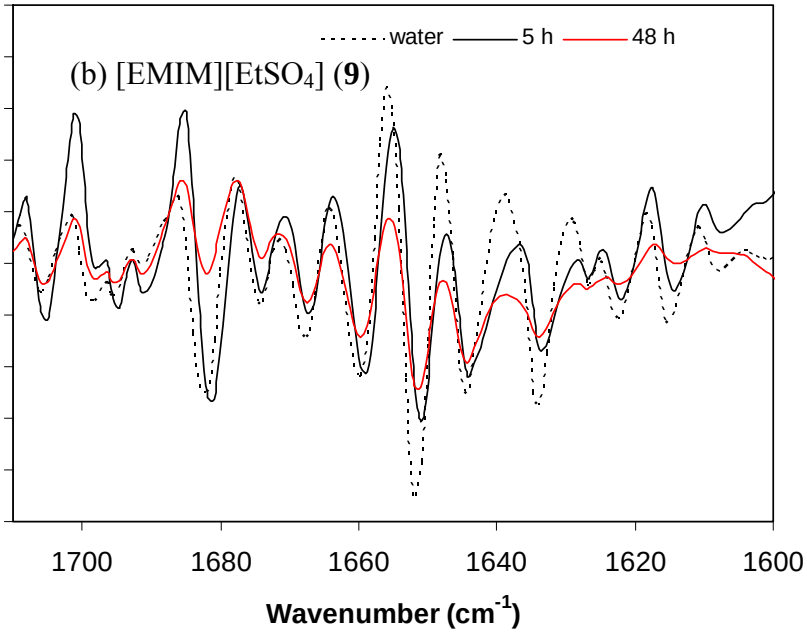
Infrared Spectra of Free CALB in ILs





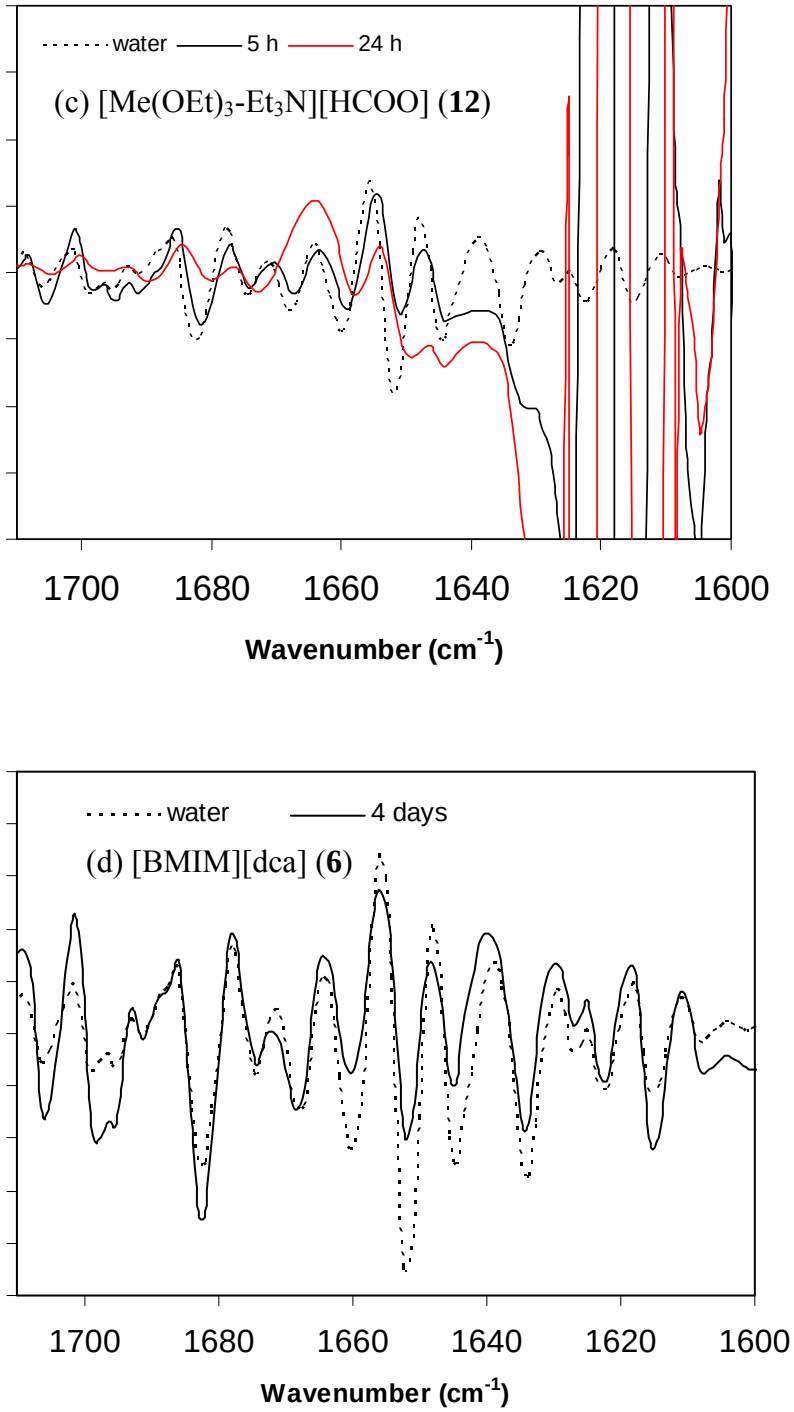


Figure S.1 Second derivative ($d^2A/d\nu^2$) spectra of free CALB in water (dashed line) and in ILs (solid lines, with different incubation times at 50 ˚C).

