SUPPLEMENTARY MATERIAL

Therapeutic Opportunities of Surface-Active Ionic Liquids: A Case Study on Acetylcholinesterase, Citrate Synthase and HeLa Cell Lines

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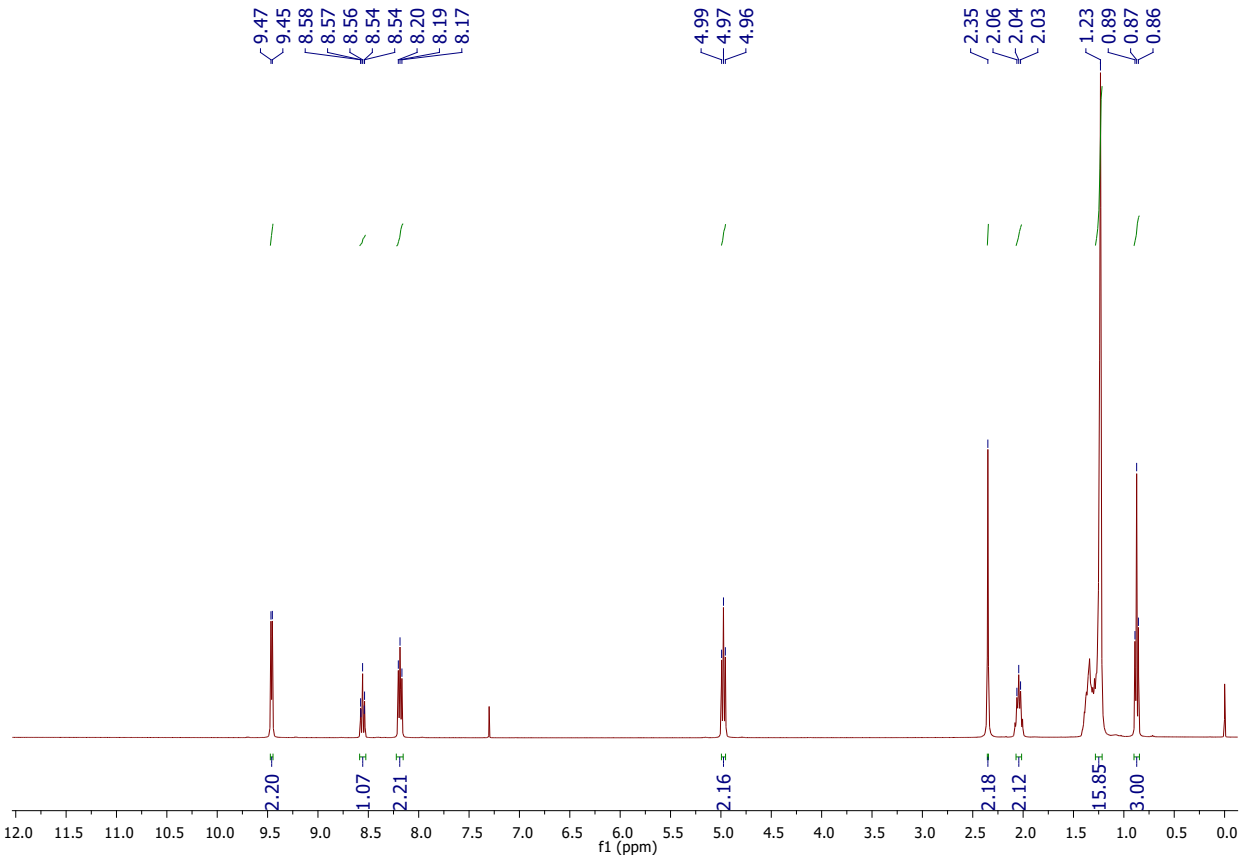
Fig. S1. HRMS spectra of N-dodecylpyridinium bromide (DPB).

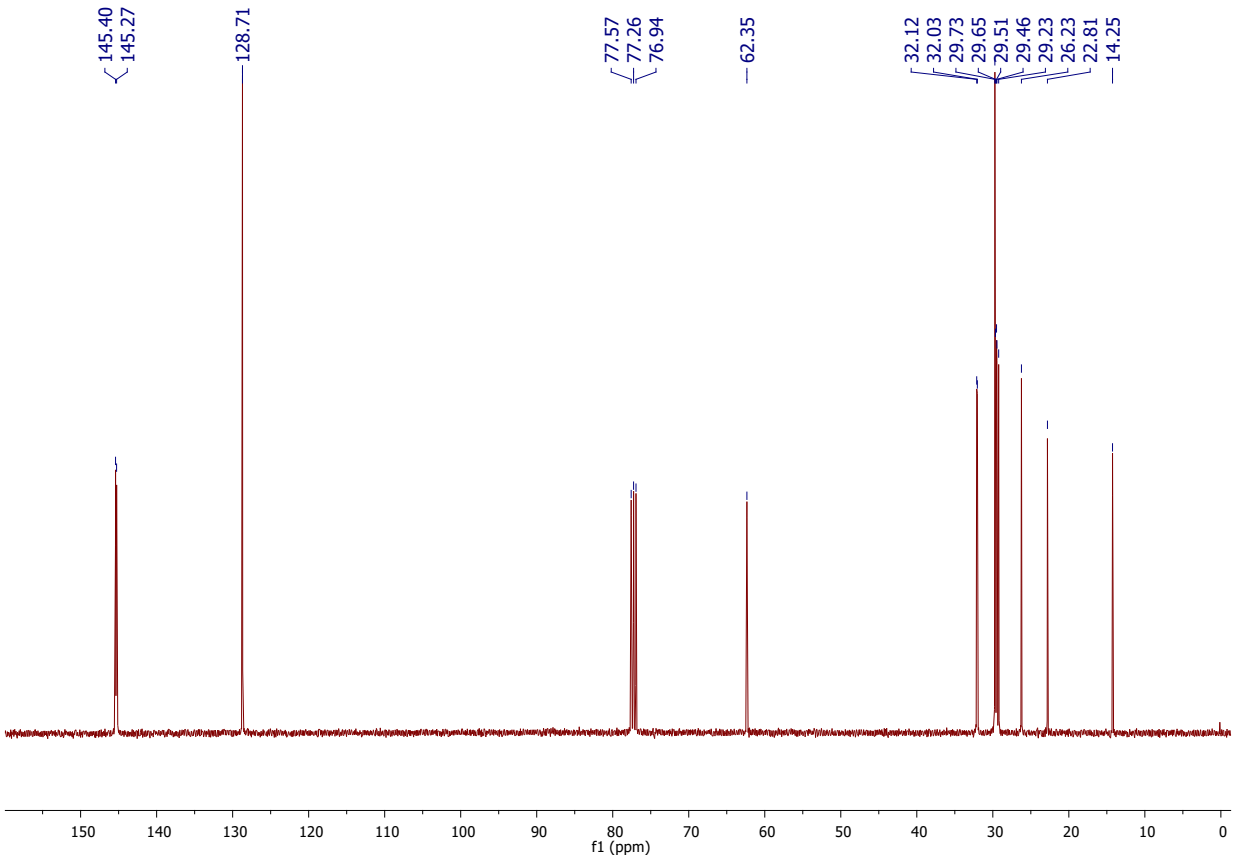
HRMS: Calculated for [M]+ (m/z): $C_{17}H_{30}N^{+}$ 248; Found: 248.

Fig. S2. ^{1}H NMR spectra of N-dodecylpyridinium bromide (DPB).



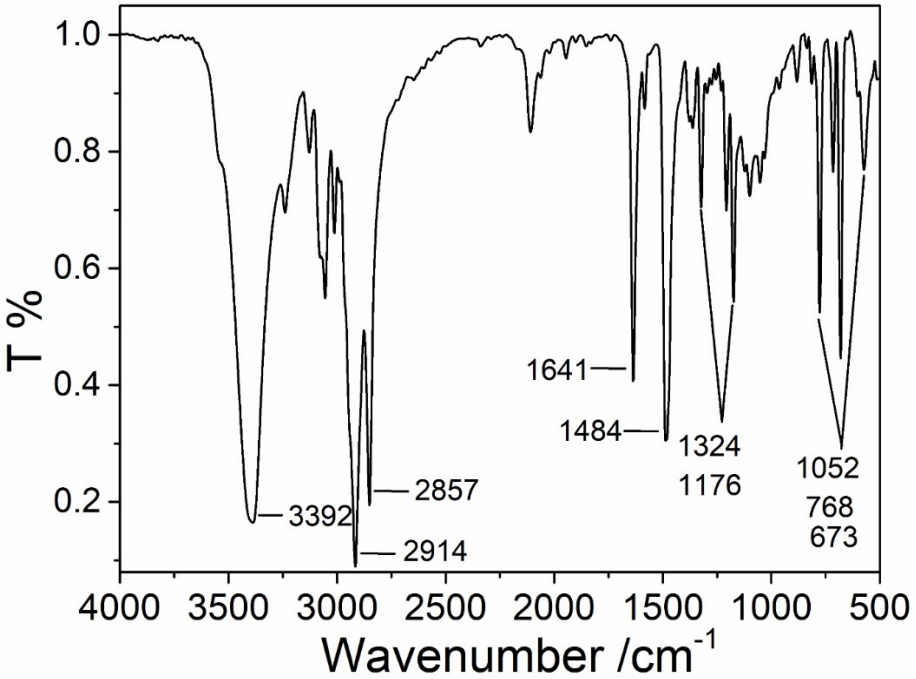
^{1}H NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 0.88 (t, j = 6 Hz, 3H, dodecyl-CH_3), 1.23 (brs, 16H, dodecyl C_4, C_5, C_6, C_7, C_8, C_9, C_{10}, C_{11}-H), 2.06 (t, j=6Hz,2H, dodecyl C_3-H), 2.35 (brs, 2H, C_2-H), 4.99 (t, j=6Hz, 2H, dodecyl C_1-H),8.20 (t, j=6Hz, 2H, $NCH(CH)_2$), 8.58 (m, 1H, NCHCHCH), 9.47 (d,j=4Hz, 2H, $N(CH)_2$) ppm.

