

The relationship between the structure and properties of Amino Acid Ionic Liquids

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SUPPLEMENTARY DATA

General Synthetic Methods The ¹H and ¹³C NMR spectra for obtained amino acid ionic liquids were recorded on a BRUKER DPX-400 spectrometer operating at 400 MHz (¹H) and 100 MHz (¹³C) as solutions in D₂O or DMSO. Chemical shifts are given in δ (ppm) and coupling constants *J* are given in Hz. Infrared spectra were recorded on Nicolet FT-IR 380 (Thermo Electron Corporation) in transmission mode on KBr pellets and are reported in wave numbers (cm⁻¹).

Tributylmethylammonium L-valinate [tBMA][L-Val]:

¹H NMR (400 MHz, DMSO-d₆) δ, ppm: 0.64 (d, 3H, *J* = 6.8 Hz, CH₃-Val); 0.78 (d, 3H, *J* = 6.9 Hz, CH₃-Val); 0.92 (t, 9H, *J* = 7.4 Hz, CH₃-cation); 1.24-1.34 (m, 6H, -CH₂- cation); 1.55-1.63 (m, 6H, -CH₂- cation); 1.83-1.90 (m, 1H, CH-Val); 2.56 (ov, 1H, -CH-Val); 2.94 (s, 3H, CH₃-cation); 3.19 (t, 6H, *J* = 8.4 Hz, -CH₂-cation); ¹³C NMR (100 MHz, DMSO-d₆) δ, ppm: 13.92 (CH₃- cation); 18.58 (CH₃-Val); 19.66 (CH₃-Val); 20.64 (-CH₂-cation); 23.55 (-CH₂-cation); 31.43 (CH-Val); 45.92 (CH₃-cation); 57.97 (-CH₂-cation); 78.70 (CH-Val); 176.26 (-COO⁻ Val).

Tributylmethylammonium L-leucinate [tBMA][L-Leu]:

¹H NMR (400 MHz, DMSO-d₆) δ, ppm: 0.77 (d, 3H, *J* = 6.6 Hz, CH₃-Leu); 0.82 (d, 3H, *J* = 6.6 Hz, CH₃-Leu); 0.92 (t, 9H, *J* = 7.4 Hz, CH₃-cation); 1.24-1.34 (m, 6H, -CH₂-cation); 1.35-1.40 (m,

1H, -CH-Leu); 1.53-1.57 (m, 6H, -CH₂-cation); 1.63-1.66 (m, 1H, -CH₂-Leu); 2.66 (ov, 1H, -CH-Leu); 2.98 (s, 3H, CH₃-cation); 3.23 (t, 6H, J = 8.4 Hz, -CH₂-cation); ¹³C NMR (100 MHz, DMSO-d₆) δ, ppm: 13.95 (CH₃-cation); 19.67 (-CH₂- cation); 22.82 (CH₃-Leu); 23.12 (CH₃-Leu); 23.55 (-CH₂-cation); 25.20 (CH-Leu); 43.62 (CH₂-Leu); 45.96 (CH₃-cation); 57.99 (-CH₂-cation); 71.05 (-CH-Leu); 177.72 (-COO⁻ Leu).

Tributylmethylammonium L-isoleucinate [tBMA][L-Ile]:

¹H NMR (400 MHz, DMSO-d₆) δ, ppm: 0.74 (d, 3H, J = 7.6 Hz, CH₃-Ile); 0.93 (t, 9H, J = 7.5 Hz, CH₃-cation); 0.99 (t, 3H, J = 8.2 Hz, CH₃-Ile); 1.22-1.36 (m, 8H, -CH₂-cation, -CH₂-Ile); 1.53-1.58 (m, 7H, -CH₂-cation, -CH-Ile); 2.64 (d, 1H, CH-Ile); 2.94 (s, 3H, CH₃-cation); 3.23 (t, 6H, J = 8.0 Hz, -CH₂-cation); ¹³C NMR (100 MHz, DMSO-d₆) δ, w ppm: 12.04 (CH₃-CH₂-Ile); 12.10 (CH₃-CH₂- cation); 15.64 (CH₃-CH₂-Ile); 19.67 (CH₃-CH₂ cation); 23.55 (-CH₂- cation); 31.43 (CH₃-CH-Ile); 38.06 (CH-CH₃-Ile); 45.93 (CH₃-N⁺ cation); 57.97 (-CH₂-N⁺ cation); 78.17 (CH-COO⁻ Ile); 176.40 (-COO⁻ Ile).