Fluorescence Spectra of Free CALB in ILs

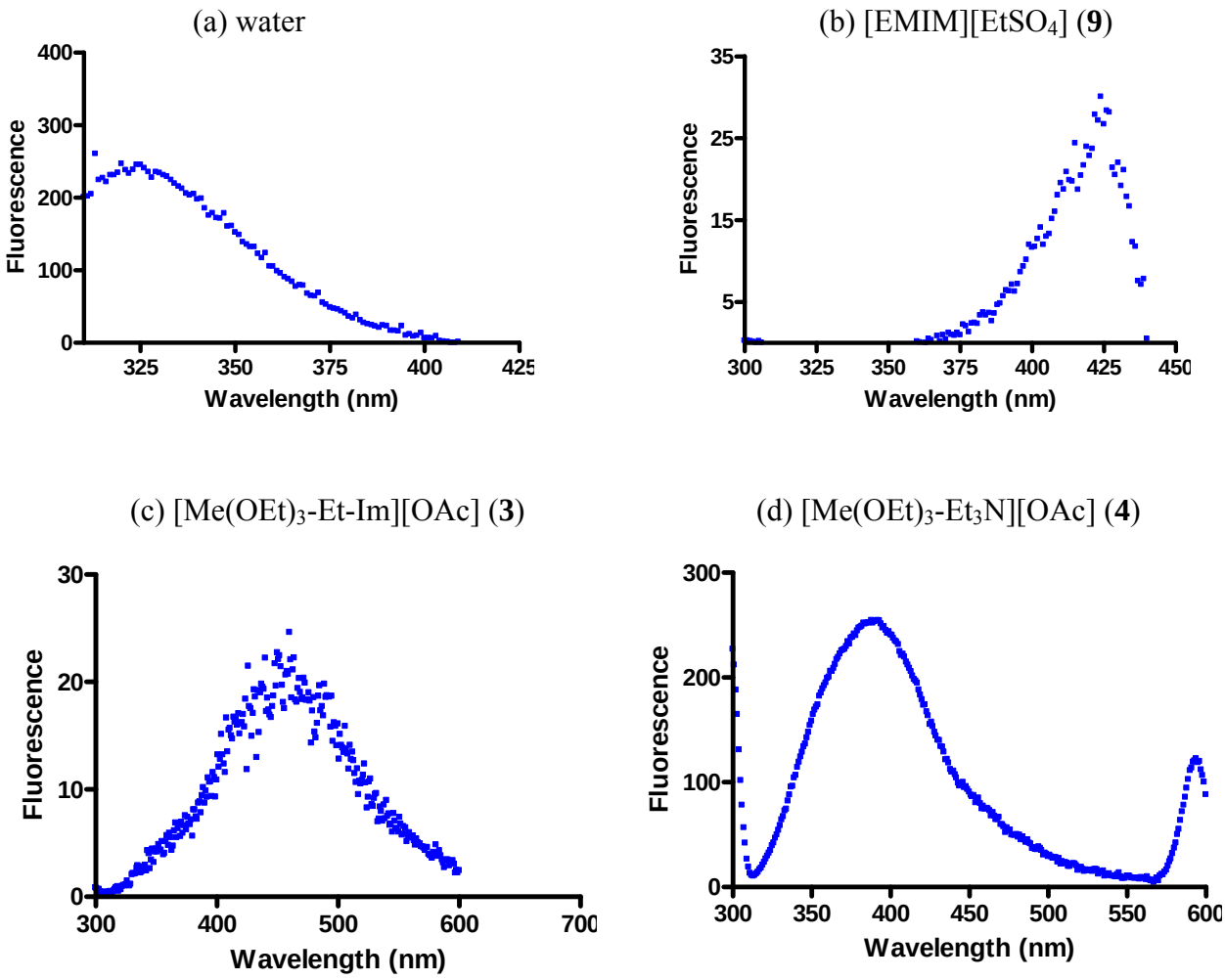


Figure S.2 Fluorescence emission spectra of free CALB in water and ILs at 50 ˚C (a Varian Eclipse BioMelt™ fluorescence spectrophotometer was used to excite the lipase at 295 nm, and the emission maximum of tryptophan (Trp) residues was observed at 325 nm in water. The enzyme concentration was 0.1 mg/mL.).