Fig. S3. ^{13}C NMR of N-dodecylpyridinium bromide (DPB).



^{13}C NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 14.25, 22.81, 26.23, 29.23,29.46, 29.51, 29.65, 29.73, 32.03, 32.12, 62.35, 128.71, 145.27, 145.40.

Fig. S4. FTIR spectra for N-dodecylpyridinium bromide (DPB).

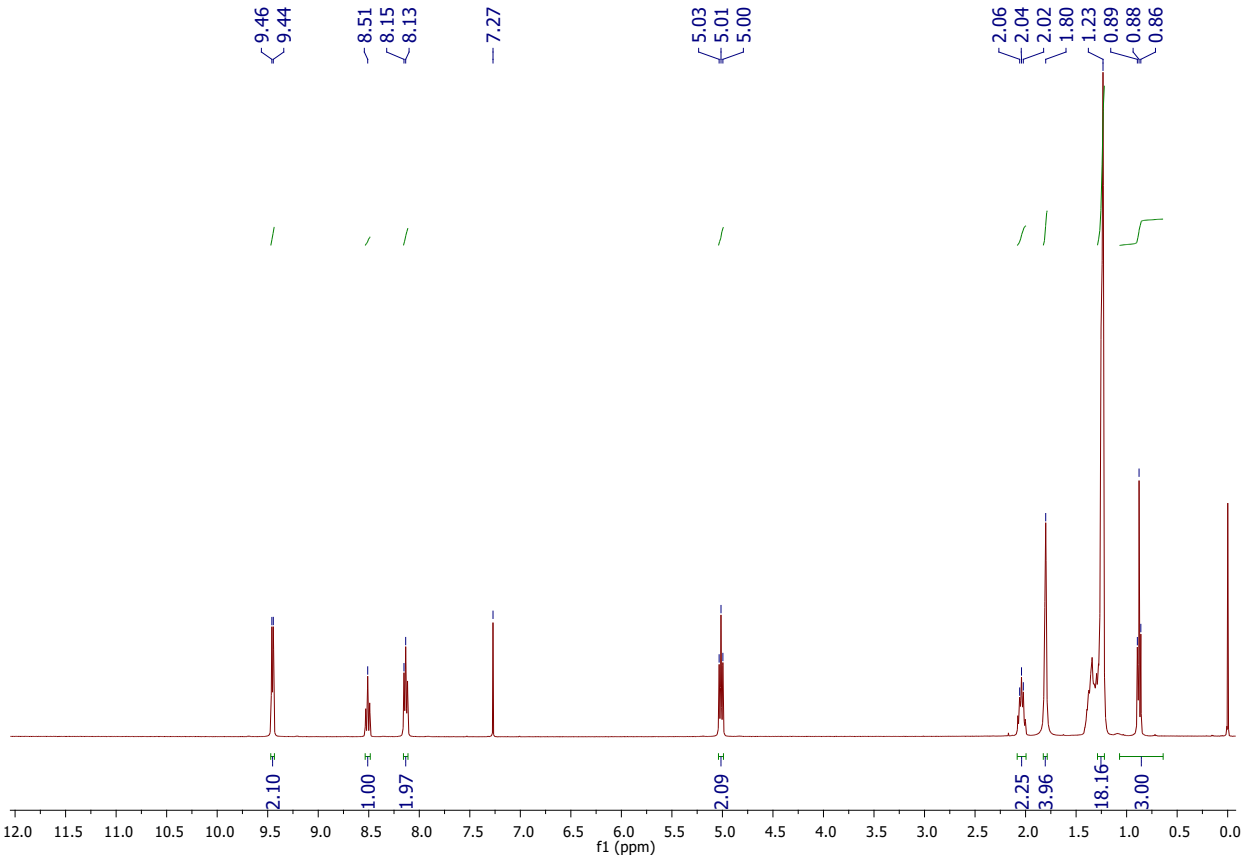


FTIR: ν_{max} (neat): 3392 cm^{-1} (aromatic C-H stretching), 2914 & 2857 cm^{-1} (aliphatic C-H stretching), 1641 cm^{-1} (C=N stretching), 1484 cm^{-1} (CH_2 bending), 1324 cm^{-1} (CH_2 bending), 1176 cm^{-1} (C-N stretching), 1052, 768, and 673 cm^{-1} (symmetrical deformations of -CH_3 groups).

Fig. S5. HRMS spectra of N-tetradecylpyridinium bromide (TPB).

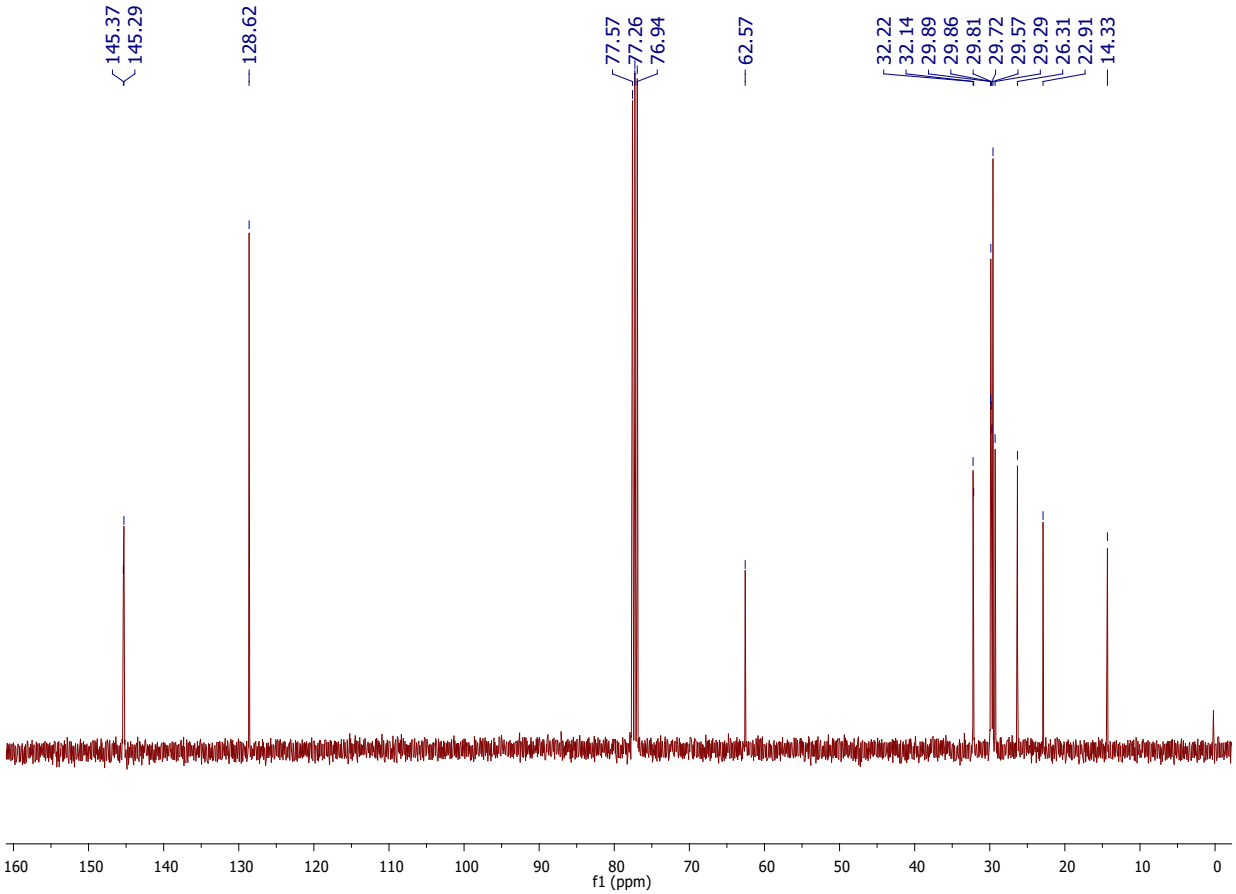
HRMS: Calculated for [M]+ (m/z): $C_{19}H_{34}N^+$ 276; Found: 276.

