

Supplementary Information

Efficient and sustainable solvents for lignin dissolution: Aqueous choline carboxylate solutions

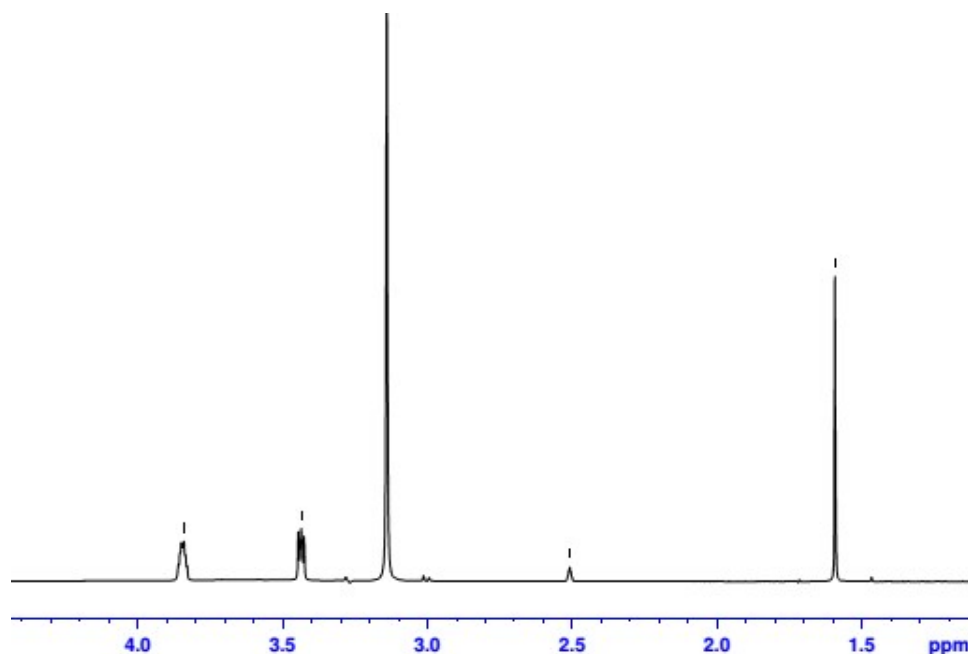
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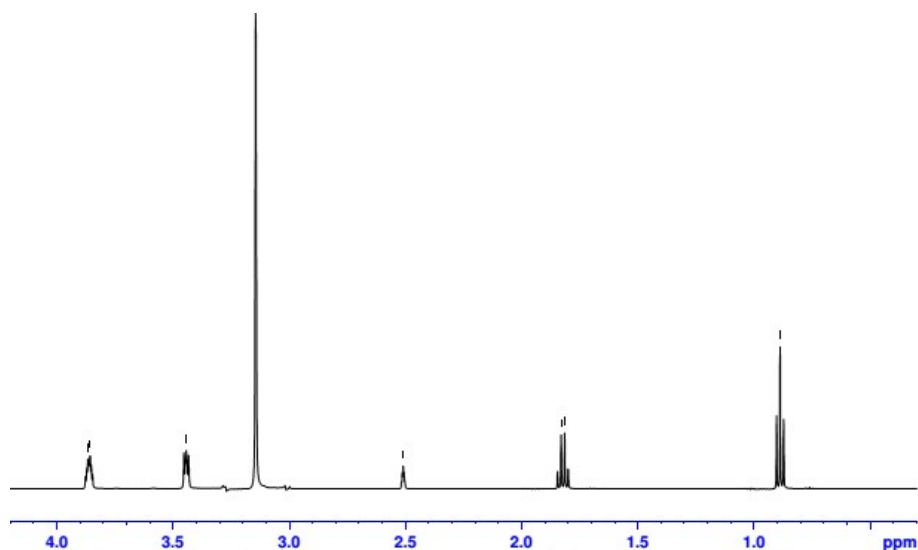
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¹H-NMR Data of the ILs

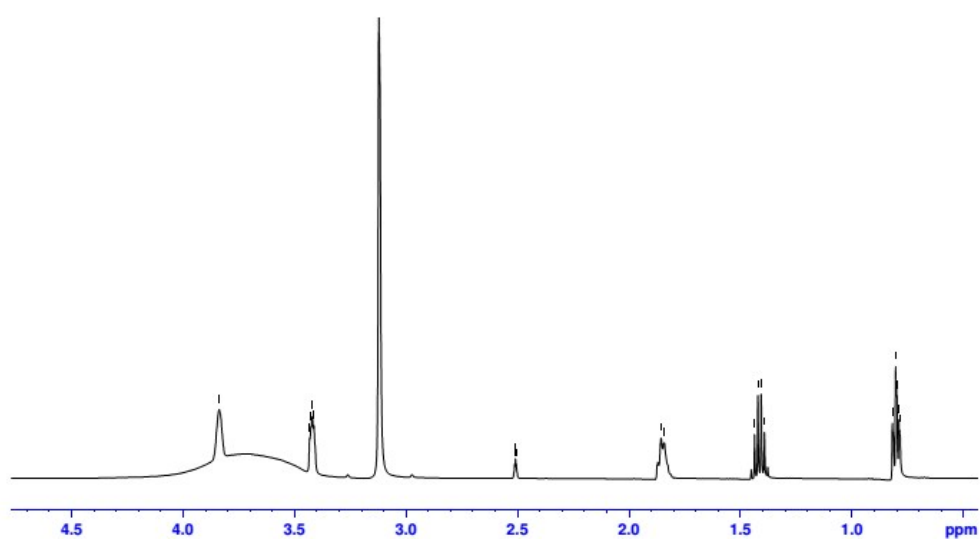
1. [Ch][CH₃COO]: ¹H NMR (500MHz: DMSO-d₆; δ /ppm relative to TMS): 1.59 (3H, s, CH₃CO₂), 3.14 (9H, s, CH₃), 3.44 (2H, t, NCH₂), 3.84 (2H, m, CH₂OH).