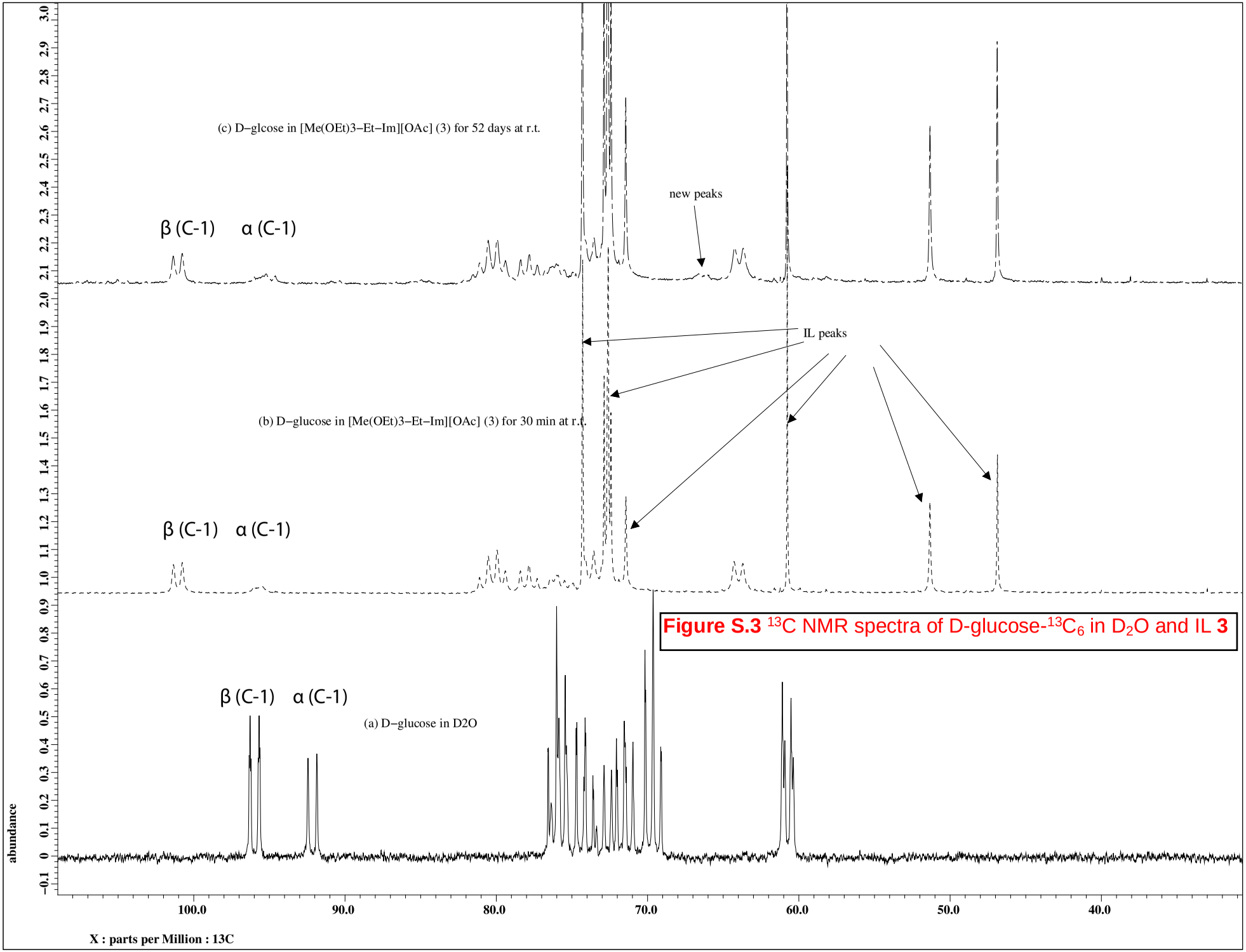


Figure S.3 ^{13}C NMR spectra of D-glucose-$^{13}C_6$ in D_2O and IL **3**