Fig. S6. [1]H NMR spectra of N-tetradecylpyridinium bromide (TPB).



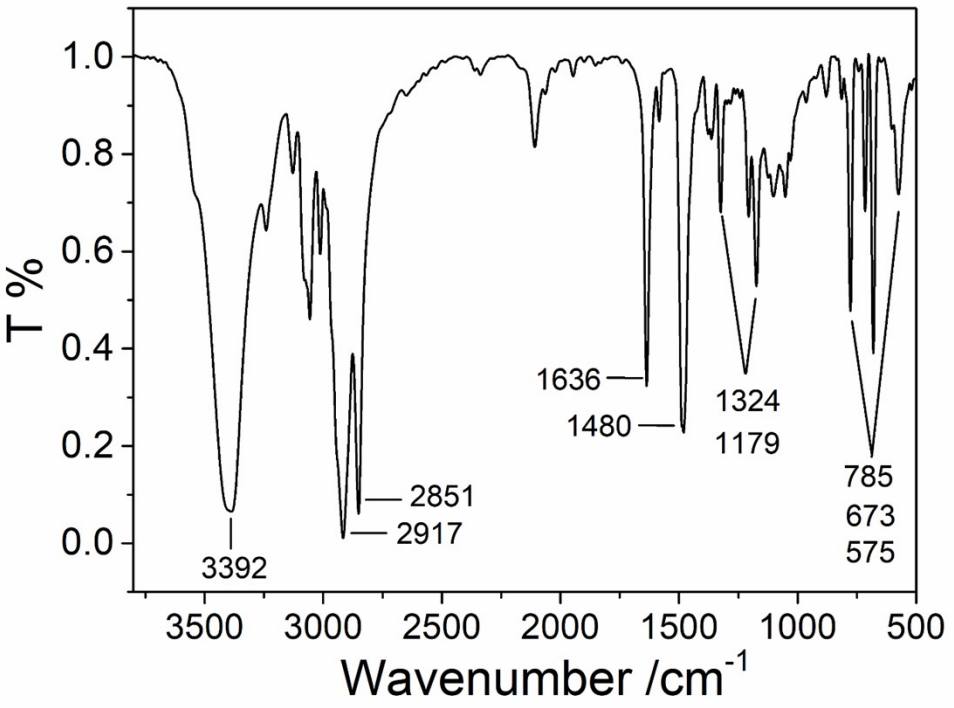
[1]H NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 0.89 (t, j=6 Hz, 3H, dodecyl-CH_3), 1.23 (br s, 18H, dodecyl C_5, C_6, C_7, C_8, C_9, C_{10}, C_{11}, C_{12}, C_{13}-H), 1.80 (br s, 4H, dodecyl C_3, C_4-H), 2.06 (t, j=8 Hz, 2H, dodecyl C_2-H), 5.03 (t, j=6 Hz, 2H, dodecyl C_1-H), 8.15 (d, j= 4Hz, 2H, $NCH(CH)_2$), 8.51 (s, 1H, NCHCHCH), 9.46 (d, j=4 Hz, 2H, $N(CH)_2$) ppm.

Fig. S7. ^{13}C NMR spectra of N-tetradecylpyridinium bromide (TPB).



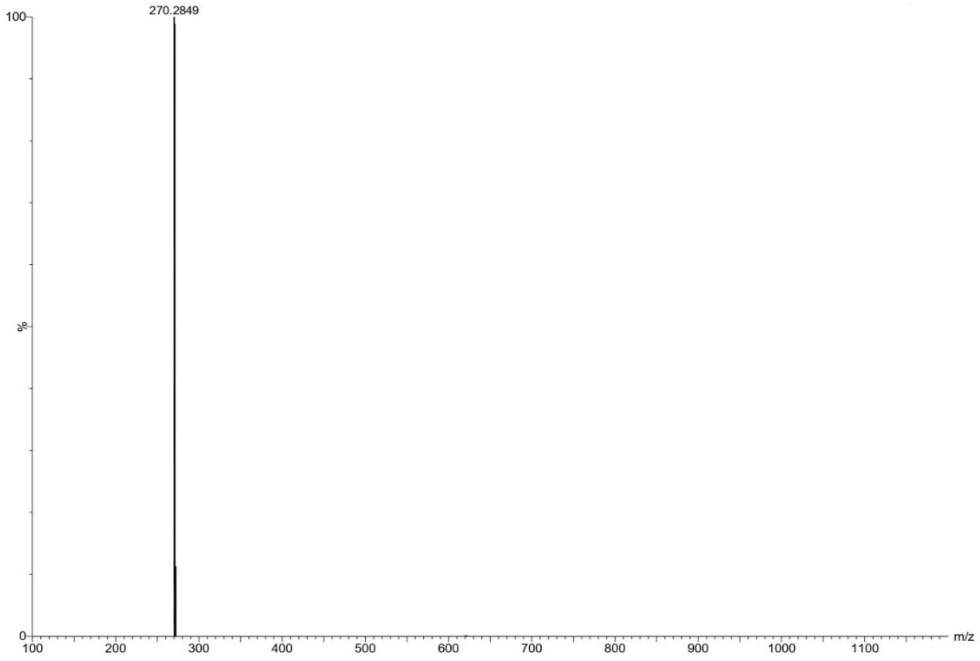
13C NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 14.33, 22.91, 26.31, 29.29, 29.57, 29.72, 29.81, 29.86, 29.89, 32.14, 32.22, 62.57, 128.62, 145.29, 145.37.

Fig. S8. FTIR spectra of N-tetradecylpyridinium bromide (TPB).



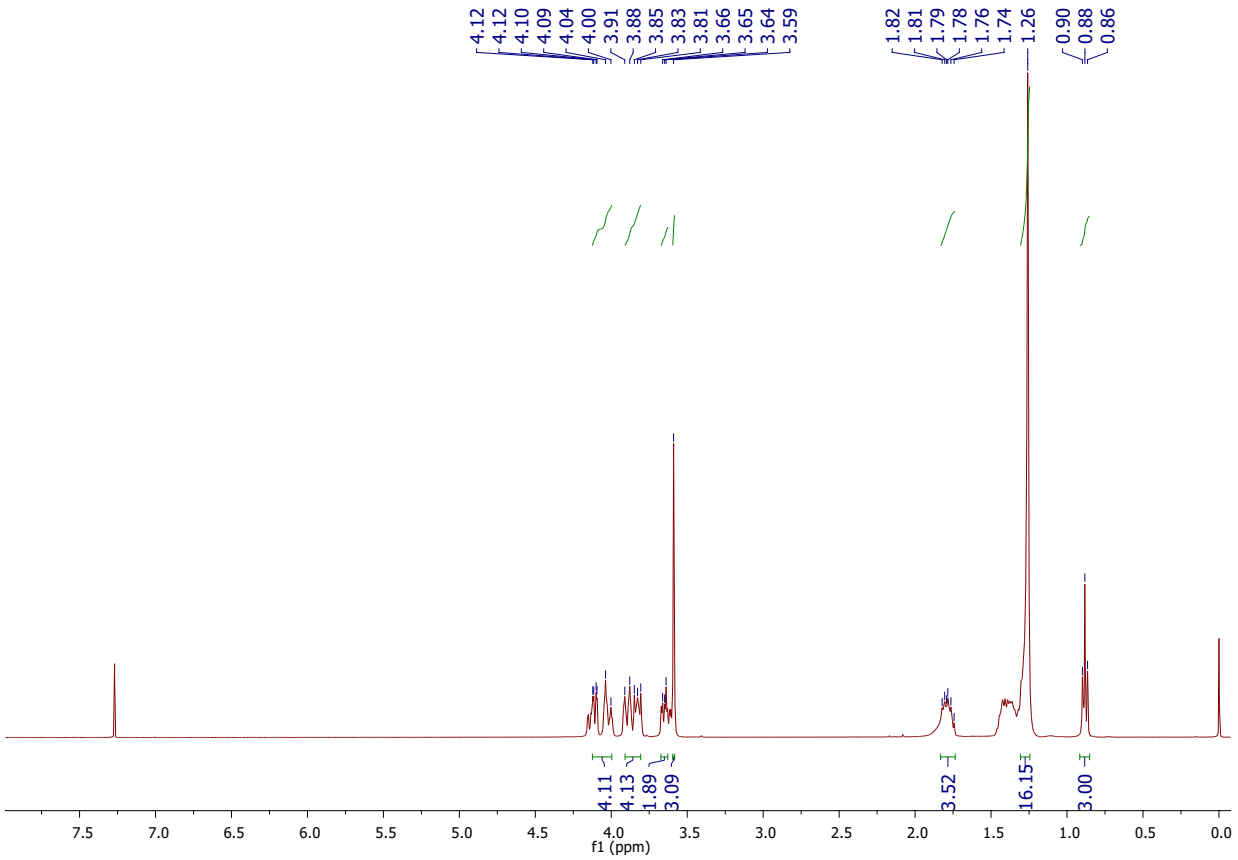
FTIR: ν_{max} (neat): 3392 cm^{-1} (aromatic C-H stretching), 2917 & 2851 cm^{-1} (aliphatic, C-H stretching), 1636 cm^{-1} (C=N stretching), 1480 cm^{-1} (CH_2 bending), 1324 cm^{-1} (CH_2 bending), 1179 cm^{-1} (C-N stretching), 785, 673, and 575 cm^{-1} (symmetrical deformations of -CH_3 groups).