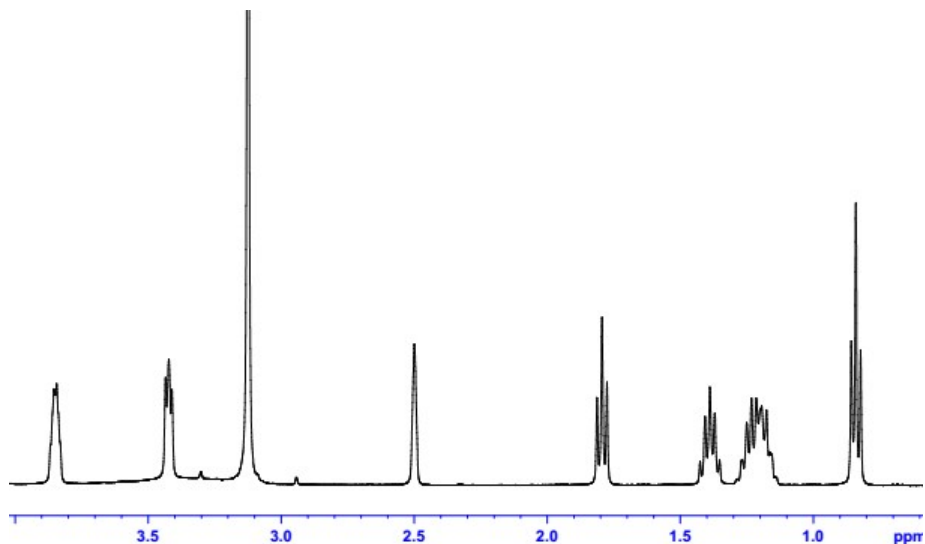
2. [Ch][CH₃CH₂COO]: ¹H NMR (500MHz: DMSO-d₆; δ/ppm relative to TMS): 0.89 (3H, t, CH₃CH₂), 1.82 (2H, m, CH₃CH₂), 3.14 (9H, s, CH₃), 3.44 (2H, t, NCH₂), 3.86 (2H, m, CH₂OH).



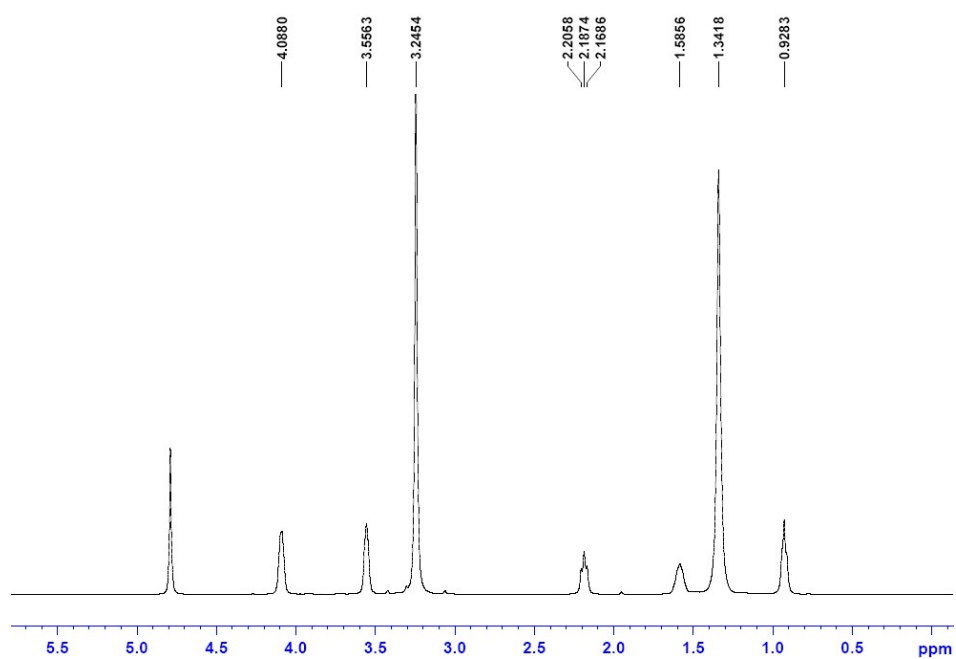
3. [Ch][CH₃(CH₂)₂COO]: ¹H NMR (500MHz: DMSO-d₆; δ/ppm relative to TMS): 0.80 (3H, t, but-CH₃), 1.41 (2H, m, CH₃CH₂), 1.86 (2H, m, CH₂CO₂), 3.12 (9H, s, CH₃N), 3.43 (2H, t, NCH₂), 3.84 (2H, s, CH₂OH).