Tributylmethylammonium L-threoninate [tBMA][L-Thr]:

¹H NMR (400 MHz, DMSO-d₆) δ, ppm: 0.98 (t, 9H, J = 4.0 Hz, CH₃-cation); 1.31 (d, 3H, J = 7.4 Hz, CH₃-Thr); 1.31-1.40 (m, 6H, -CH₂-cation); 1.62-1.70 (m, 6H, -CH₂-cation); 3.05 (s, 3H, CH₃-cation); 3.36 (t, 6H, J = 8.4 Hz, CH₂-cation); 2.92 (d, 1H, J = 4.9 Hz, CH-Thr); 3.54-3.60 (m, 1H, CH-Thr); ¹³C NMR (100 MHz, DMSO-d₆) δ, ppm: 13.94 (CH₃-cation); 19.67 (-CH₂-cation); 20.15 (CH₃-Thr); 23.53 (-CH₂-cation); 45.97 (CH₃-cation); 57.98 (-CH₂-cation); 67.97 (-CH-Thr); 77.07 (CH-Thr); 175.76 (-COO⁻ Thr).

Tributylmethylammonium L-histidinate [tBMA][L-His]:

¹H NMR (400 MHz, DMSO-d₆) δ, ppm: 0.98 (t, 9H, J = 7.4 Hz, CH₃-cation); 1.31-1.40 (m, 6H, -CH₂-cation); 1.62-1.70 (m, 6H, -CH₂-cation); 2.50 (d, 1H, J = 1.6 Hz, CH(H)-His); 2.90 (d, 1H, J = 10.7 Hz, CH(H)-His); 3.04 (s, 3H, CH₃-cation); 3.29 (t, 6H, J = 8.4 Hz, CH₂-cation); 3.93 (t, 1H, CH-His); 6.68 (s, 1H, CH(Ar)-His); 7.46 (s, 1H, CH(Ar)-His); ¹³C NMR (100 MHz, DMSO-d₆) δ, ppm: 13.91 (CH₃-cation); 19.65 (-CH₂-cation); 23.56 (-CH₂-cation); 29.00 (CH₂-His); 47.01 (CH-His); 57.99 (-CH₂-cation); 116.99 (CH(Ar)-His); 134.18 (CH(Ar)-His); 136.33 (CH(Ar)-His); 176.59 (-COO⁻ His).

Dodecyltrimethylammonium glycinate ([DDTMA][Gly]):

^1H NMR (400 MHz, D_2O) δ , ppm: 0.85-0.90 (t, 3H, CH_3 -DDTMA, d, 6H, CH_3 -DDTMA); 1.16-1.34 (m, 18H, $-\text{CH}_2$ -DDTMA); 1.63-1.73 (m, 2H, $-\text{CH}_2$ -DDTMA); 3.03 (s, 9H, CH_3 -DDTMA); 3.09 (s, 2H, $-\text{CH}_2$ -Gly); 3.21 (t, 2H, $J = 8.7$ Hz, $-\text{CH}_2$ -DDTMA); ^{13}C NMR (100 MHz, D_2O) δ , ppm: 13.89 (CH_3 -DDTMA); 22.60 ($-\text{CH}_2$ -DDTMA); 25.95 ($-\text{CH}_2$ -DDTMA); 28.91 ($-\text{CH}_2$ -DDTMA); 29.31 ($-\text{CH}_2$ -DDTMA); 29.46 ($-\text{CH}_2$ -DDTMA); 29.59 ($-\text{CH}_2$ -DDTMA); 31.87 ($-\text{CH}_2$ -DDTMA); 44.74 ($-\text{CH}_2$ -Gly); 52.87 ($-\text{CH}_3$ DDTMA); 66.70 ($-\text{CH}_2$ -DDTMA); 181.69 ($-\text{COO}^-$ Gly); FT-IR ν_{max} (KBr, thin film): 3600-3000 (br), 2918, 2850, 1578, 1487, 1472, 1396, 1298, 963, 911, 720 cm^{-1} ;

Dodecyltrimethylammonium L-leucinate ([DDTMA][L-Leu]):

