

Electronic Supplementary Information

Structural-property relationships of antibacterial amphiphilic polymers derived from 2-aminoethyl acrylate

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N-Boc protection of 2-(Ethylamino)ethanol, 2-(Propylamino)ethanol, and 2-(Butylamino)ethanol

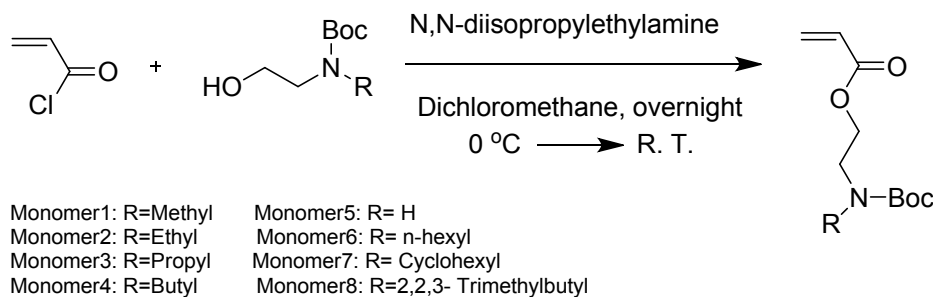
For Boc protection of 2-(Ethylamino)ethanol, 2-(Propylamino)ethanol, and 2-(Butylamino)ethanol, higher reaction time (24 to 48 hours) and slightly modified work-up procedure was employed. After the completion of reaction, organic and aqueous layers were separated. Ethyl acetate (30 mL) was added into organic layer, and washed with distilled water (3 × 125 mL). Organic layer was dried over sodium sulfate, and excess solvent removed using rotavapor to yield pure product.

2-(N-Boc-ethylamino)ethanol: ¹H NMR (300 MHz, CDCl₃): δ 1.13 (t, 3H), 1.48 (s, 9H), 3.18-3.46 (d, 4H), 3.75 (s, 2H).

2-(N-Boc-propylamino)ethanol: ¹H NMR (300 MHz, CDCl₃): δ 0.91 (t, 3H), 1.45-1.62 (bs, 11H), 3.2 (s, 2H), 3.4 (s, 2H), 3.77 (s, 2H).

2-(N-Boc-butylamino)ethanol: ¹H NMR (300 MHz, CDCl₃): δ 0.92 (t, 3H), 1.29 (m, 2H), 1.38-1.6 (bs, 11H), 3.21 (s, 2H), 3.37 (s, 2H), 3.71 (s, 2H).

¹H NMR spectra of monomers



Scheme S1. Synthetic procedure indicating the structures of various monomers synthesized

Monomer 1 (R=Methyl): ¹H NMR (600 MHz, CDCl₃): 1.41 (s, 9H), 2.88 (s, 3H), 3.48 (s, 2H), 4.23 (s, 2H), 5.81 (d, 1H), 6.09 (q, 1H), 6.38 (d, 1H).

Monomer 2 (R=Ethyl): ¹H NMR (600 MHz, CDCl₃): 1.11 (t, 3H), 1.45 (s, 9H), 3.3 (s, 2H), 3.5 (s, 2H), 4.3 (s, 2H), 5.9 (d, 1H), 6.14 (q, 1H), 6.4 (d, 1H).

Monomer 3 (R=Propyl): $^1\text{H NMR}$ (600 MHz, CDCl_3): 0.86 (t, 3H), 1.39-1.59 (bs, 11H), 3.19 (s, 2H), 3.47 (s, 2H), 4.25 (s, 2H), 5.84 (d, 1H), 6.12 (q, 1H), 6.4 (d, 1H).

Monomer 5 (R=H): $^1\text{H NMR}$ (600 MHz, CDCl_3): 1.50 (s, 9H), 3.47 (t, 2H), 4.27 (t, 2H), 4.83 (s, 1H), 5.93 (d, 1H), 6.15 (q, 1H), 6.45 (d, 1H).

Monomer 6 (R=n-Hexyl): $^1\text{H NMR}$ (600 MHz, CDCl_3): 0.86 (t, 3H), 1.28 (m, 4H), 1.34 (m, 2H), 1.63 (m, 2H), 4.11 (t, 2H), 5.77 (d, 1H), 6.08 (q, 1H), 6.35 (d, 1H).

Monomer 7 (R=Cyclohexyl): $^1\text{H NMR}$ (600 MHz, CDCl_3): 1.18-1.56 (m, 6H), 1.71 (m, 2H), 1.85 (m, 2H), 4.81 (m, 1H), 5.76 (dd, 1H), 6.08 (q, 1H), 6.35 (dd, 1H).