Fig. S9. HRMS spectra of N-dodecyl-N-methylmorpholinium Bromide (DMB).



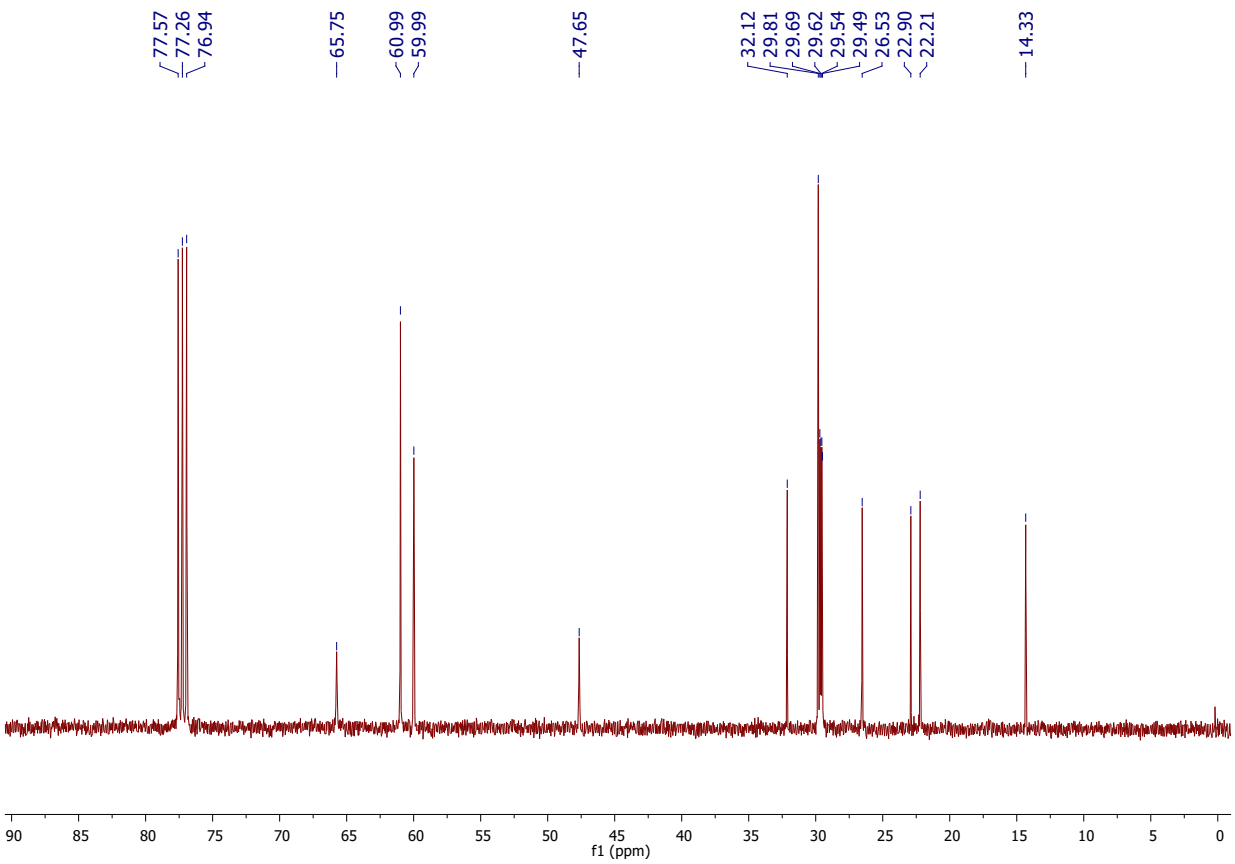
HRMS: Calculated for [M]+ (m/z): $C_{17}H_{36}ON^{+}$ 270; Found: 270.

Fig. S10. [1]H NMR spectra of N-dodecyl-N-methylmorpholinium Bromide (DMB).



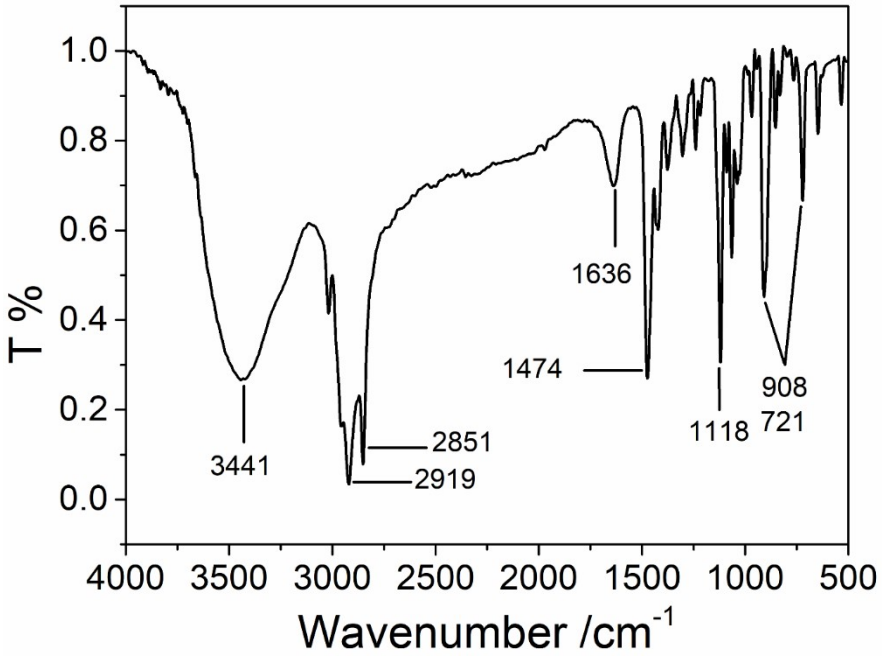
[1]H-NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 0.90 (t, 3H, dodecyl-CH_3), 1.26 (br s, 16H, dodecyl C_7, C_8, C_9, C_{10}, C_{11}, C_{12}, C_{13}-H), 1.82 (m, 4H, dodecyl C_5,C_6), 3.59 (br s, 3H, NCH_3),3.66 (t, j= 2H, NCH_2),3.91 (m,4H, $N(CH_2)_2$),4.12 (m,4H, $O(CH_2)_2$).

Fig. S11. ^{13}C NMR of N-dodecyl-N-methylmorpholinium Bromide (DMB).



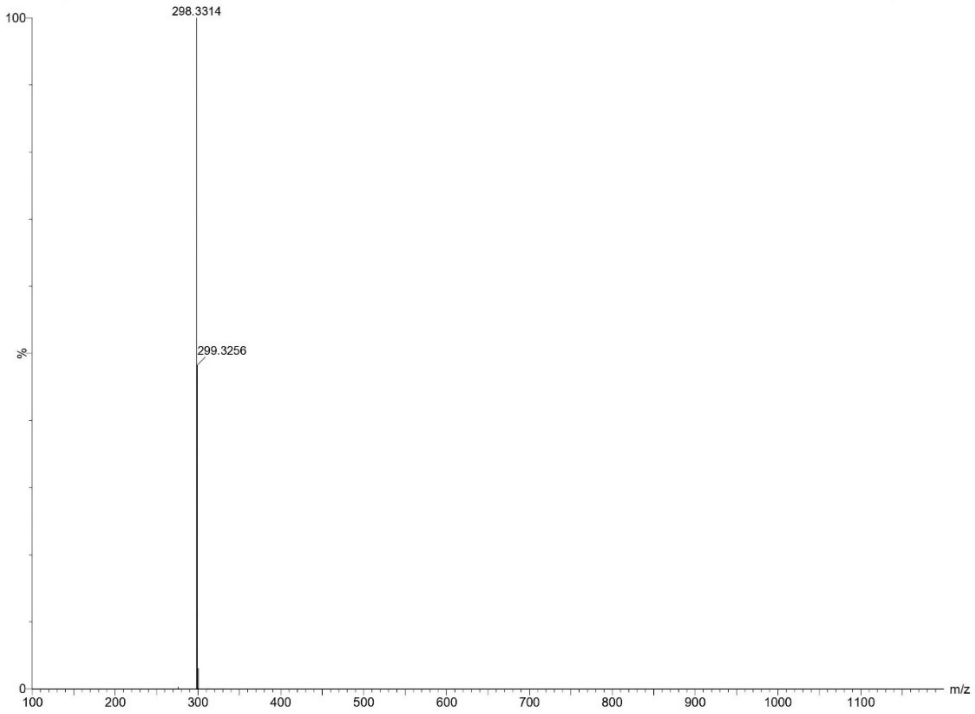
^{13}C NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 14.33, 22.21, 22.90, 26.53, 29.49, 29.54, 29.62, 29.69, 29.81, 32.12, 47.65, 59.99, 60.99, 65.75.