^1H NMR (400 MHz, D_2O) δ , ppm: 0.74 (t, 3H, $J = 6.9$ Hz, CH_3 -DDTMA); 0.78 (d, 3H, $J = 6.6$ Hz, CH_3 -Leu); 0.80 (d, 3H, $J = 6.6$ Hz, CH_3 -Leu); 1.10-1.25 (m, 18H, $-\text{CH}_2$ -DDTMA); 1.29-1.34 (m, 1H, $-\text{CH}$ -Leu); 1.40-1.44 (m, 1H, $-\text{CH}(\text{H})$ -Leu); 1.52-1.56 (m, 1H, $-\text{CH}(\text{H})$ -Leu); 1.60-1.66 (m, 2H, $-\text{CH}_2$ -DDTMA); 2.98 (s, 9H, CH_3 -DDTMA); 3.16 (t, 2H, $J = 8.7$ Hz, $-\text{CH}_2$ -DDTMA); 3.25 (t, 1H, $J = 8.7$ Hz, $-\text{CH}$ -Leu); ^{13}C NMR (100 MHz, D_2O) δ , ppm: 13.88 (CH_3 -HDTMA); 21.43 ($-\text{CH}_3$ Leu); 21.87 ($-\text{CH}_3$ Leu); 22.58 ($-\text{CH}_2$ -HDTMA); 22.67 ($-\text{CH}$ -Leu); 24.54 ($-\text{CH}_2$ -HDTMA); 26.01 ($-\text{CH}_2$ -HDTMA); 28.94 ($-\text{CH}_2$ -HDTMA); 29.27 ($-\text{CH}_2$ -HDTMA); 28.27 ($-\text{CH}_2$ -HDTMA); 29.32 ($-\text{CH}_2$ -HDTMA); 29.45 ($-\text{CH}_2$ -HDTMA); 29.56 ($-\text{CH}_2$ -HDTMA); 29.58 ($-\text{CH}_2$ -HDTMA); 31.84 ($-\text{CH}_2$ -HDTMA); 43.13 ($-\text{CH}$ -Leu); 52.96 ($-\text{CH}_3$ HDTMA); 54.38 ($-\text{CH}$ -Leu); 66.75 ($-\text{CH}_2$ -HDTMA); 181.37 ($-\text{COO}^-$ Leu); FT-IR ν_{max} (KBr, thin film): 3600-3000 (br), 2918, 2850, 1580, 1514, 1468, 1395, 964, 911, 720 cm^{-1} ;

Dodecyltrimethylammonium L-isoleucinate ([DDTMA][L-Ile]):

^1H NMR (400 MHz, D_2O) δ , ppm: 0.84-0.90 (d, 6H, CH_3 -Ile, t, 3H, CH_3 -DDTMA); 1.10-1.15 (m, 1H, $-\text{CH}(\text{H})$ -Ile); 1.24-1.38 (m, 18H, $-\text{CH}_2$ -DDTMA); 1.39-1.45 (m, 1H, $-\text{CH}(\text{H})$ -Ile); 1.60-1.68 (m, 1H, $-\text{CH}$ -Ile); 1.71-1.79 (m, 2H, $-\text{CH}_2$ -DDTMA); 3.05 (d, 1H, $J = 5.4$ Hz, $-\text{CH}$ -Ile); 3.10 (s, 9H, CH_3 -DDTMA); 3.28 (t, 2H, $J = 8.6$ Hz, $-\text{CH}_2$ -DDTMA); ^{13}C NMR (100 MHz, D_2O) δ , ppm: 11.29 (CH_3 -Ile); 13.89 (CH_3 -DDTMA); 15.56 ($-\text{CH}_2$ -Ile); 22.64 ($-\text{CH}_2$ -DDTMA); 22.71 ($-\text{CH}_2$ -DDTMA); 24.29 (CH_3 -Ile); 26.10 ($-\text{CH}_2$ -DDTMA); 29.11 ($-\text{CH}_2$ -DDTMA); 29.42 ($-\text{CH}_2$ -

DDTMA); 29.53 (-CH₂-DDTMA); 29.65 (-CH₂-DDTMA); 29.73 (-CH₂-DDTMA); 29.78 (-CH₂-DDTMA); 31.94 (-CH₂-DDTMA); 38.33 (-CH-Ile); 52.89 (-CH₃ DDTMA); 60.89 (-CH-Ile); 66.59 (-CH₂-DDTMA); 180.58 (-COO⁻ Ile); FT-IR ν_{\max} (KBr, thin film): 3600-3000 (br), 2918, 2851, 1579, 1513, 1487, 1464, 1395, 964, 911, 719 cm⁻¹;

Dodecyltrimethylammonium L-methioninate ([DDTMA][L-Met]):

¹H NMR (400 MHz, D₂O) δ , ppm: 0.94 (t, 3H, J = 6.4 Hz, CH₃-DDTMA); 1.29-1.46 (m, 18H, -CH₂-DDTMA); 1.79-1.87 (m, 2H, -CH₂-DDTMA, m, 1H, CH(H)-Met); 1.94-2.03 (m, 1H, CH(H)-Met); 2.16 (s, 3H, CH₃-Met); 2.61 (t, 2H, J = 7,8 Hz, -CH₂-Met); 3.18 (s, 9H, CH₃-DDTMA); 3.34-3.38 (t, 2H, -CH₂-DDTMA, t, 1H, -CH-Met); ¹³C NMR (100 MHz, D₂O) δ , ppm: 13.93 (CH₃-DDTMA); 14.33 (-CH₃ Met); 22.64 (-CH₂-DDTMA); 22.70 (-CH₂-DDTMA); 26.07 (-CH₂-DDTMA); 29.06 (-CH₂-DDTMA); 29.38 (-CH₂-DDTMA); 29.45 (-CH₂-DDTMA); 29.58 (-CH₂-DDTMA); 29.67 (-CH₂-DDTMA); 30.02 (-CH₂-DDTMA); 30.06 (-CH₂-Met); 31.92 (-CH₂-DDTMA); 34.45 (-CH₂-Met); 52.89 (-CH₃ DDTMA); 55.42 (-CH-Met); 66.63 (-CH₂-DDTMA); 182.22 (-COO⁻ Met); FT-IR ν_{\max} (KBr, thin film): 3600-3000 (br), 2918, 2851, 1581, 1509, 1487, 1464, 1395, 964, 720 cm⁻¹;

