

Novel biocompatible cholinium-based ionic liquids - toxicity and biodegradability

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Cholinium ethanoate: ¹H NMR (D₂O, 400 MHz): δ/ppm = 1.86 (s, 3H, CH₃COO); 3.15 (s, 9H, N(CH₃)₃); 3.46 (t, *J* = 4.8 Hz, 2H, CH₂OH); 4.01 (m, 2H, NCH₂). ¹³C NMR (D₂O, 100 MHz): δ/ppm = 23.591 (CH₃COO); 54.404 (t, N(CH₃)₃); 56.038 (CH₂OH); 67.839 (t, NCH₂); 181.714 (COO). MS ES+ *m/z* (% rel. Intensity): 104 M⁺ (100). Calc. 104.1075, found 104.1078.

Cholinium propanoate: ^1H NMR (D_2O , 400 MHz): $\delta/\text{ppm} = 0.88$ (t, $J = 7.7$ Hz, 3H, CH_3CH_2); 1.99 (q, $J = 7.5$ Hz, 2H, CH_2COO); 3.02 (s, 9H, $\text{N}(\text{CH}_3)_3$); 3.34 (t, $J = 5.0$ Hz, 2H, CH_2OH); 3.87 (m, 2H, NCH_2). ^{13}C NMR (D_2O , 100 MHz): $\delta/\text{ppm} = 10.21$ (CH_3CH_2); 30.65 (CH_2COO); 53.77 (t, $\text{N}(\text{CH}_3)_3$); 55.47 (CH_2OH); 57.33 (t, NCH_2); 184.21 (COO). MS ES+ m/z (% rel. Intensity): 104 M^+ (100). Calc. for $\text{C}_5\text{H}_{14}\text{NO}$ 104.1075, found 104.1079. MS ES- m/z (% rel. Intensity): 73 M^- (100). Calc. for $\text{C}_3\text{H}_5\text{O}_2$ 73.0710, found 73.0290.

Cholinium butanoate: ^1H NMR (D_2O , 400 MHz): $\delta/\text{ppm} = 0.76$ (t, $J = 7.5$ Hz, 3H, CH_3CH_2); 1.42 (m, 2H, CH_3CH_2); 2.02 (t, $J = 7.1$ Hz, 2H, CH_2COO); 3.07 (s, 9H, $\text{N}(\text{CH}_3)_3$); 3.38 (t, $J = 4.7$ Hz, 2H, CH_2OH); 3.92 (m, 2H, NCH_2). ^{13}C NMR (D_2O , 100 MHz): $\delta/\text{ppm} = 13.26$ (CH_3CH_2); 19.34 (CH_3CH_2); 39.62 (CH_2COO); 53.81 (t, $\text{N}(\text{CH}_3)_3$); 55.52 (CH_2OH); 67.6 (t, NCH_2); 183.79 (COO). MS ES+ m/z (% rel. Intensity): 104 M^+ (100). Calc. for $\text{C}_5\text{H}_{14}\text{NO}$ 104.1075, found 104.1076. MS ES- m/z (% rel. Intensity): 87 M^- (100). Calc. for $\text{C}_4\text{H}_7\text{O}_2$ 87.0446, found 87.0443.

Cholinium pentanoate: ^1H NMR (D_2O , 400 MHz): $\delta/\text{ppm} = 0.86$ (t, $J = 6.0$ Hz, 3H, CH_3CH_2); 1.27 (m, 2H, CH_3CH_2); 1.50 (m, 2H, $\text{CH}_3\text{CH}_2\text{CH}_2$); 2.15 (t, $J = 6.0$ Hz, 2H, CH_2COO); 3.17 (s, 9H, $\text{N}(\text{CH}_3)_3$); 3.49 (t, $J = 6.0$ Hz, 2H, CH_2OH); 4.02 (m, 2H, NCH_2). ^{13}C NMR (D_2O , 100 MHz): $\delta/\text{ppm} = 13.73$ (CH_3CH_2); 22.55 (CH_3CH_2); 28.74 ($\text{CH}_3\text{CH}_2\text{CH}_2$); 37.66 (CH_2COO); 54.26 (t, $\text{N}(\text{CH}_3)_3$); 55.98 (CH_2OH); 67.77 (t, NCH_2); 184.24 (COO). MS ES+ m/z (% rel. Intensity): 104 M^+ (100). Calc. for $\text{C}_5\text{H}_{14}\text{NO}$ 104.1075, found 104.1079. MS ES- m/z (% rel. Intensity): 115 M^- (100). Calc. for $\text{C}_5\text{H}_9\text{O}_2$ 101.0603, found 101.0622.

Cholinium hexanoate: ^1H NMR (D_2O , 400 MHz): δ/ppm = 0.76 (t, J = 7.2 Hz, 3H, CH_3CH_2); 1.17 (m, 4H, $\text{CH}_3(\text{CH}_2)_2$); 1.43 (m, 2H, $\text{CH}_2\text{CH}_2\text{COO}$); 2.04 (t, J = 7.6 Hz, 2H, CH_2COO); 3.08 (s, 9H, $\text{N}(\text{CH}_3)_3$); 3.40 (t, J = 5.0 Hz, 2H, CH_2OH); 3.94 (m, 2H, NCH_2). ^{13}C NMR (D_2O , 100 MHz): δ/ppm = 13.30 (CH_3CH_2); 21.77 (CH_3CH_2); 25.58 ($\text{CH}_3\text{CH}_2\text{CH}_2$); 31.01 ($\text{CH}_2\text{CH}_2\text{COO}$); 37.63 (CH_2COO); 53.82 (t, $\text{N}(\text{CH}_3)_3$); 55.53 (CH_2OH); 67.37 (t, NCH_2); 184.00 (COO). MS ES+ m/z (% rel. Intensity): 104 M^+ (100). Calc. for $\text{C}_5\text{H}_{14}\text{NO}$ 104.1075, found 104.1077. MS ES- m/z (% rel. Intensity): 115 M^- (100). Calc. for $\text{C}_6\text{H}_{11}\text{O}_2$ 115.0759, found 115.0758.