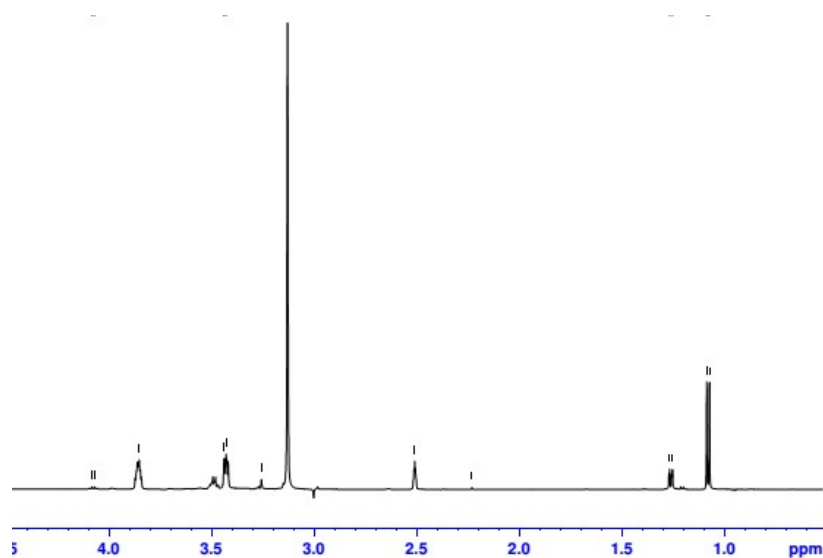
4. $[\text{Ch}][\text{CH}_3(\text{CH}_2)_4\text{COO}]$: ^1H NMR (500MHz: DMSO-d_6 ; δ/ppm relative to TMS): 0.84 (3H, t, CH_3), 1.16-1.27 (4H, m, $\text{CH}_3(\text{CH}_2)_2$), 1.35-1.43 (2H, m, $\text{CH}_2\text{-CH}_2\text{-CH}_2\text{CO}_2$), 1.79 (2H, t, CH_2CO_2)



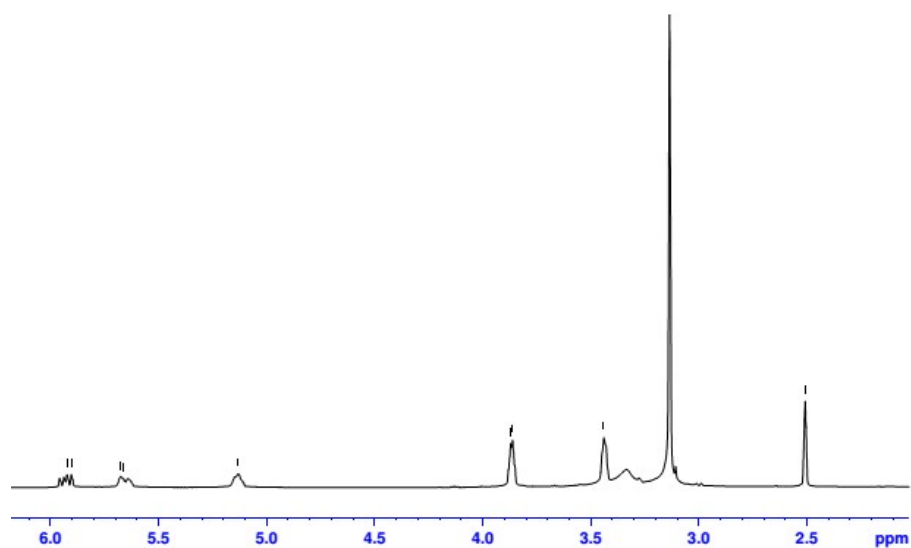
5. $[\text{Ch}][\text{CH}_3(\text{CH}_2)_{10}\text{COO}]$: ^1H NMR (500MHz: D_2O ; δ/ppm relative to TMS): 0.93 (3H, t, CH_3), 1.34 (16H, m, $\text{CH}_3\text{CH}_2\text{CH}_2(\text{CH}_2)_8$), 1.59 (2H, m, CH_3CH_2), 2.19 (2H, m, $\text{CH}_3\text{CH}_2\text{CH}_2$), 3.25 (9H, s, CH_3N), 3.56 (2H, t, NCH_2), 4.09 (2H, t, CH_2OH)