Hexadecyltrimethylammonium glycinate ([HDTMA][Gly]):

¹H NMR (400 MHz, D₂O) δ , ppm: 0.92 (t, 3H, J = 6.0 Hz, CH₃-HDTMA); 1.28-1.42 (m, 26H, -CH₂-HDTMA); 1.73-1.83 (m, 2H, -CH₂-HDTMA); 3.14 (s, 9H, CH₃-HDTMA); 3.25 (s, 2H, -CH₂-Gly); 3.32 (t, 2H, -CH₂-HDTMA); ¹³C NMR (100 MHz, D₂O) δ , ppm: 13.88 (CH₃-HDTMA); 22.63 (-CH₂-HDTMA); 26.02 (-CH₂-HDTMA); 29.06 (-CH₂-HDTMA); 29.51 (-CH₂-HDTMA); 29.68 (-CH₂-HDTMA); 29.78 (-CH₂-HDTMA); 29.87 (-CH₂-HDTMA); 29.89 (-CH₂-HDTMA); 31.96 (-CH₂-HDTMA); 43.90 (-CH₂-Gly); 52.81 (-CH₃ HDTMA); 66.53 (-CH₂-HDTMA); 179.07 (-COO⁻ Gly); FT-IR ν_{\max} (KBr, thin film): 2918, 2850, 1585, 1487, 1473, 1463, 1407, 1334, 1303, 961, 912, 829 cm⁻¹;

Hexadecyltrimethylammonium L-valinate ([HDTMA][L-Val]):

¹H NMR (400 MHz, D₂O) δ , ppm: 0.76 (d, 3H, CH₃-Val, t, 3H, CH₃-HDTMA); 0.81 (d, 3H, J = 7.1 Hz, CH₃-Val); 1.09-1.30 (m, 26H, -CH₂-HDTMA); 1.57-1.67 (m, 2H, -CH₂-HDTMA); 1.83-1.88 (m, 1H, -CH-Val); 2.99 (d, 1H, -CH-Val; s, 9H, CH₃-HDTMA); 3.17 (t, 2H, J = 8.4 Hz, -

CH₂-HDTMA); ¹³C NMR (100 MHz, D₂O) δ, ppm: 13.86 (CH₃-HDTMA); 16.81 (-CH₃ Val); 18.99 (-CH₃ Val); 22.63 (-CH₂-HDTMA); 22.67 (-CH₂-HDTMA); 26.09 (-CH₂-HDTMA); 29.16 (-CH₂-HDTMA); 29.48 (-CH₂-HDTMA); 29.81 (-CH₂-HDTMA); 29.93 (-CH₂-HDTMA); 29.96 (-CH₂-HDTMA); 31.25 (-CH-Val); 31.97 (-CH₂-HDTMA); 52.82 (-CH₃ HDTMA); 61.55 (-CH-Val); 66.45 (-CH₂-HDTMA); 180.35 (-COO⁻Val); FT-IR ν_{max} (KBr, thin film): 3600-3100 (br), 2920, 2851, 1584, 1507, 1464, 1396, 1329, 964, 911, 718 cm⁻¹;

Hexadecyltrimethylammonium L-leucinate ([HDTMA][L-Leu]):

¹H NMR (400 MHz, D₂O) δ, ppm: 0.75 (t, 3H, J = 7.1 Hz, CH₃-HDTMA); 0.79 (d, 3H, J = 6.6 Hz, CH₃-Leu); 0.81 (d, 3H, J = 6.6 Hz, CH₃-Leu); 1.12-1.27 (m, 26H, -CH₂-HDTMA); 1.30-1.34 (m, 1H, -CH-Leu); 1.42-1.45 (m, 1H, -CH(H)-Leu); 1.52-1.57 (m, 1H, -CH(H)-Leu); 1.59-1.65 (m, 2H, -CH₂-HDTMA); 2.99 (s, 9H, CH₃-HDTMA); 3.17 (t, 2H, J = 8,6 Hz, -CH₂-HDTMA); 3.25 (t, 1H, J = 8,8 Hz, -CH-Leu); ¹³C NMR (100 MHz, D₂O) δ, ppm: 13.87 (CH₃-HDTMA); 21.37 (-CH₃ Leu); 22.61 (-CH₃ Leu); 22.65 (-CH₂-HDTMA); 22.74 (-CH-Leu); 24.48 (-CH₂-HDTMA); 26.18 (-CH₂-HDTMA); 29.25 (-CH₂-HDTMA); 29.50 (-CH₂-HDTMA); 29.70 (-CH₂-HDTMA); 29.84 (-CH₂-HDTMA); 29.93 (-CH₂-HDTMA); 29.97 (-CH₂-HDTMA); 30.00 (-CH₂-HDTMA); 31.99 (-CH₂-HDTMA); 43.14 (-CH-Leu); 52.87 (-CH₃ HDTMA); 54.24 (-CH-Leu); 66.48 (-CH₂-HDTMA); 180.69 (-COO⁻ Leu); FT-IR ν_{max} (KBr, thin film): 3600-3000 (br), 2918, 2850, 1580, 1515, 1463, 1395, 964, 912, 719 cm⁻¹;