Fig. S12. FTIR spectra of N-dodecyl-N-methylmorpholinium Bromide (DMB).



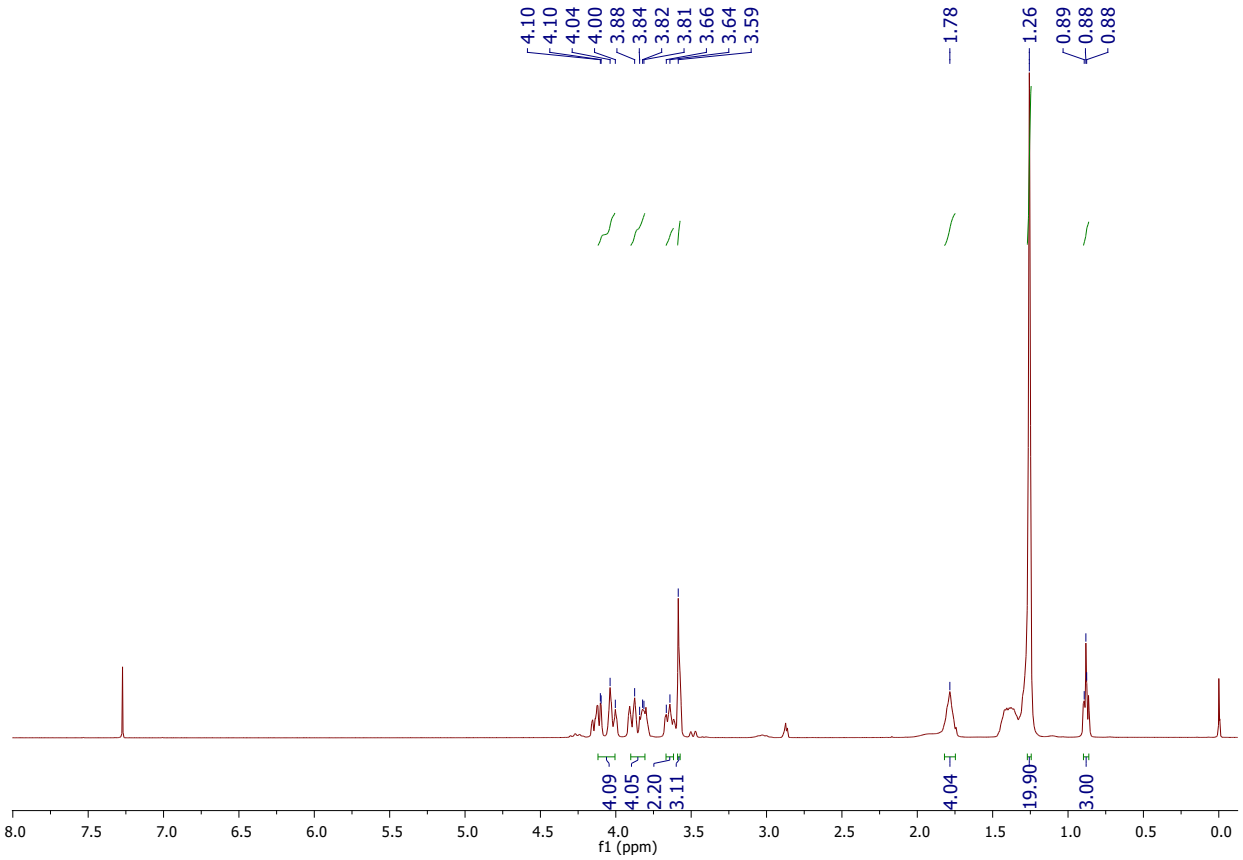
FTIR: ν_{max} (neat): 3441 cm^{-1} (O-H stretching), 2919 and 2851 cm^{-1} (aliphatic, C-H stretching), 1636 cm^{-1} (C=N stretching), 1474 cm^{-1} (CH_2 bending), 1118 cm^{-1} (C-N stretching), 908, and 721 cm^{-1} (symmetrical deformations of -CH_3 groups).

Fig. S13. HRMS spectra of N-tetradecyl-N-methylmorpholinium Bromide (TMB).



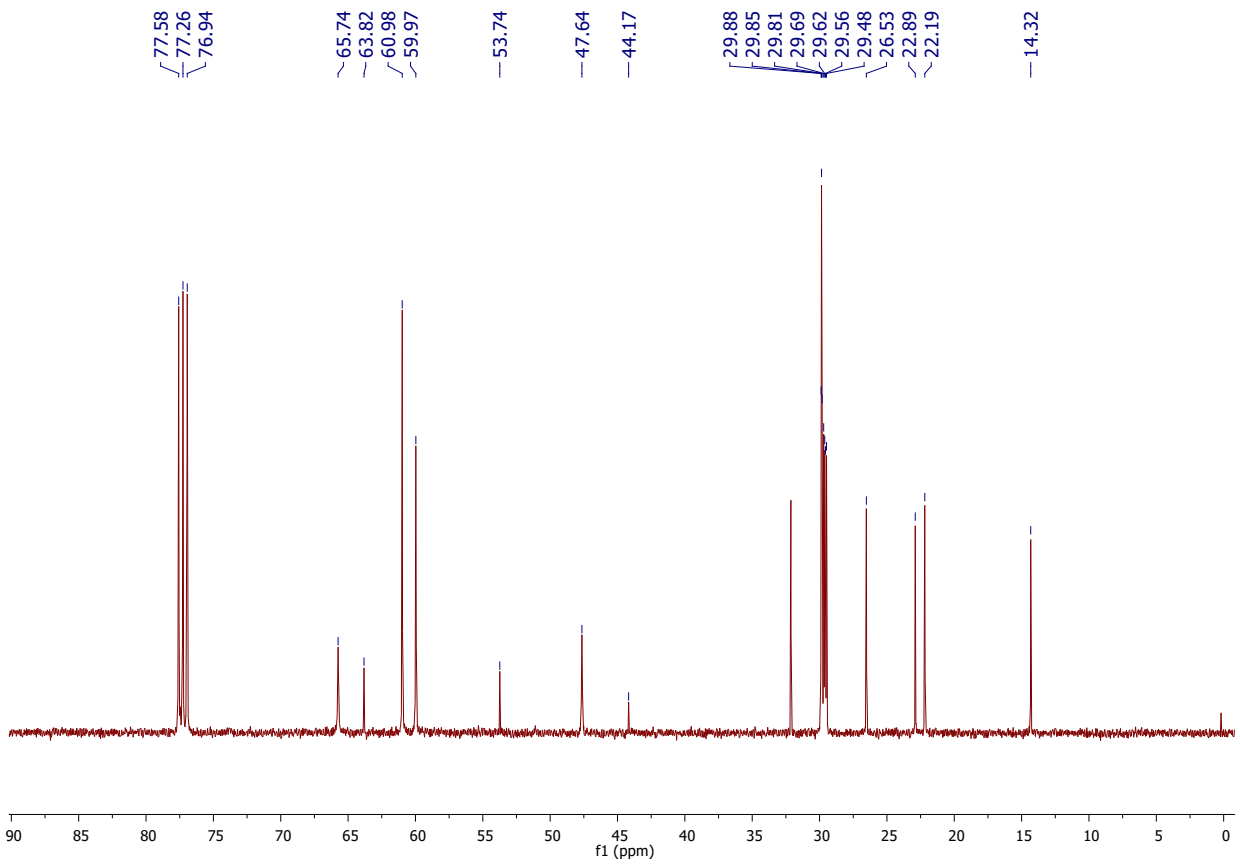
HRMS: Calculated for [M]+ (m/z): $C_{19}H_{40}ON^{+}$ 298; Found: 298.

Fig. S14. [1]H NMR spectra of N-tetradecyl-N-methylmorpholinium Bromide (TMB).



