

¹H-NMR SPECTRA DATA – COMPOUND STRUCTURE CONFIRMATION

For each δ (ppm) chemical shift stated, only the respective Hs are shown

m-7NH-m series

12-7NH-12 (1,9-bis(dodecyl)-1,1,9,9-tetramethyl-5-amino-1,9-nonanediammonium dibromide)

¹H-NMR data for 12-7NH-12 are consistent with data from our previous report.^a

16-7NH-16 (1,9-bis(hexadecyl)-1,1,9,9-tetramethyl-5-amino-1,9-nonanediammonium dibromide)

δ_{H} /ppm (500 MHz, CDCl₃, Me₄Si):

0.88 (6H, t, Me), 1.25-1.35 (52H, m, -(CH₂)₁₃), 1.74 (4H, m, ⁺N-C-CH₂), 2.19 (4H, m, ⁺N-C-CH₂-C-N), 2.90 (1H, br s, NH), 2.98 (4H, m, ⁺N-C₂-CH₂-N), 3.32 (12H, s, ⁺NMe), 3.36-3.45 (4H, m, ⁺N-CH₂), 4.08-4.12 (4H, m, ⁺N-CH₂-C₂-N).

18-7NH-18 (1,9-bis(octadecyl)-1,1,9,9-tetramethyl-5-amino-1,9-nonanediammonium dibromide)

δ_{H} /ppm (500 MHz, CDCl₃, Me₄Si):

0.87 (6H, t, Me), 1.26-1.38 (60H, m, -(CH₂)₁₅), 1.76 (4H, m, ⁺N-C-CH₂), 2.04 (1H, br s, NH), 2.53 (4H, m, ⁺N-C-CH₂-C-N), 2.88 (4H, m, ⁺N-C₂-CH₂-N), 3.30 (4H, m, ⁺N-CH₂), 3.40 (12H, s, ⁺NMe), 4.10-4.18 (4H, m, ⁺N-CH₂-C₂-N).

18:1-7NH-18:1 (1,9-bis(*cis*-oleyl)-1,1,9,9-tetramethyl-5-imino-1,9-nonanediammonium dibromide)

δ_{H} /ppm (500 MHz, CDCl₃, Me₄Si):

0.85 (6H, t, Me), 1.20-1.40 (44H, m, (CH₂)₅-C-C=C-C-(CH₂)₆), 1.77 (4H, m, ⁺N-C-CH₂), 1.90 (1H, br s, NH), 2.03 (8H, m, allylic Hs), 2.10 (2H, m, ⁺N-C-CH₂-C-N), 2.68 (4H, m, ⁺N-C₂-CH₂-N), 3.23 (4H, m, ⁺N-CH₂), 3.49 (12H, s, ⁺NMe), 4.10-4.15 (4H, m, ⁺N-CH₂-C₂-N), 5.30-5.40 (4H, t, vinyl Hs).

m-3-m series

12-3-12 (1,3-propanediyl-bis(dimethyl-dodecylammonium) dibromide)

¹H-NMR data for 12-3-12 are consistent with data from our previous report.^b

16-3-16 (1,3-propanediyl-bis(dimethyl-hexadecylammonium) dibromide)

¹H-NMR data for 16-3-16 are consistent with data from our previous report.^c

18-3-18 (1,3-propanediyl-bis(dimethyl-octadecylammonium) dibromide)

δ_{H} /ppm (500 MHz, CDCl_3 , Me_4Si):

0.88 (6H, t, Me), 1.26-1.40 (60H, m, $-(\text{CH}_2)_{15}$), 1.82 (4H, m, $^+\text{N}-\text{C}-\text{CH}_2$), 2.83 (2H, m, $\text{N}^+-\text{C}-\text{CH}_2-\text{C}-\text{N}^+$), 3.40 (12H, s, ^+NMe), 3.46 (4H, m, $^+\text{N}-\text{CH}_2$), 3.98 (4H, m, $^+\text{N}-\text{CH}_2-\text{C}-\text{CH}_2-\text{N}^+$).

18:1-3-18:1 (1,3-propanediyl-bis(dimethyl-*cis*-oleylammonium) dibromide)

$^1\text{H-NMR}$ data for 18:1-3-18:1 are consistent with data from our previous report.^d

m-7-m series

12-7-12 (1,7-heptanediyl-bis(dimethyldodecylammonium) dibromide)

δ_{H} /ppm (500 MHz, CDCl_3 , Me_4Si):

0.89 (6H, t, Me), 1.20-1.38 (36H, m, $-(\text{CH}_2)_9$), 1.55 (6H, m, $^+\text{N}-\text{C}_2-(\text{CH}_2)_3-\text{C}_2-\text{N}^+$), 1.78 (2H, m, $^+\text{N}-\text{C}-\text{CH}_2-$), 1.85 (4H, m, $^+\text{N}-\text{C}-\text{CH}_2-\text{C}_3-\text{CH}_2-\text{C}-\text{N}^+$), 3.33 (12H, s, ^+NMe), 3.48 (4H, m, $^+\text{N}-\text{CH}_2$), 3.98 (4H, m, $^+\text{N}-\text{CH}_2-\text{C}_5-\text{CH}_2-\text{N}^+$).

16-7-16 (1,7-heptanediyl-bis(dimethylhexadecylammonium) dibromide)

δ_{H} /ppm (500 MHz, CDCl_3 , Me_4Si):

0.87 (6H, t, Me), 1.26-1.38 (52H, m, $-(\text{CH}_2)_{13}$), 1.58 (6H, m, $^+\text{N}-\text{C}_2-(\text{CH}_2)_3-\text{C}_2-\text{N}^+$), 1.72 (2H, m, $^+\text{N}-\text{C}-\text{CH}_2-$), 1.88 (4H, m, $^+\text{N}-\text{C}-\text{CH}_2-\text{C}_3-\text{CH}_2-\text{C}-\text{N}^+$), 3.23 (12H, s, ^+NMe), 3.43 (4H, m, $^+\text{N}-\text{CH}_2$), 3.91 (4H, m, $^+\text{N}-\text{CH}_2-\text{C}_5-\text{CH}_2-\text{N}^+$).

18-7-18 (1,7-heptanediyl-bis(dimethyl-octadecylammonium) dibromide)

δ_{H} /ppm (500 MHz, CDCl_3 , Me_4Si):

0.88 (6H, t, Me), 1.20-1.36 (60H, m, $-(\text{CH}_2)_{15}$), 1.57 (6H, m, $^+\text{N}-\text{C}_2-(\text{CH}_2)_3-\text{C}_2-\text{N}^+$), 1.72 (2H, m, $^+\text{N}-\text{C}-\text{CH}_2-$), 1.86 (4H, m, $^+\text{N}-\text{C}-\text{CH}_2-\text{C}_3-\text{CH}_2-\text{C}-\text{N}^+$), 3.35 (12H, s, ^+NMe), 3.49 (4H, m, $^+\text{N}-\text{CH}_2$), 3.88 (4H, m, $^+\text{N}-\text{CH}_2-\text{C}_5-\text{CH}_2-\text{N}^+$).

REFERENCES:

^a Ref ²¹, ^b Ref ⁴⁷ and #236 therein, ^c Ref ⁴⁷ and #222 therein, ^d Ref ⁴⁴ – see main article's bibliography.