Monomer 8 (R=2,2,3-Trimethylbutyl): $^1\text{H NMR}$ (600 MHz, CDCl_3): 0.95 (s, 9H), 1.19 (d, 3H), 4.78 (q, 1H), 5.81 (d, 1H), 6.13 (q, 1H), 6.40 (d, 1H).

$^1\text{H NMR}$ of homopolymer poly(N-ethyl)-1.6k.

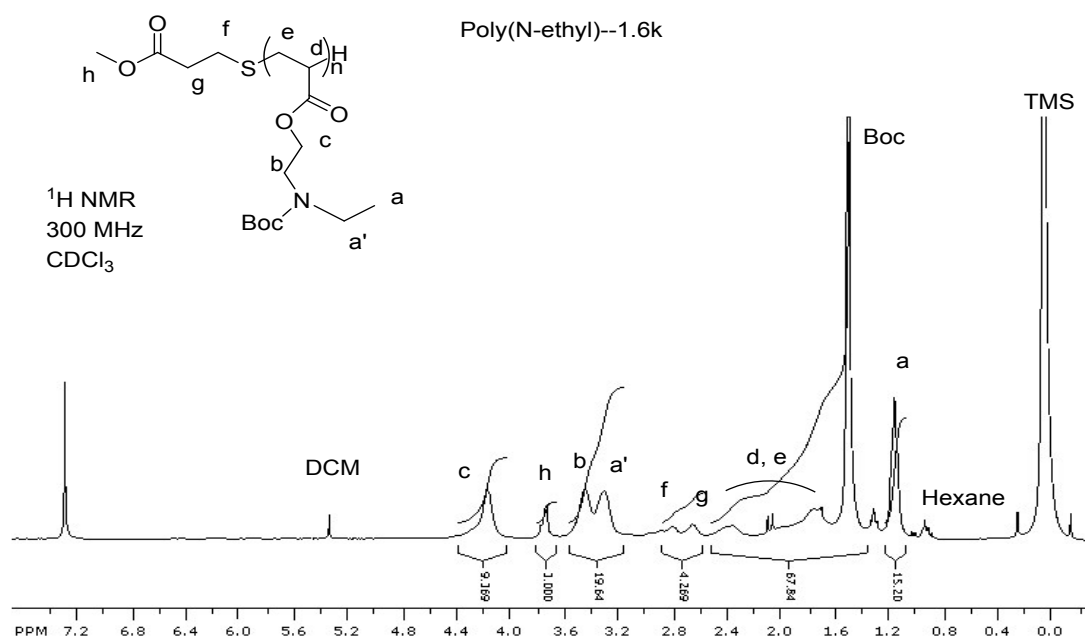


Figure S1. $^1\text{H NMR}$ (300 MHz, CDCl_3) spectrum of poly(N-ethyl)-1.6k before Boc removal.