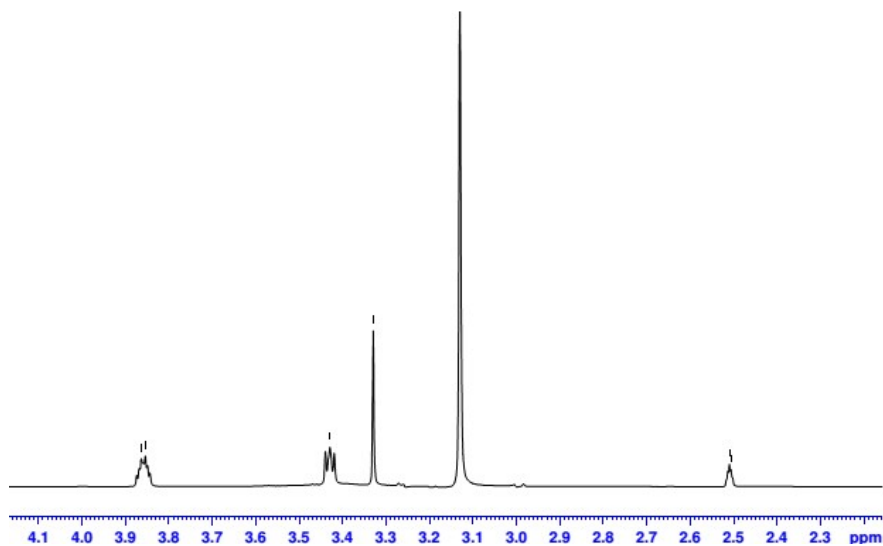
6. [Ch][CH₃CH(OH)COO]: ¹H NMR (500MHz: DMSO-d₆; δ/ppm relative to TMS): 1.08 (3H, d, CH₃CH), 1.25 (1H, m, CH₃CH), 3.13 (9H, s, CH₃), 3.43 (2H, t, NCH₂), 3.85 (2H, m, CH₂OH)



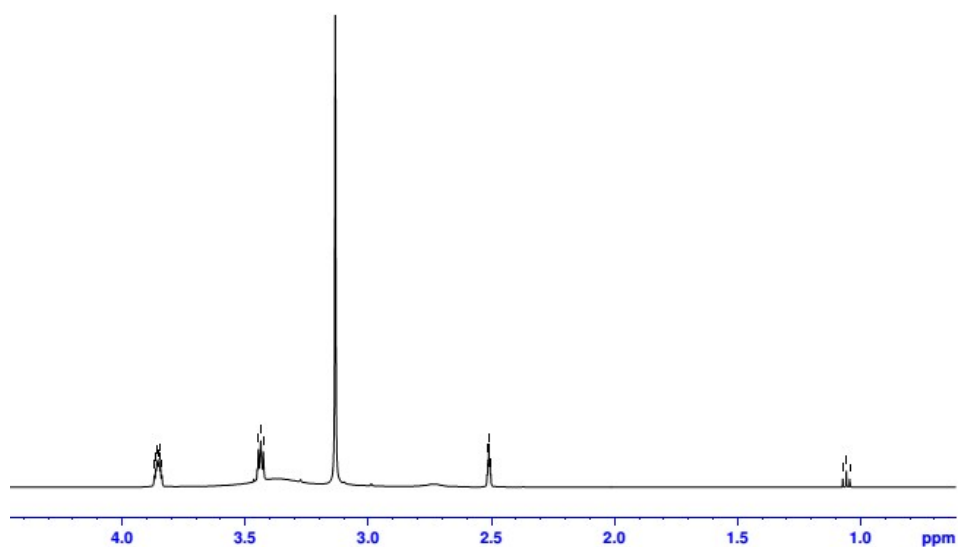
7. [Ch][CH₂=CHCOO]: ¹H NMR (500MHz: DMSO-d₆; δ/ppm relative to TMS): 3.14 (9H, s, CH₃), 3.44 (2H, t, NCH₂), 3.86 (2H, m, CH₂OH), 5.13, 5.91 (2H, m, CH₂CH), 5.68 (1H, t, CH₂CH).