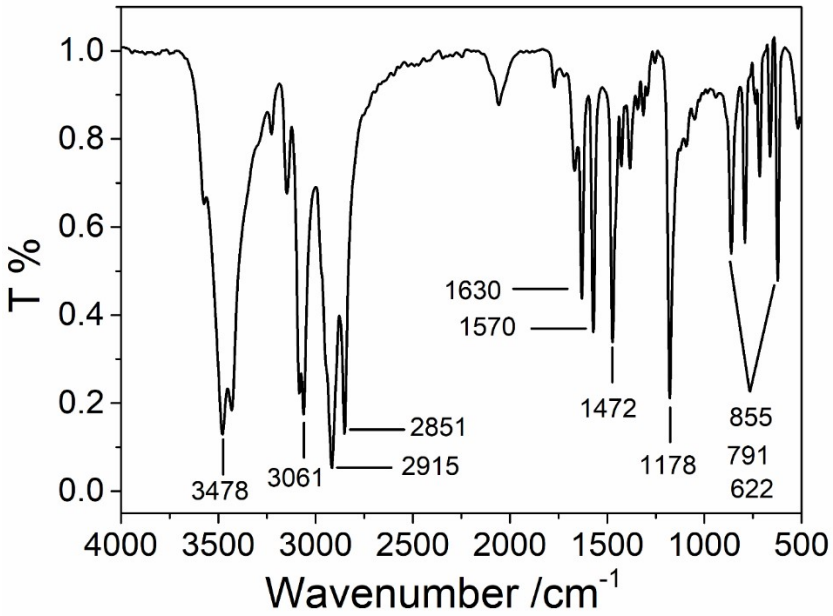
[1]H-NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 0.90 (t, j=8 Hz, 3H, dodecyl-CH_3), 1.26 (br s, 20H, dodecyl C_4, C_5, C_6, C_7, C_8, C_9, C_{10}, C_{11}, C_{12}, C_{13}-H), 1.78 (t, j=4Hz,2H, dodecyl C_2), 2.37 (brs, 2H, dodecyl C_3), 3.59 (s, 3H, NCH_3), 3.66 (d, j=8Hz, 2H, dodecyl C_1), 3.88 (m, 2H, $N(CH_2)_2$),4.10 (m,4H, $O(CH_2)_2$).

Fig. S15. ^{13}C NMR spectra of N-tetradecyl-N-methylmorpholinium Bromide (TMB).



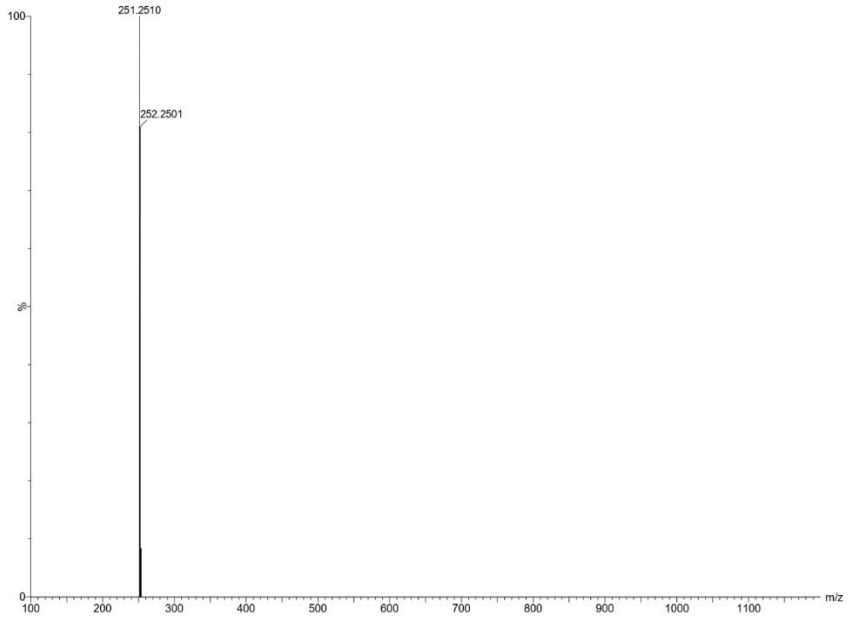
^{13}C-NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS):14.32, 22.19, 22.89, 26.53, 29.48, 29.56, 29.62, 29.69, 29.81, 29.85, 29.88, 32.13, 44.17, 47.64, 53.74, 59.97, 60.98, 63.82.

Fig. S16. FTIR spectra of N-tetradecyl-N-methylmorpholinium Bromide (TMB).



FTIR: ν_{max} (neat): 3478 (O-H stretching), 3061 (N-H axial deformation), 2915 and 2851 cm^{-1} (aliphatic, C-H stretching), 1630 and 1570 cm^{-1} (C=N stretching), 1472 cm^{-1} (CH_2 bending), 1178 cm^{-1} (C-N stretching), 855, 791, and 622 cm^{-1} (symmetrical deformations of -CH_3 groups).

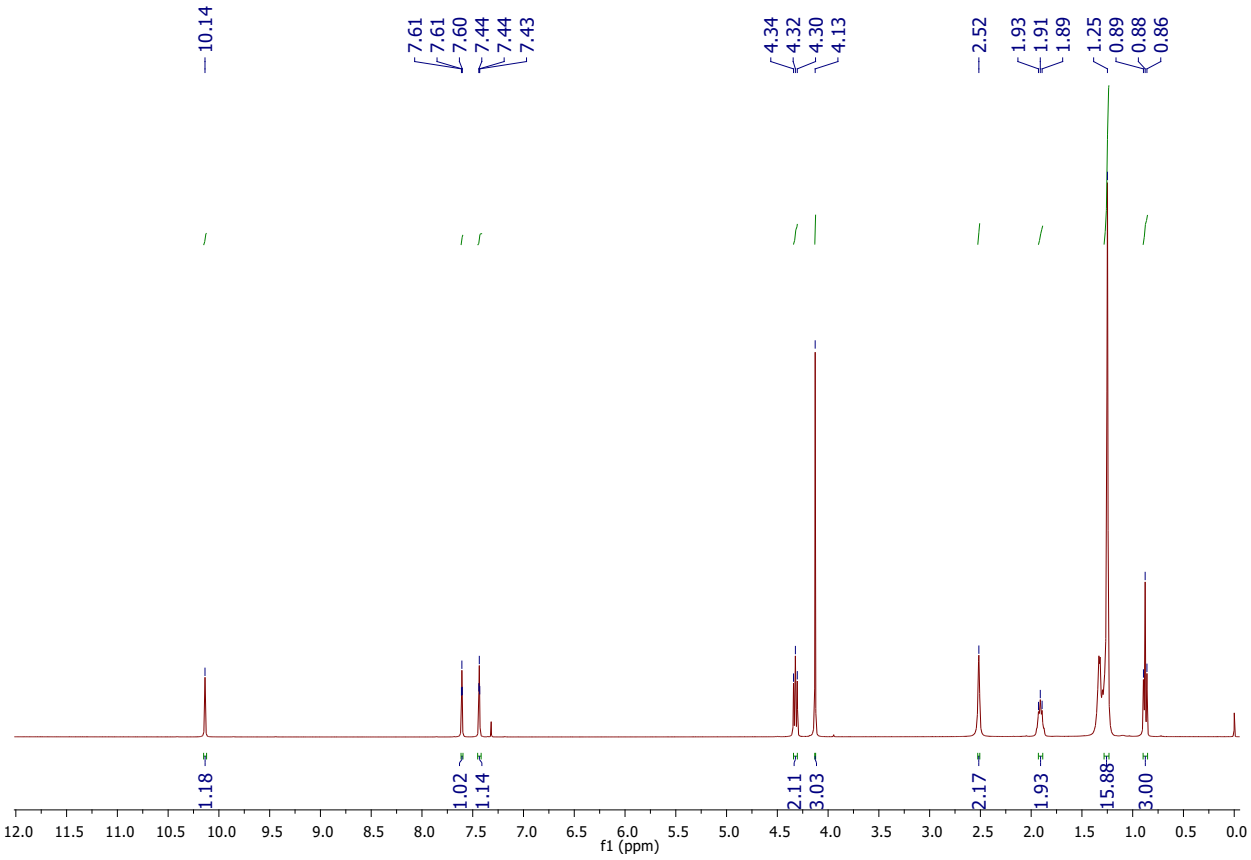
Fig. S17. HRMS spectra of 1-dodecyl-3-methylimidazolium Bromide (DIB).



HRMS: Calculated for [M]+ (m/z): $C_{16}H_{31}N_2^+$ 251; Found: 251.