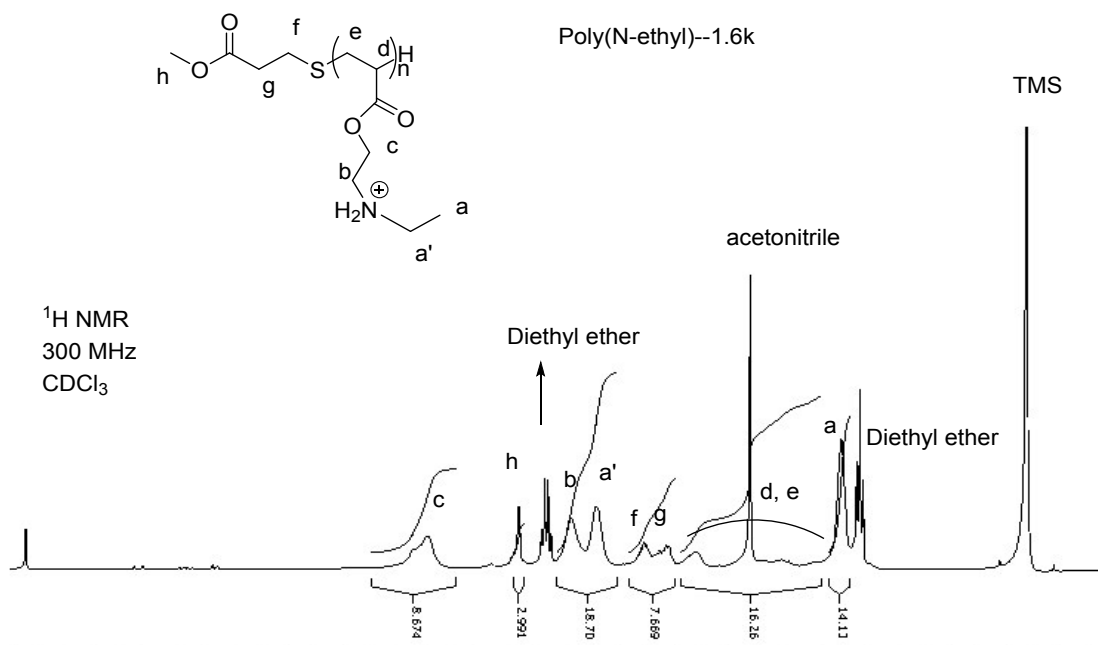
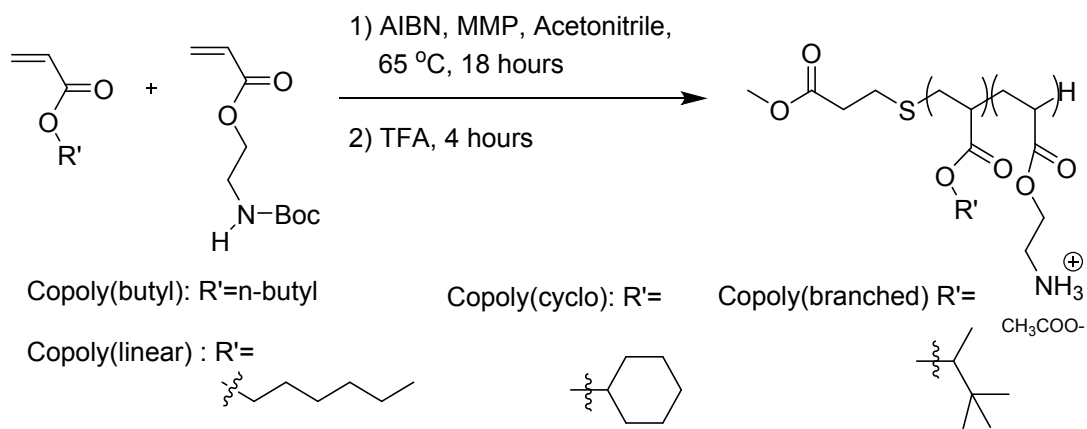


Figure S2. ^1H NMR (300 MHz, CDCl_3) spectrum of Poly(N-ethyl)-1.6K after complete removal of Boc groups using trifluoroacetic acid.

Synthesis of random copolymers



Scheme S2. Free radical copolymerization of amine functionalized acrylate monomer with lipophilic acrylate comonomers.

For the synthesis of copoly(butyl)-6K, butyl acrylate (3.1 g, 24.2 mmol) was charged into a 100 mL, 3 neck round bottom flask, loaded with Monomer 5 (*N*-(*tert*-butoxycarbonyl)aminoethyl acrylate, 5.21 g, 24.2 mmol), AIBN (0.08 g), MMP (0.268 mL), and acetonitrile (49 mL). The reaction mixture was purged with dry nitrogen for 20 minutes, and stirred at 65 °C for 18 hours. Acetonitrile was evaporated and copolymer was redissolved in 2 mL dichloromethane, followed by repeated precipitation in hexane. For the synthesis of Copoly(linear)-6k,

Copoly(cyclo)-6k, and Copoly(branched)3; higher mole percentage (60%) of Monomer 5 was used to facilitate the solubility of copolymers in aqueous medium. Deprotection of Boc protected copolymers was carried out as explained above. Relative percentage of monomers in copolymers were confirmed with ^1H NMR spectra and found to be in agreement with the monomer feed ratio.