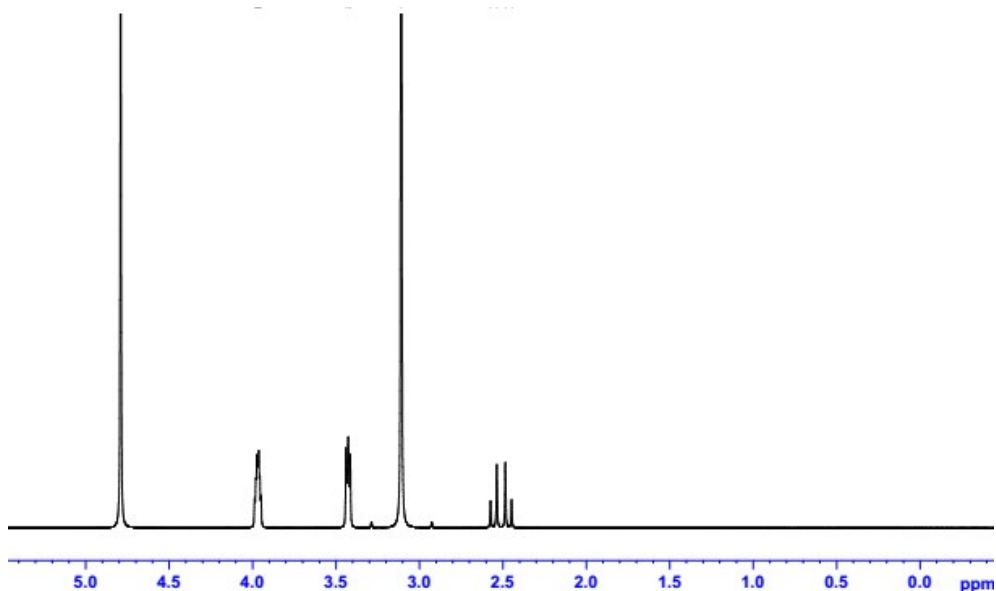
8. [Ch][HOCH₂COO]: ¹H NMR (500MHz: DMSO-d₆; δ/ppm relative to TMS): 3.13 (9H, s, CH₃), 3.33 (2H, s, CH₂CO₂), 3.43 (2H, t, NCH₂), 3.85 (2H, m, CH₂OH).



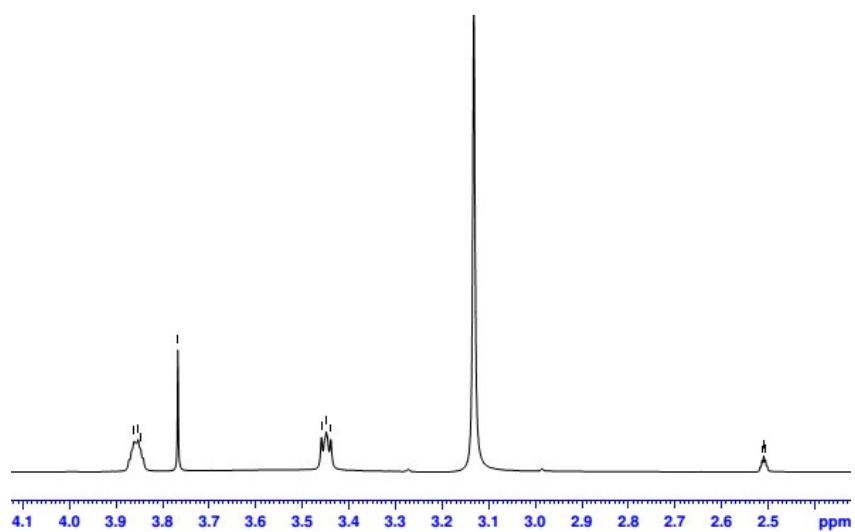
9. [Ch][NH₂CH₂COO]: ¹H NMR (500MHz: DMSO-d₆; δ/ppm relative to TMS): 3.13 (9H, s, CH₃), 3.45 (2H, t, NCH₂), 3.85 (2H, m, HOCH₂)



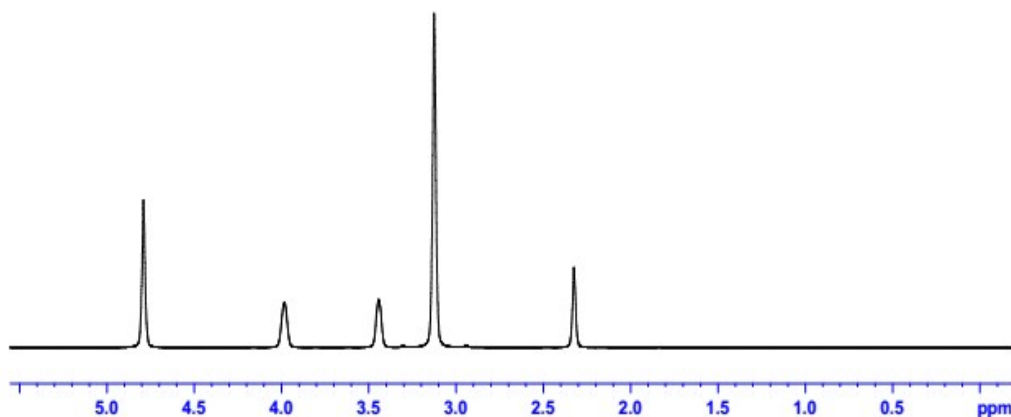
10 $[\text{Ch}]_3[\text{OOCCH}_2(\text{HO})\text{C}(\text{COO})\text{CH}_2\text{COO}]$: ^1H NMR (500MHz: D_2O ; δ/ppm relative to TMS): 2.51 (4H, m, CH_2COO), 3.11 (27H, s, CH_3N), 3.43 (6H, t, CH_2N), 3.97 (6H, m, CH_2OH)