Hexadecyltrimethylammonium L-isoleucinate ([HDTMA][Gly]):

¹H NMR (400 MHz, D₂O) δ, ppm: 0.90-0.92 (d, 3H, J = 8.0 Hz, CH₃-Ile, t, 6H, J = 4.0 Hz, CH₃-Ile, CH₃-HDTMA); 1.12-1.19 (m, 1H, -CH(H)-Ile); 1.33-1.39 (m, 26H, -CH₂-HDTMA); 1.47-1.50 (m, 1H, -CH(H)-Ile); 1.63-1.70 (m, 1H, -CH-Ile); 1.74-1.85 (m, 2H, -CH₂-HDTMA); 3.09 (t, 1H, J = 8.0 Hz, -CH-Ile); 3,16 (s, 9H, CH₃-HDTMA); 3.34 (t, 2H, J = 8.0 Hz, -CH₂-HDTMA); ¹³C NMR (100 MHz, D₂O) δ, ppm: 11.32 (CH₃-Ile); 13.86 (CH₃-HDTMA); 15.70 (-CH₂-Ile); 22.64 (-CH₂-HDTMA); 22.70 (-CH₂-HDTMA); 24.26 (CH₃-Ile); 26.13 (-CH₂-HDTMA); 29.20 (-CH₂-HDTMA); 29.48 (-CH₂-HDTMA); 29.67 (-CH₂-HDTMA); 29.81 (-CH₂-HDTMA); 29.91 (-CH₂-HDTMA); 29.97 (-CH₂-HDTMA); 31.97 (-CH₂-HDTMA); 38.88 (-CH-Ile); 52.82 (-CH₃ HDTMA); 61.15 (-CH-Ile); 66.46 (-CH₂-HDTMA); 181.82 (-COO⁻ Ile); FT-IR ν_{max} (KBr, thin film): 3600-3000 (br), 2920, 2851, 1576, 1513, 1464, 1395, 964, 911, 720 cm⁻¹;

Hexadecylltrimethylammonium L-methioninate ([HDTMA][L-Met]):

^1H NMR (400 MHz, D_2O) δ , ppm: 0.87 (t, 3H, $J = 6.0$ Hz, $\text{CH}_3\text{-HDTMA}$); 1.24-1.42 (m, 26H, $-\text{CH}_2\text{-HDTMA}$); 1.71-1.78 (m, 2H, $-\text{CH}_2\text{-HDTMA}$); 1.79-1.84 (m, 1H, CH(H)-Met); 1.92-1.97 (m, 1H, CH(H)-Met); 2.08 (s, 3H, $\text{CH}_3\text{-Met}$); 2.55 (t, 2H, $J = 8.0$ Hz, $-\text{CH}_2\text{-Met}$); 3.11 (s, 9H, $\text{CH}_3\text{-HDTMA}$); 3.29 (t, 2H, $J = 8.0$ Hz, $-\text{CH}_2\text{-HDTMA}$); 3.36 (t, 1H, $J=4.0$ Hz, $-\text{CH-Met}$); ^{13}C NMR (100 MHz, D_2O) δ , ppm: 13.86 ($\text{CH}_3\text{-HDTMA}$); 14.36 ($-\text{CH}_3\text{ Met}$); 22.65 ($-\text{CH}_2\text{-HDTMA}$); 22.73 ($-\text{CH}_2\text{-HDTMA}$); 26.17 ($-\text{CH}_2\text{-HDTMA}$); 29.24 ($-\text{CH}_2\text{-HDTMA}$); 29.49 ($-\text{CH}_2\text{-HDTMA}$); 29.69 ($-\text{CH}_2\text{-HDTMA}$); 29.83 ($-\text{CH}_2\text{-HDTMA}$); 29.93 ($-\text{CH}_2\text{-HDTMA}$); 29.96 ($-\text{CH}_2\text{-HDTMA}$); 29.99 ($-\text{CH}_2\text{-Met}$); 31.98 ($-\text{CH}_2\text{-HDTMA}$); 34.49 ($-\text{CH}_2\text{-Met}$); 52.83 ($-\text{CH}_3\text{ HDTMA}$); 55.37 ($-\text{CH-Met}$); 66.48 ($-\text{CH}_2\text{-HDTMA}$); 181.77 ($-\text{COO}^- \text{Met}$); FT-IR ν_{max} (KBr, thin film): 3700-3000 (br), 2920, 2851, 1581, 1510, 1465, 1391, 965, 911, 720 cm^{-1} ;