Cholinium octanoate: ^1H NMR (D_2O , 400 MHz): δ/ppm = 0.76 (t, J = 7.0 Hz, 3H, CH_3CH_2); 1.18 (m, 8H, $\text{CH}_3(\text{CH}_2)_4$); 1.43 (m, 2H, $\text{CH}_2\text{CH}_2\text{COO}$); 2.05 (t, J = 7.7 Hz, 2H, CH_2COO); 3.09 (s, 9H, $\text{N}(\text{CH}_3)_3$); 3.40 (t, J = 4.9 Hz, 2H, CH_2OH); 3.94 (m, 2H, NCH_2). ^{13}C NMR (D_2O , 100 MHz): δ/ppm = 13.55 (CH_3CH_2); 22.12 (CH_3CH_2); 26.02 ($\text{CH}_3\text{CH}_2\text{CH}_2$); 28.45 ($\text{CH}_3(\text{CH}_2)_2\text{CH}_2$); 28.91 ($\text{CH}_3(\text{CH}_2)_3\text{CH}_2$); 31.22 ($\text{CH}_2\text{CH}_2\text{COO}$); 37.74 (CH_2COO); 53.85 (t, $\text{N}(\text{CH}_3)_3$); 55.54 (CH_2OH); 67.40 (t, NCH_2); 183.65 (COO). MS ES+ m/z (% rel. Intensity): 104 M^+ (100). Calc. for $\text{C}_5\text{H}_{14}\text{NO}$ 104.1075, found 104.1077. MS ES- m/z (% rel. Intensity): 143 M^- (100). Calc. for $\text{C}_8\text{H}_{15}\text{O}_2$ 143.1072, found 143.1060.

Cholinium decanoate: ^1H NMR (D_2O , 400 MHz): δ/ppm = 0.78 (t, J = 7.0 Hz, 3H, CH_3CH_2); 1.19 (m, 12H, $\text{CH}_3(\text{CH}_2)_6$); 1.44 (m, 2H, $\text{CH}_2\text{CH}_2\text{COO}$); 2.05 (t, J = 7.5 Hz, 2H, CH_2COO); 3.10 (s, 9H, $\text{N}(\text{CH}_3)_3$); 3.41 (t, J = 4.9 Hz, 2H, CH_2OH); 3.95 (m, 2H, NCH_2). ^{13}C NMR (D_2O , 100 MHz): δ/ppm = 13.73 (CH_3CH_2); 22.45 (CH_3CH_2); 26.25 ($\text{CH}_3\text{CH}_2\text{CH}_2$); 29.16 ($\text{CH}_3(\text{CH}_2)_2\text{CH}_2$); 29.29 ($\text{CH}_3(\text{CH}_2)_3\text{CH}_2$); 29.43 ($\text{CH}_3(\text{CH}_2)_4\text{CH}_2$); 29.44 ($\text{CH}_3(\text{CH}_2)_5\text{CH}_2$); 31.74 ($\text{CH}_2\text{CH}_2\text{COO}$); 37.85 (CH_2COO); 53.86 (t, $\text{N}(\text{CH}_3)_3$);

55.56 (CH₂OH); 67.44 (t, NCH₂); 183.03 (COO). MS ES+ *m/z* (% rel. Intensity): 104 M⁺ (100). Calc. for C₅H₁₄NO 104.1075, found 104.1075. MS ES- *m/z* (% rel. Intensity): 171 M⁻ (100). Calc. for C₁₀H₁₉O₂ 171.1385, found 171.1384.

Cholinium 2-methylpropanoate: ¹H NMR (D₂O, 400 MHz): δ/ppm = 0.9 (d, *J* = 7.0 Hz, 6H, (CH₃)₂CH); 2.35 (m, H, CH(CH₃)₂); 3.17 (s, 9H, N(CH₃)₃); 3.48 (t, *J* = 3.0 Hz, 2H, CH₂OH); 4.03 (m, 2H, NCH₂). ¹³C NMR (D₂O, 100 MHz): δ/ppm = 19.38 ((CH₃)₂CH); 35.89 (CHCOO); 53.81 (t, N(CH₃)₃); 55.53 (CH₂OH); 57.36 (t, NCH₂); 187.58 (COO). MS ES+ *m/z* (% rel. Intensity): 104 M⁺ (100). Calc. for C₅H₁₄NO 104.1075, found 104.1078. MS ES- *m/z* (% rel. Intensity): 87 M⁻ (100). Calc. for C₄H₇O₂ 87.0446, found 87.0448.

Cholinium 2,2-dimethylpropanoate: ¹H NMR (D₂O, 400 MHz): δ/ppm = 1.00 (s, 9H, C(CH₃)₃); 3.10 (s, 9H, N(CH₃)₃); 3.41 (t, *J* = 5.0 Hz, 2H, CH₂OH); 3.96 (m, 2H, NCH₂). ¹³C NMR (D₂O, 100 MHz): δ/ppm=27.47 (C(CH₃)₃); 39.76 (C(CH₃)₃); 53.82 (t, N(CH₃)₃); 55.54 (CH₂OH); 67.37 (t, NCH₂); 188.83 (COO). MS ES+ *m/z* (% rel. Intensity): 104 M⁺ (100). Calc. for C₅H₁₄NO 104.1075, found 104.1079. MS ES- *m/z* (% rel. Intensity): 101 M⁻ (100). Calc. for C₅H₉O₂ 101.0603, found 101.0603.