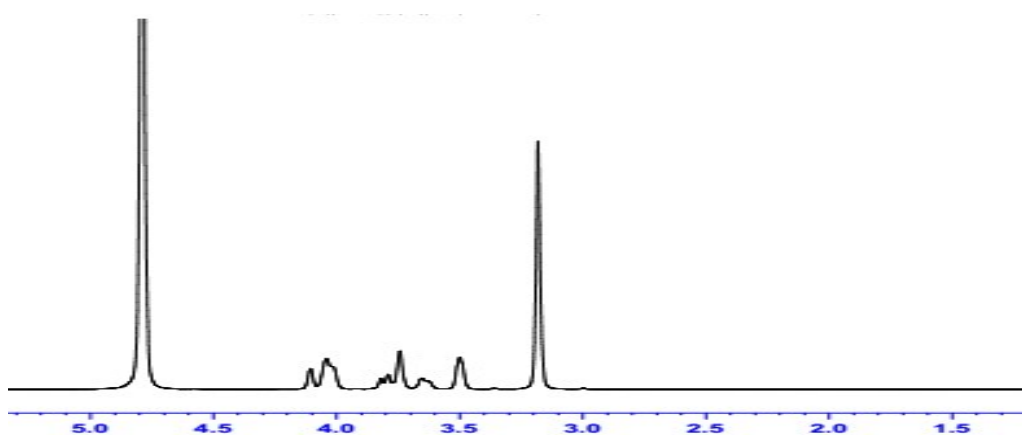
11. $[\text{Ch}]_2[\text{OOC}(\text{CHOH})_2\text{COO}]$: ^1H NMR (500MHz: DMSO-d_6 ; δ/ppm relative to TMS): 3.13 (18H, s, CH_3), 3.45 (4H, t, NCH_2), 3.77 (2H, s, CHCO_2), 3.85 (4H, m, CH_2OH).



12. $[\text{Ch}]_2[\text{OOC}(\text{CH}_2)_2\text{COO}]$: ^1H NMR (500MHz: D_2O ; δ/ppm relative to TMS): 2.33 (4H, t, CH_2CO_2), 3.13 (18H, s, CH_3N), 3.44 (4H, t, NCH_2), 3.98 (4H, t, CH_2O).



13. $[\text{Ch}][\text{HOCH}_2(\text{CHOH})_4\text{COO}]$: ^1H NMR (500MHz: D_2O ; δ/ppm relative to TMS): 3.18 (9H, s, CH_3), 3.50 (2H, t, NCH_2), 3.63 (1H, d, CH), 3.74 (2H, m, $\text{CH}_2\text{OH}(\text{NCH}_2\text{CH}_2\text{OH})$), 3.80 (1H, d, CH), 4.01 (1H, s, CH), 4.04 (2H, m, $\text{HOCH}_2(\text{HOCH}_2(\text{CHOH})_4\text{COO})$), 4.10 (1H, t, CH).



The ^{13}C NMR and ^{15}N NMR spectra of $[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ in $\text{H}_2\text{O}-[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ solvent and $\text{H}_2\text{O}-[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ -lignin (8 wt%) solution

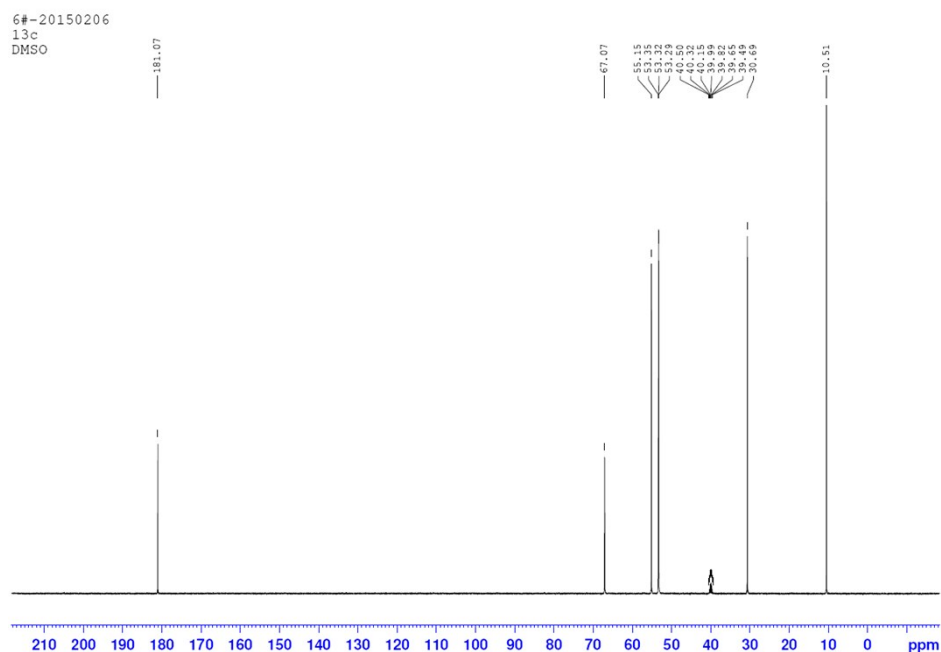


Fig. S1 ^{13}C NMR spectra of $[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ in $\text{H}_2\text{O}-[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ solvent