Hexadecylltrimethylammonium L-histidinate ([HDTMA][L-His]):

^1H NMR (400 MHz, D_2O) δ , ppm: 0.75 (t, 3H, $J = 6.4$ Hz, $\text{CH}_3\text{-HDTMA}$); 1.06-1.26 (m, 26H, $-\text{CH}_2\text{-HDTMA}$); 1.52-1.67 (m, 2H, $-\text{CH}_2\text{-HDTMA}$); 2.70 (d, 1H, $J = 7.8$ Hz, $-\text{CH(H)-His}$); 2.86 (d, 1H, $J = 5.0$ Hz, $-\text{CH(H)-His}$); 2.95 (s, 9H, $\text{CH}_3\text{-HDTMA}$); 3.12 (t, 2H, $J = 8.4$ Hz, $-\text{CH}_2\text{-HDTMA}$); 3.41 (t, 1H, $J = 6.5$ Hz, $-\text{CH-His}$); 6.76 (s, 1H, $-\text{CH(H)-His}$); 7.51 (s, 1H, $-\text{CH(H)-His}$); ^{13}C NMR (100 MHz, D_2O) δ , ppm: 13.88 ($\text{CH}_3\text{-HDTMA}$); 22.61 ($-\text{CH}_2\text{-HDTMA}$); 26.00 ($-\text{CH}_2\text{-HDTMA}$); 29.04 ($-\text{CH}_2\text{-HDTMA}$); 29.43 ($-\text{CH}_2\text{-HDTMA}$); 29.48 ($-\text{CH}_2\text{-HDTMA}$); 29.65 ($-\text{CH}_2\text{-HDTMA}$); 29.75 ($-\text{CH}_2\text{-HDTMA}$); 29.83 ($-\text{CH}_2\text{-HDTMA}$); 29.85 ($-\text{CH}_2\text{-HDTMA}$); 31.36 ($-\text{CH}_2\text{-His}$); 31.93 ($-\text{CH}_2\text{-HDTMA}$); 52.77 ($-\text{CH-His}$); 52.86 ($-\text{CH}_3\text{ HDTMA}$); 66.52 ($-\text{CH}_2\text{-HDTMA}$); 117.98 ($-\text{CH}_2\text{-His}$); 133.01 ($-\text{CH-His}$); 135.77 ($-\text{CH}_2\text{-His}$); 180.36 ($-\text{COO}^- \text{His}$); FT-IR ν_{max} (KBr, thin film): 3650-3000 (br), 2917, 2848, 1633, 1570, 1486, 1462, 1417, 964, 836, 730, 624 cm^{-1} ;

Hexadecylltrimethylammonium L-argininate ([HDTMA][L-Arg]):

^1H NMR (400 MHz, D_2O) δ , ppm: 0.93 (t, 3H, $J = 6.9$ Hz, $\text{CH}_3\text{-HDTMA}$); 1.28-1.43 (m, 26H, $-\text{CH}_2\text{-HDTMA}$); 1.61-1.66 (m, 4H, $-\text{CH}_2\text{-Arg}$); 1.75-1.84 (m, 2H, $-\text{CH}_2\text{-HDTMA}$); 3.16 (s, 9H, $\text{CH}_3\text{-HDTMA}$); 3.22 (t, 2H, $J = 6.6$ Hz, $-\text{CH}_2\text{-HDTMA}$); 3.27 (t, 1H, $J = 5.0$ Hz, $-\text{CH-Arg}$); 3.33 (t, 2H, $J = 8.6$ Hz, $-\text{CH}_2\text{-Arg}$); ^{13}C NMR (100 MHz, D_2O) δ , ppm: 13.86 ($\text{CH}_3\text{-HDTMA}$); 22.63 ($-\text{CH}_2\text{-HDTMA}$); 24.44 ($-\text{CH}_2\text{-HDTMA}$); 26.02 ($-\text{CH}_2\text{-HDTMA}$); 28.12 ($-\text{CH}_2\text{-Arg}$); 29.07 ($-\text{CH}_2\text{-$