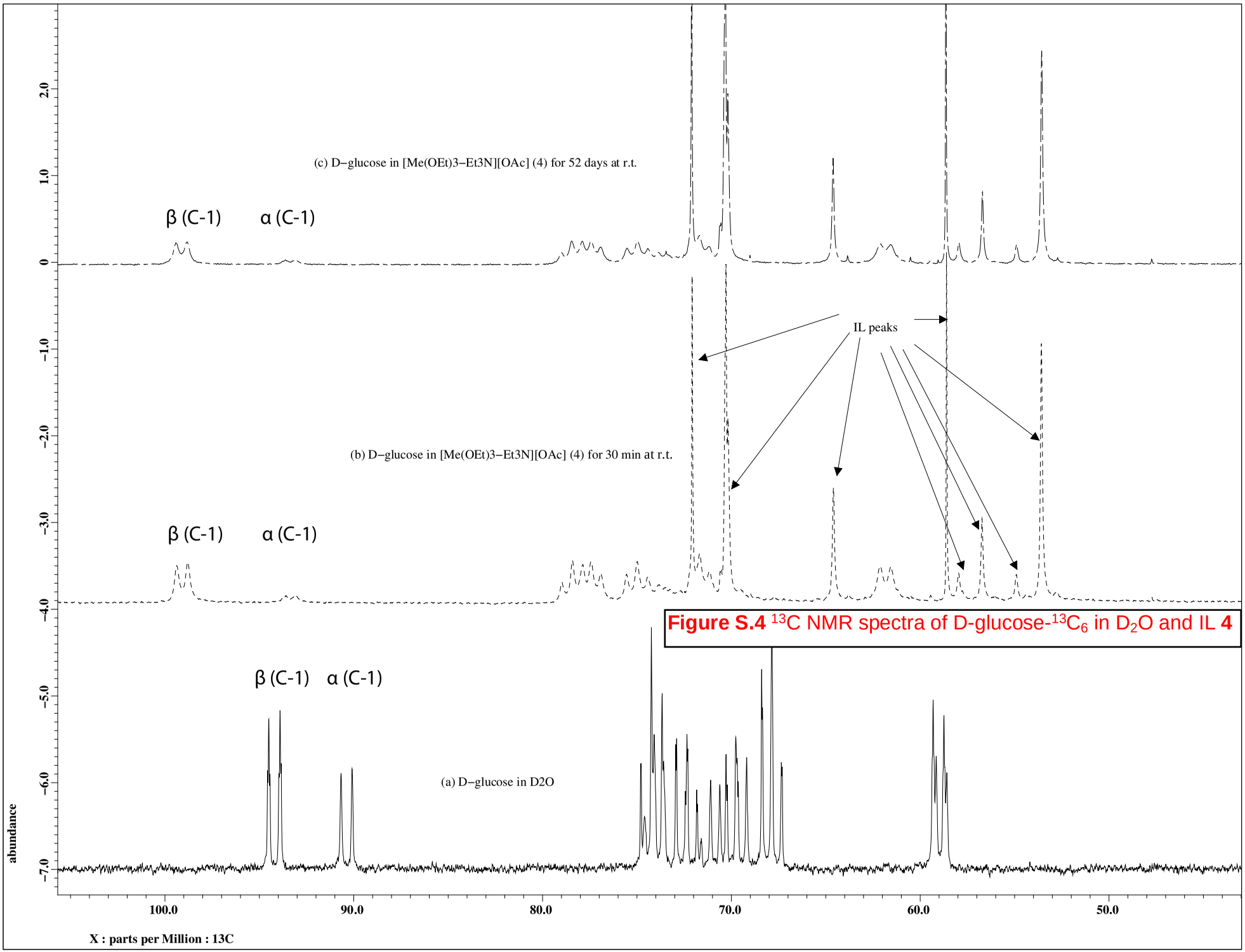


Figure S.4 ^{13}C NMR spectra of D-glucose-$^{13}C_6$ in D_2O and IL **4**