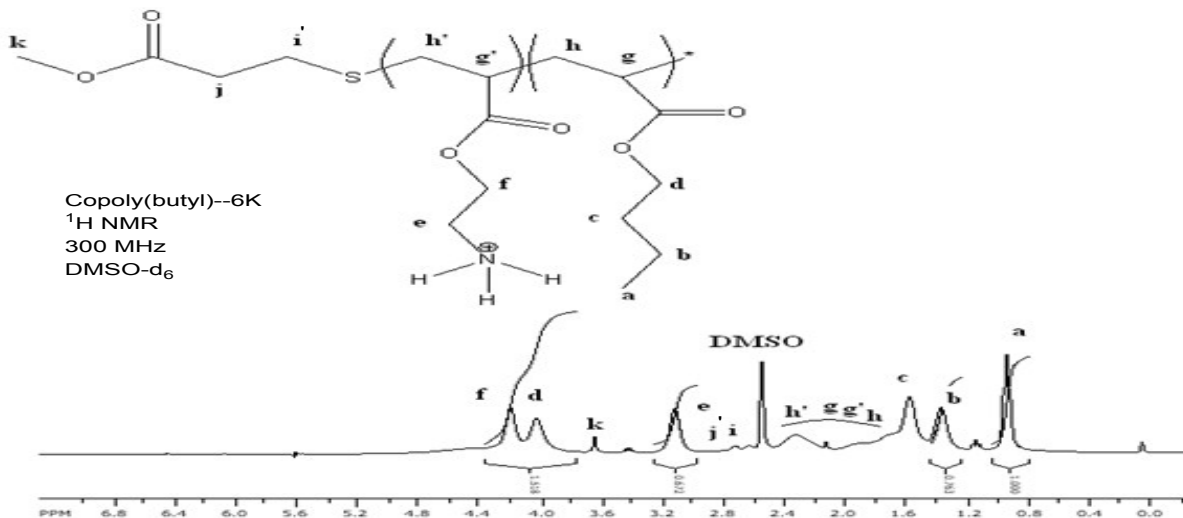


Figure S3. ^1H NMR (300 MHz, dms o - d_6) spectra of Copoly(butyl)-6k.

Calculation of Degree of polymerization: Figure S4 represents the ^1H NMR spectrum of Poly(N-methyl)-6K. A broad single peak at δ 2.9-3.1 (integral value =57.33) belongs to methyl protons in the monomer repeat unit. A single peak at δ 3.68 belongs to methyl proton at the polymer end chain (integral value=3). Degree of polymerization (DP) of polymer is calculated as below:

$$\text{D. P.} = (57.33/3) \div (3/3)$$

$$\text{D. P.} = 19$$

Similarly, DP values for all polymers and copolymers were calculated.

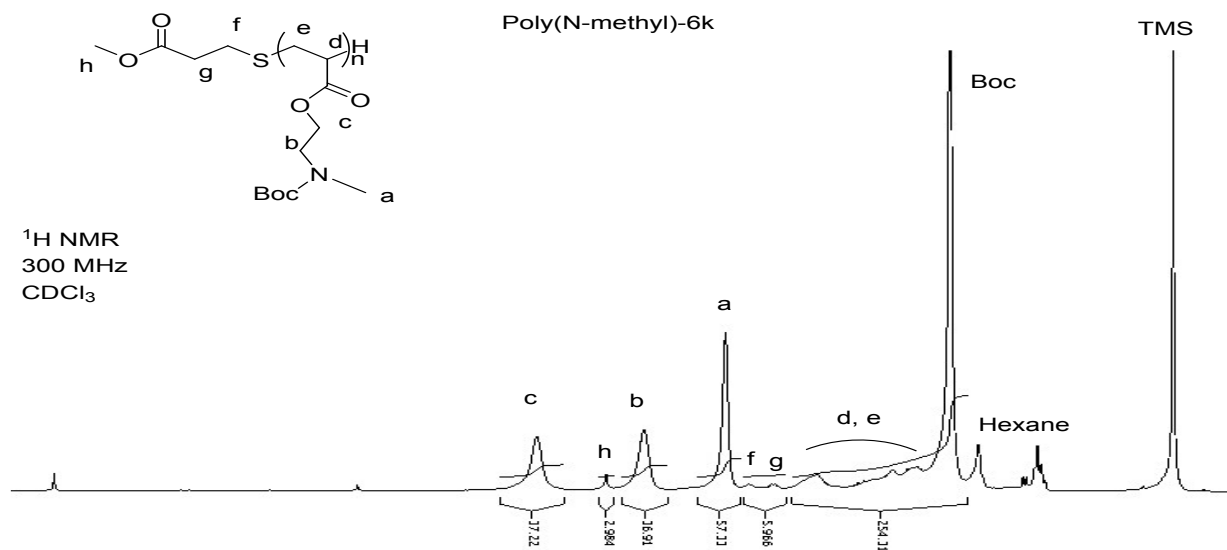


Figure S4. Calculation of degree of polymerization of poly(N-methyl)-6k through ¹H NMR (300 MHz, dmsO-d₆).