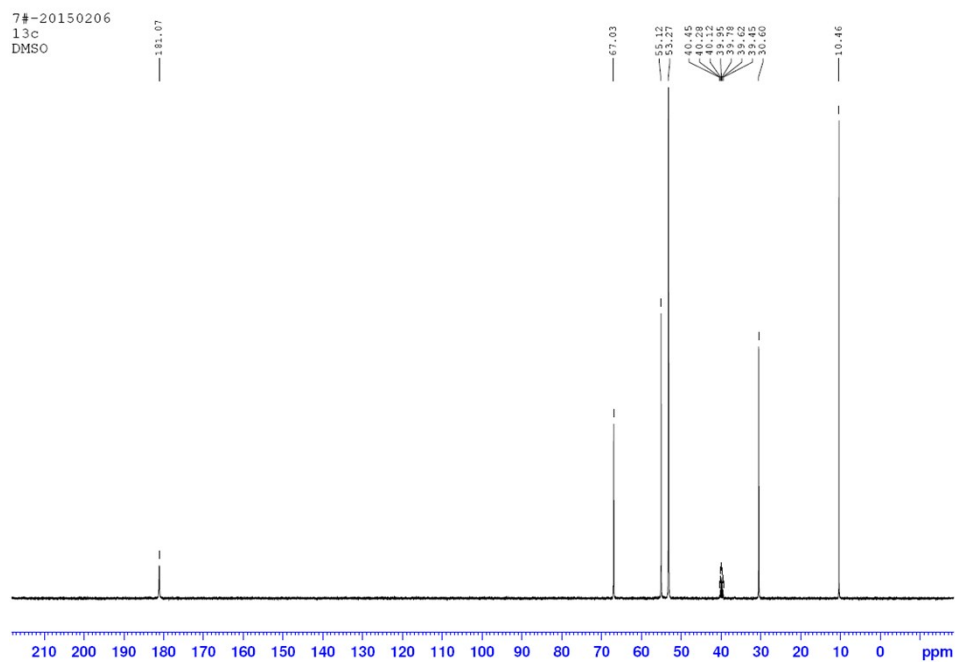


Fig. S2 The ^{13}C NMR spectra of $[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ in $\text{H}_2\text{O}-[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ -lignin (8 wt%) solution

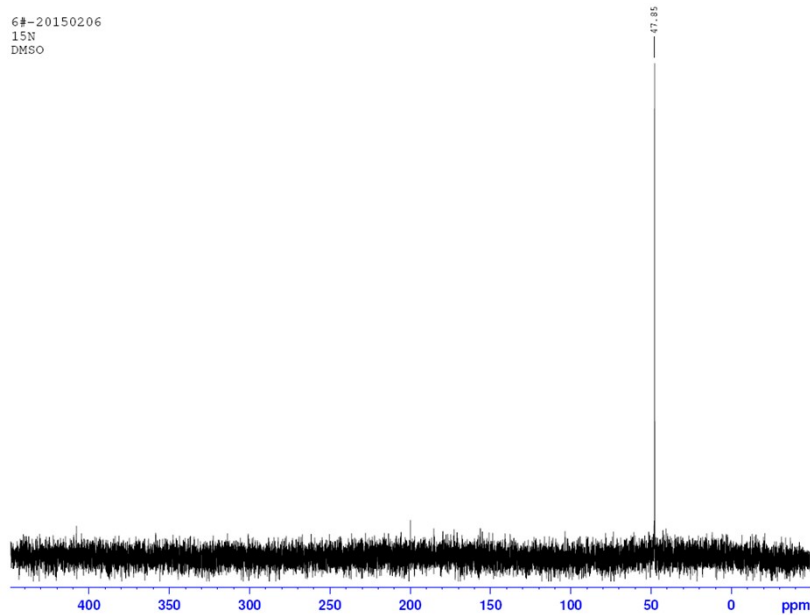


Fig. S3 The ^{15}N NMR spectra of $[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ in $\text{H}_2\text{O}-[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ solvent.