HDTMA); 29.47 (-CH₂-HDTMA); 29.52 (-CH₂-HDTMA); 29.70 (-CH₂-HDTMA); 29.88 (-CH₂-HDTMA); 29.91 (-CH₂-HDTMA); 31.60 (-CH₂-Arg); 31.96 (-CH₂-HDTMA); 40.93 (-CH₂-Arg); 52.81 (-CH₃ HDTMA); 55.53 (-CH-Arg); 66.50 (-CH₂-HDTMA); 156.86 (-CH-Arg); 183.18 (-COO⁻ Arg); FT-IR ν_{\max} (KBr, thin film): 3600-3000 (br), 2917, 2850, 1647, 1570, 1507, 1487, 1462, 1407, 1330, 961, 730 cm⁻¹;

Octadecylltrimethylammonium L-valinate ([HDTMA][L-Val]):

¹H NMR (400 MHz, D₂O) δ , ppm: 0.73-0.76 (d, 3H, CH₃-Val, t, 3H, CH₃-ODTMA); 0.82 (d, 3H, J = 6.8 Hz, CH₃-Val); 1.12-1.26 (m, 30H, -CH₂-ODTMA); 1.55-1.69 (m, 2H, -CH₂-ODTMA); 1.83-1.87 (m, 1H, -CH-Val); 2.97-3.00 (s, 9H, CH₃-ODTMA, m, 1H, -CH-Val); 3.18 (t, 2H, J = 8.6 Hz, -CH₂-ODTMA); ¹³C NMR (100 MHz, D₂O) δ , ppm: 13.86 (CH₃-ODTMA); 16.88 (-CH₃ Val); 19.11 (-CH₃ Val); 22.66 (-CH₂-ODTMA); 22.70 (-CH₂-ODTMA); 26.14 (-CH₂-ODTMA); 29.23 (-CH₂-ODTMA); 29.53 (-CH₂-ODTMA); 29.71 (-CH₂-ODTMA); 29.86 (-CH₂-ODTMA); 29.96 (-CH₂-ODTMA); 30.00 (-CH₂-ODTMA); 30.03 (-CH₂-ODTMA); 30.06 (-CH₂-ODTMA); 31.43 (-CH-Val); 32.00 (-CH₂-ODTMA); 52.82 (-CH₃ ODTMA); 61.66 (-CH-Val); 66.42 (-CH₂-ODTMA); 180.59 (-COO⁻Val); FT-IR ν_{\max} (KBr, thin film): 3600-3000 (br), 2918, 2849, 1669, 1569, 1473, 1463, 1408, 1296, 1165, 965, 912, 719 cm⁻¹;

Octadecylltrimethylammonium L-methioninate ([HDTMA][L-Met]):

¹H NMR (400 MHz, D₂O) δ , ppm: 0.76 (t, 3H, J = 7.0 Hz, CH₃-ODTMA); 1.11-1.28 (m, 30H, -CH₂-ODTMA); 1.62-1.67 (m, 2H, -CH₂-ODTMA, m, 1H, CH(H)-Met); 1.80-1.86 (m, 1H, CH(H)-Met); 1.97 (s, 3H, CH₃-Met); 2.44 (t, 2H, J = 8.3 Hz, -CH₂-Met); 3.00 (s, 9H, CH₃-ODTMA); 3.20 (t, 2H, -CH₂-ODTMA, t, 1H, -CH-Met); ¹³C NMR (100 MHz, D₂O) δ , ppm: 13.87 (CH₃-ODTMA); 14.31 (-CH₃ Met); 22.66 (-CH₂-ODTMA); 22.73 (-CH₂-ODTMA); 26.17 (-CH₂-ODTMA); 29.24 (-CH₂-ODTMA); 29.51 (-CH₂-ODTMA); 29.71 (-CH₂-ODTMA); 29.84 (-CH₂-ODTMA); 29.94 (-CH₂-ODTMA); 29.97 (-CH₂-ODTMA); 30.02 (-CH₂-Met); 31.99 (-CH₂-ODTMA); 34.11 (-CH₂-Met); 52.85 (-CH₃ ODTMA); 55.24 (-CH-Met); 66.48 (-CH₂-ODTMA); 181.12 (-COO⁻ Met); FT-IR ν_{\max} (KBr, thin film): 3700-3000 (br), 2919, 2850, 1582, 1509, 1487, 1473, 1463, 1407, 1317, 719 cm⁻¹;

Octadecylltrimethylammonium L-histidinate ([HDTMA][L-His]):