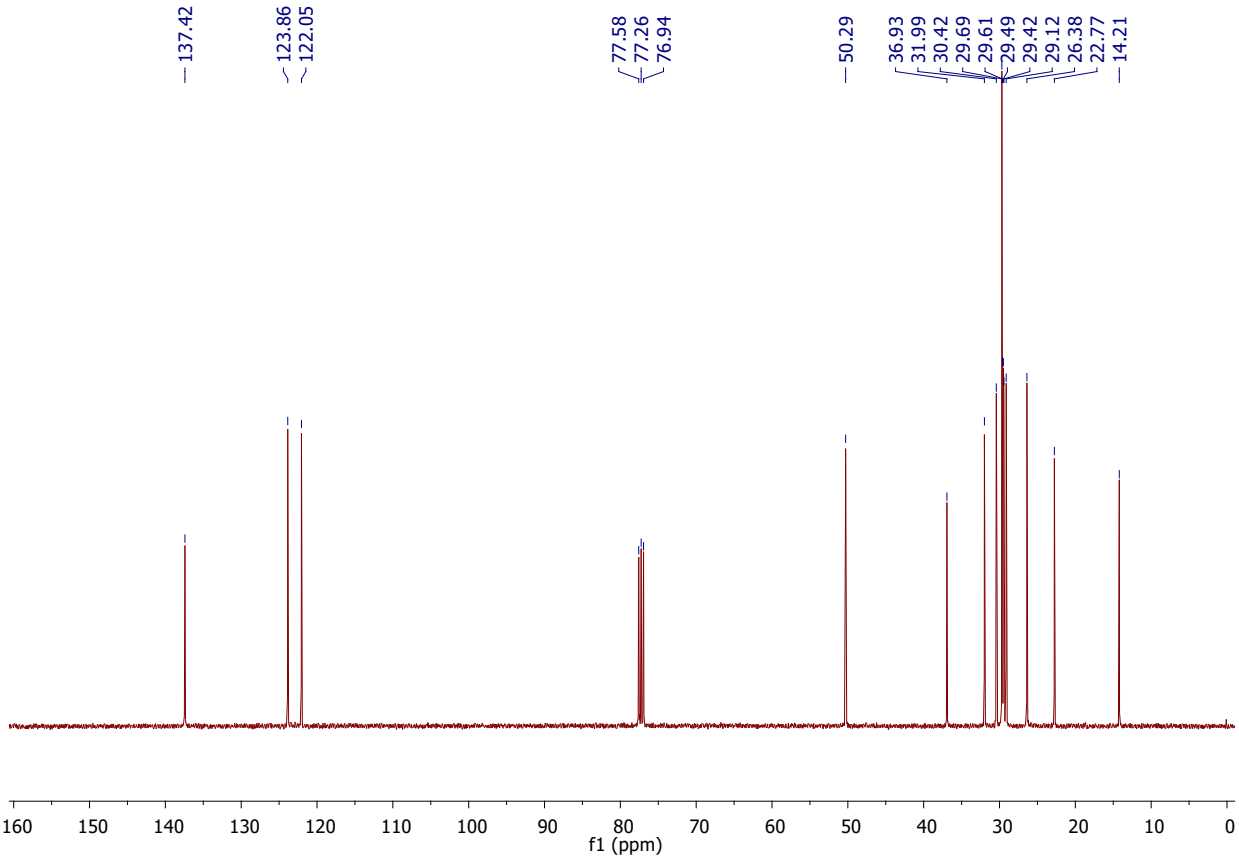
.

Fig. S18. ^{1}H NMR spectra of 1-dodecyl-3-methylimidazolium Bromide (DIB).



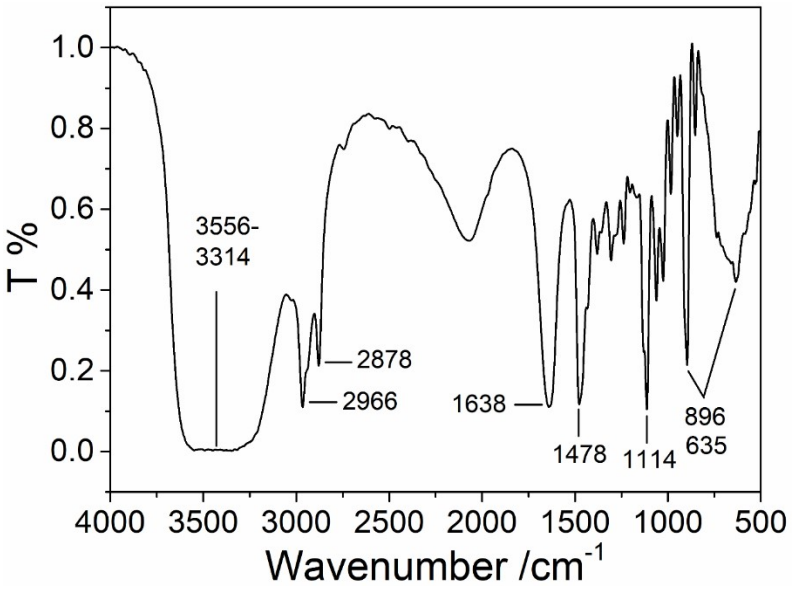
^{1}H NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 0.89 (t, j=6 Hz, 3H, dodecyl-CH_3), 1.25 (br s, 16H, dodecyl C_4, C_5, C_6, C_7, C_8, C_9, C_{10}, C_{11}-H), 1.93 (t, j=8Hz, 2H, dodecyl C_3-H), 2.52 (brs, 2H, dodecyl C_2-H), 4.13 (s, 3H, NCH_3), 4.34 (t, j=8Hz, 2H, dodecyl C_1-H), 7.44 (t, j=2Hz, 1H, C_4-H), 7.61 (t, j=2Hz, 1H, C_5-H), 10.14 (s, 1H, C_2-H).

Fig. S19. ^{13}C NMR spectra of 1-dodecyl-3-methylimidazolium Bromide (DIB).



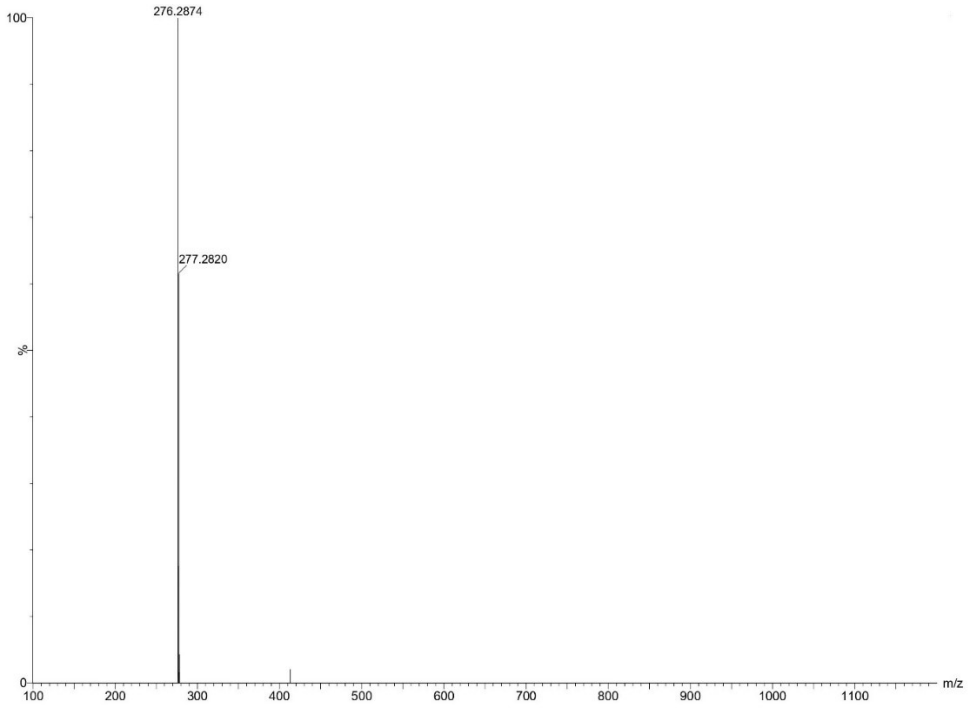
^{13}C NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS):14.21, 22.77, 26.38, 29.12, 29.42, 29.49, 29.61, 29.69, 30.42, 31.99, 36.93, 50.29, 122.05, 123.86, 137.42.

Fig. S20. FTIR spectra of 1-dodecyl-3-methylimidazolium Bromide (DIB).