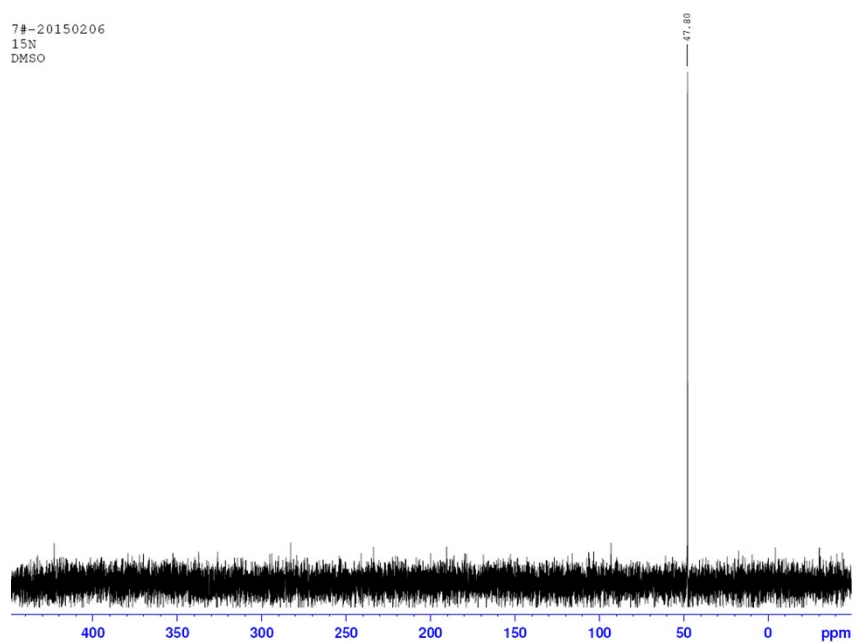


Fig. S4 The ^{15}N NMR spectra of $[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ in $\text{H}_2\text{O}-[\text{Ch}][\text{CH}_3\text{CH}_2\text{COO}]$ -lignin (8 wt%) solution

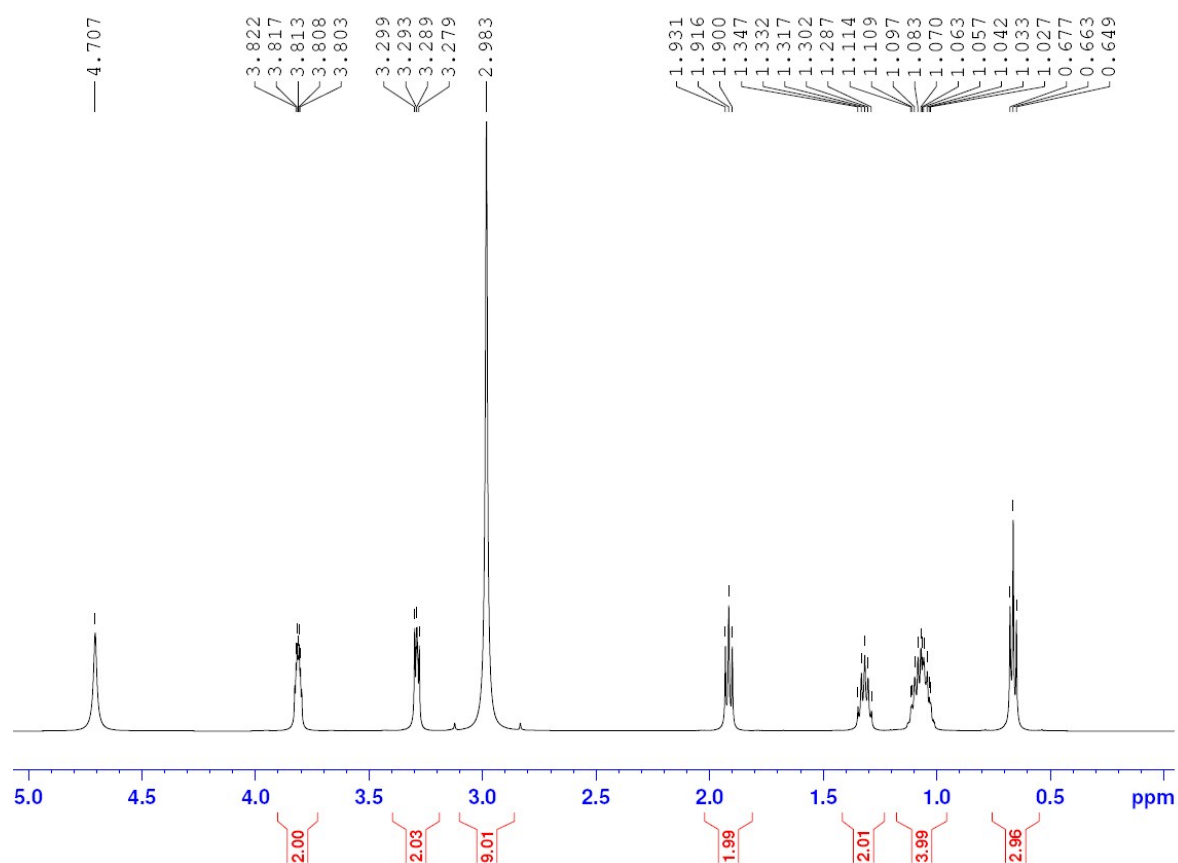


Fig. S5 ^1H NMR spectrum of the recovered $[\text{Ch}][\text{CH}_3(\text{CH}_2)_4\text{COO}]$ at room temperature. D_2O is used as an internal standard.

Table S1 Solubility of lignin in $\text{H}_2\text{O}-[\text{C}_4\text{mim}][\text{CH}_3\text{COO}]$ solvents at $25\text{ }^\circ\text{C}$

Entry	R	Solubility (gram per 100g of solvent)
1	1	47
2	3	58
3	6	67
4	9	70
5	12	62
6	15	0

R is the molar ratio of H_2O to $[\text{C}_4\text{mim}][\text{CH}_3\text{COO}]$.