^1H NMR (400 MHz, D_2O) δ , ppm: 0.74 (t, 3H, $J = 6.7$ Hz, $\text{CH}_3\text{-ODTMA}$); 1.05-1.23 (m, 30H, $-\text{CH}_2\text{-ODTMA}$); 1.50-1.64 (m, 2H, $-\text{CH}_2\text{-ODTMA}$); 2.71 (d, 1H, $J = 7.9$ Hz, $-\text{CH(H)-His}$); 2.87 (d, 1H, $J = 5.2$ Hz, $-\text{CH(H)-His}$); 2.94 (s, 9H, $\text{CH}_3\text{-ODTMA}$); 3.12 (t, 2H, $J = 8.5$ Hz, $-\text{CH}_2\text{-ODTMA}$); 3.43 (t, 1H, $J = 5.1$ Hz, $-\text{CH-His}$); 6.77 (s, 1H, $-\text{CH(H)-His}$); 7.50 (s, 1H, $-\text{CH(H)-His}$); ^{13}C NMR (100 MHz, D_2O) δ , ppm: 13.89 ($\text{CH}_3\text{-ODTMA}$); 22.65 ($-\text{CH}_2\text{-ODTMA}$); 26.08 ($-\text{CH}_2\text{-ODTMA}$); 29.17 ($-\text{CH}_2\text{-ODTMA}$); 29.50 ($-\text{CH}_2\text{-ODTMA}$); 29.62 ($-\text{CH}_2\text{-ODTMA}$); 29.79 ($-\text{CH}_2\text{-ODTMA}$); 29.83 ($-\text{CH}_2\text{-ODTMA}$); 29.92 ($-\text{CH}_2\text{-ODTMA}$); 29.96 ($-\text{CH}_2\text{-ODTMA}$); 30.01 ($-\text{CH}_2\text{-ODTMA}$); 31.30 ($-\text{CH}_2\text{-His}$); 31.98 ($-\text{CH}_2\text{-ODTMA}$); 52.77 ($-\text{CH-His}$); 52.82 ($-\text{CH}_3\text{ ODTMA}$); 66.50 ($-\text{CH}_2\text{-ODTMA}$); 117.95 ($-\text{CH}_2\text{-His}$); 132.99 ($-\text{CH-His}$); 135.76 ($-\text{CH}_2\text{-His}$); 180.08 ($-\text{COO}^- \text{His}$); FT-IR ν_{max} (KBr, thin film): 3650-3000 (br), 2918, 2850, 1634, 1578, 1463, 1342, 1315, 1250, 966, 912, 834, 720, 624 cm^{-1} ;

Octadecylltrimethylammonium L-argininate ([HDTMA][L-Arg]):

^1H NMR (400 MHz, D_2O) δ , ppm: 0.80 (t, 3H, $J = 7.0$ Hz, $\text{CH}_3\text{-ODTMA}$); 1.17-1.30 (m, 30H, $-\text{CH}_2\text{-ODTMA}$); 1.49-1.52 (m, 4H, $-\text{CH}_2\text{-Arg}$); 1.64-1.70 (m, 2H, $-\text{CH}_2\text{-ODTMA}$); 3.04 (s, 9H, $\text{CH}_3\text{-ODTMA}$); 3.10 (t, 2H, $J = 7.5$ Hz, $-\text{CH}_2\text{-Arg}$); 3.15 (t, 1H, $J = 5.1$ Hz, $-\text{CH-Arg}$); 3.20 (t, 2H, $J = 7.9$ Hz, $-\text{CH}_2\text{-ODTMA}$); ^{13}C NMR (100 MHz, D_2O) δ , ppm: 13.87 ($\text{CH}_3\text{-ODTMA}$); 22.68 ($-\text{CH}_2\text{-ODTMA}$); 24.44 ($-\text{CH}_2\text{-ODTMA}$); 26.11 ($-\text{CH}_2\text{-ODTMA}$); 29.18 ($-\text{CH}_2\text{-Arg}$); 29.56 ($-\text{CH}_2\text{-ODTMA}$); 29.65 ($-\text{CH}_2\text{-ODTMA}$); 29.84 ($-\text{CH}_2\text{-ODTMA}$); 29.90 ($-\text{CH}_2\text{-ODTMA}$); 30.00 ($-\text{CH}_2\text{-ODTMA}$); 30.02 ($-\text{CH}_2\text{-ODTMA}$); 30.04 ($-\text{CH}_2\text{-ODTMA}$); 30.10 ($-\text{CH}_2\text{-ODTMA}$); 31.55 ($-\text{CH}_2\text{-Arg}$); 32.03 ($-\text{CH}_2\text{-ODTMA}$); 40.95 ($-\text{CH}_2\text{-Arg}$); 52.87 ($-\text{CH}_3\text{ ODTMA}$); 55.53 ($-\text{CH-Arg}$); 66.51 ($-\text{CH}_2\text{-ODTMA}$); 156.74 ($-\text{CH-Arg}$); 183.05 ($-\text{COO}^- \text{Arg}$); FT-IR ν_{max} (KBr, thin film): 3600-3000 (br), 2918, 2849, 1669, 1569, 1473, 1463, 1408, 1296, 1165, 965, 924, 719 cm^{-1} ;