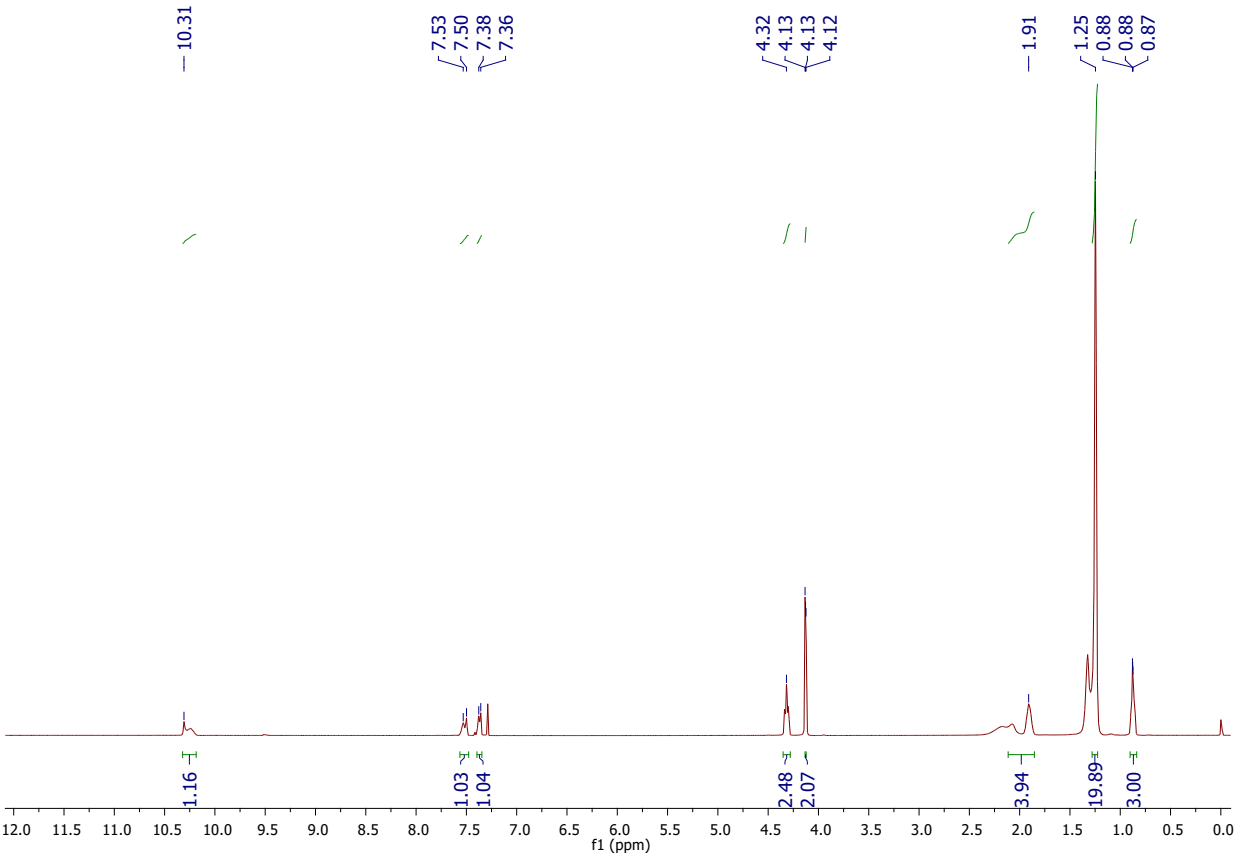
FTIR: ν_{max} (neat): 3556-3314 cm^{-1} (aromatic C–H stretching), 2966, 2878 (aliphatic C–H stretching), 1638 cm^{-1} (C=N stretching), 1478 (CH_2 bending), 1114 cm^{-1} (C–N stretching), 896, and 635 cm^{-1} (symmetrical deformations of -CH_3 groups).

Fig.S21. HRMS spectra of 1-tetradecyl-3-methylimidazolium Bromide (TIB).



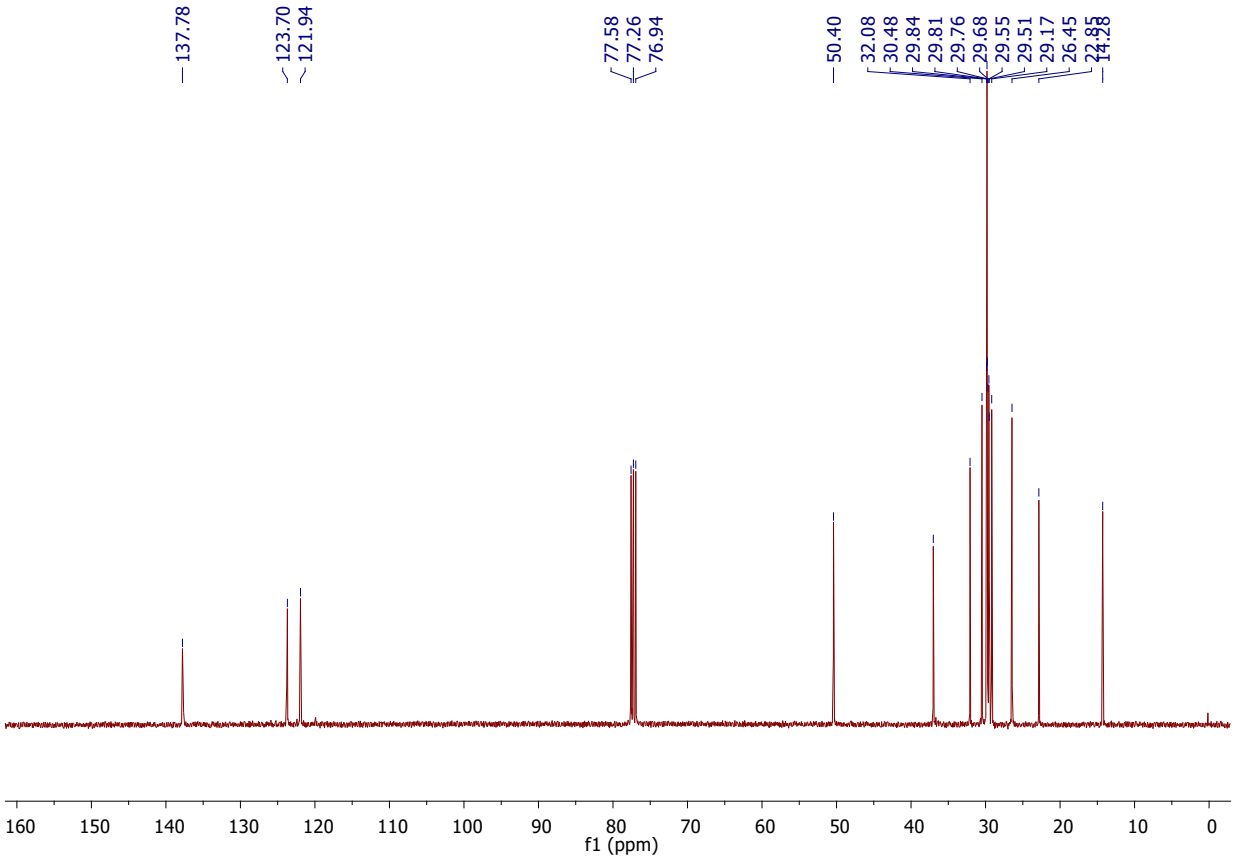
HRMS: Calculated for [M]+ (m/z): $C_{18}H_{35}N_2^+$ 279; Found: 276.

Fig. S22. [1]H NMR spectra of 1-tetradecyl-3-methylimidazolium Bromide (TIB).



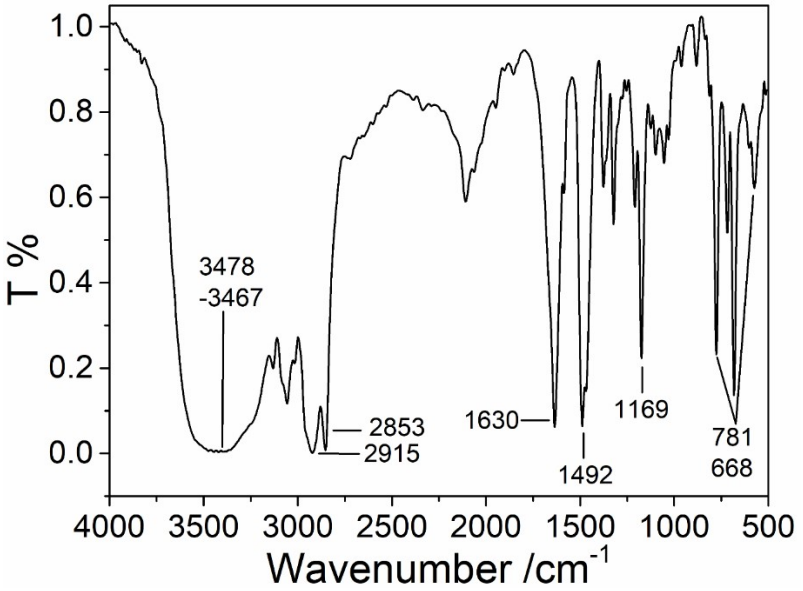
[1]H NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 0.88 (t, j= 2Hz, 3H, dodecyl-CH_3), 1.25 (br s, 18H, dodecyl C_4, C_5, C_6, C_7, C_8, C_9, C_{10},C_{11}, C_{12}, C_{13}-H), 1.91 (brs, 4H, dodecyl C_2, C_3-H), 4.13 (t, j=2 Hz,2H, dodecyl C_1-H), 4.32 (s, 3H, NCH_3), 7.38 (d, j= 4 Hz, 1H, C_4-H), 7.53 (d, j= 6 Hz, 1H, C_5-H), 10.31 (s, 1H, C_2-H).

Fig. S23. HRMS spectra of 1-tetradecyl-3-methylimidazolium Bromide (TIB).



^{13}C NMR (400 MHz: $CDCl_3$, δ/ppm relative to TMS): 14.28, 22.85, 26.45, 29.17, 29.51, 29.55, 29.68, 29.76, 29.81, 29.84, 30.48, 37.01, 50.40, 121.94, 123.70, 137.78.

Fig. S24. FTIR spectra of 1-tetradecyl-3-methylimidazolium Bromide (TIB).



FTIR: ν_{max} (neat): 3478-3467 cm^{-1} (aromatic C–H stretching), 2915, 2853 cm^{-1} (aliphatic C–H stretching), 1630 cm^{-1} (C=N stretching), 1492 cm^{-1} (CH_2 bending), 1169 cm^{-1} (C–N stretching), 781, 668 cm^{-1} (symmetrical deformations of -CH_3 groups).