

Supplementary Information

Methacrylamide based antibiotic polymers with no detectable bacterial resistance

Anju Tyagi, Abhijit Mishra

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Supplementary Information Text

Characterization of Polymer by ^1H NMR. Unique peak assignments were made for each polymer structure, and the composition of homopolymer and random copolymers were calculated via peak integration of pendant methylene protons (Figure S1). Analysis of representative proton NMR spectrum of copolymer AB-19 provided in detail (Table S1).

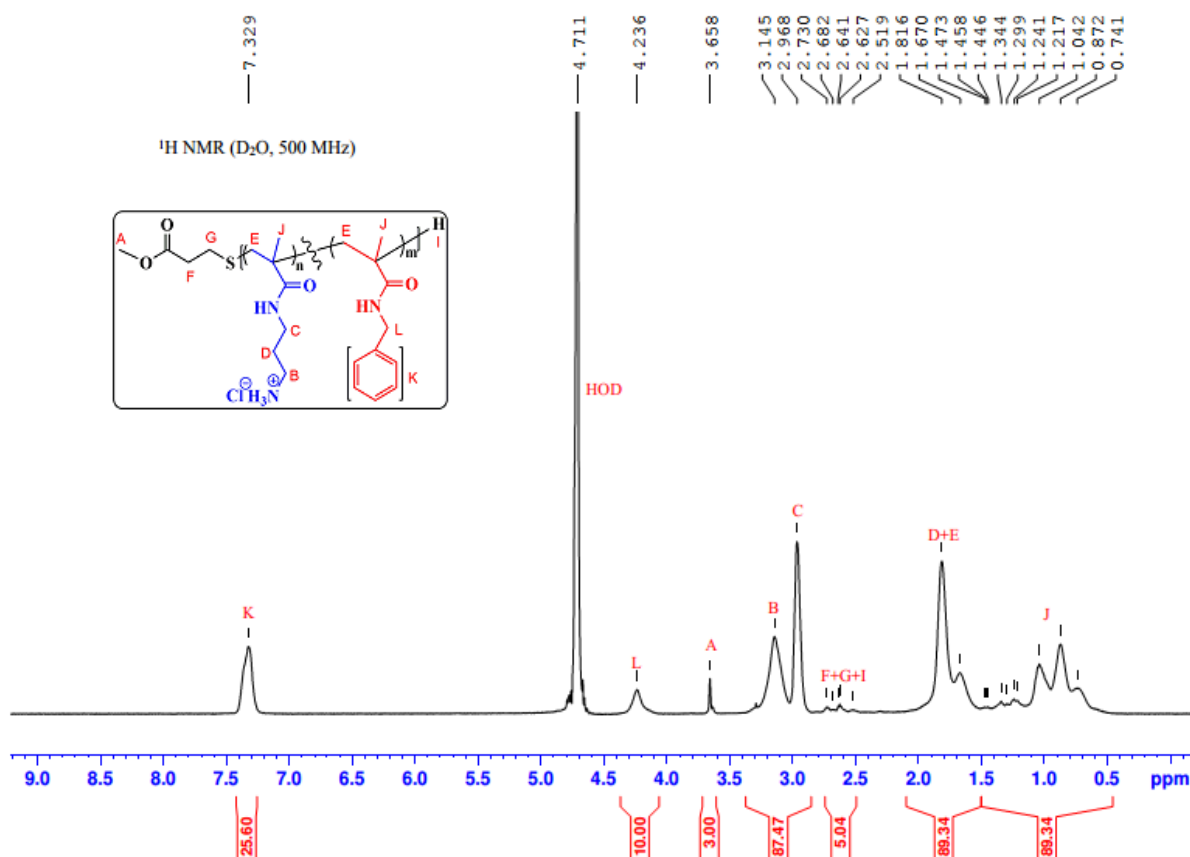


Figure S1. Chemical structure and ^1H NMR spectrum of copolymer AB-19, poly[(APMA)-*ran*-(BMA)] in deuterium oxide

Table S1: Characterization and ^1H NMR peaks assignment of copolymer AB-19

Chemical Entity	Proton (in bold)	Peak	Assigned Alphabet	Chemical Shift (ppm)
BMA	-C₆H₅	Broad multiplet	K	7.42– 7.24
BMA	-CH₂-	Broad singlet	L	4.23
End group	CH₃OOC-	Sharp singlet	A	3.65
APMA	-CH₂NH₃⁺ -CH₂NHCO-	Broad singlet	B + C	3.14 – 2.96
End group	-OOCCH₂CH₂SH-	Broad multiplet	F,G and I	2.72–2.51
APMA and	-CH₂-	Broad multiplet	D + E	2.31–1.67
End group	-SCH₂-			
APMA and BMA	-CH₃	Broad multiplet	J	1.47–0.74

Peak A was assigned to a polymer terminal group of methyl ester that appears at 3.66 ppm as a sharp singlet. Therefore the integrated peak area was normalized to 3 protons per individual polymer chain. Comparing the integration of this peak to those arising from pendant methylene protons from polymer side chains gives the DP and f_{benzyl} of the polymer. For instance, peaks B and C adjacent to protonated amine and amide group seen at 3.37 to 2.89 ppm constitutes 4 protons of the APMA monomer. Therefore, the average number of protonated amine-functionalized repeat units per polymer chain equates to $87.47/4 = 21.86$.

Similarly, the peak L seen at 4.36 to 4.06 ppm is for methylene protons adjacent to the benzene ring. Hence the average number of methylene protons (N_{benzyl}) per individual polymer chain corresponds to $10/2 = 5$.

Degree of polymerization (DP) is the average of the total number of each monomer units present in an individual polymer chain, therefore, equal to

$$DP = N_{\text{amine}} + N_{\text{benzyl}}$$

$$= 21.86 + 5 = 26.86 \text{ which is rounded to a DP value of } 27.$$

The mole fraction of the methylene group next to the benzene ring in the copolymers (f_{benzyl}) is calculated by interpreting the signals arising from amine and benzyl side groups and calculated by the formula given below:

$$f_{\text{benzyl}} = \frac{\text{Number of methylene units present in benzyl group}}{\text{Total number of monomer units per individual polymer chain}}$$

$$f_{\text{benzyl}} = 5/27 = 0.19 \text{ for this polymer.}$$

For finding the number average molecular weight (M_n), the respective molecular weight of each monomer unit is multiplied by the total number of each repeat unit and added to the molecular weight of the chain transfer agent. [Molecular weights of N-(3-aminopropyl)methacrylamide hydrochloride = 178.7 g/mol-1, N-Benzylmethacrylamide = 175.2, and methyl mercaptopropionate (CTP) = 120.17 g/mol-1]

$$M_n = (21.8675 \times 178.7) + (5.3 \times 175.2) + 120.17 = 4956 \text{ g mol}^{-1}$$

No signals were observed in the 5.2 to 6.0 ppm region, showing that there was no traceable quantity of unreacted monomer remaining in the product, and it was entirely removed by dialysis during purification.

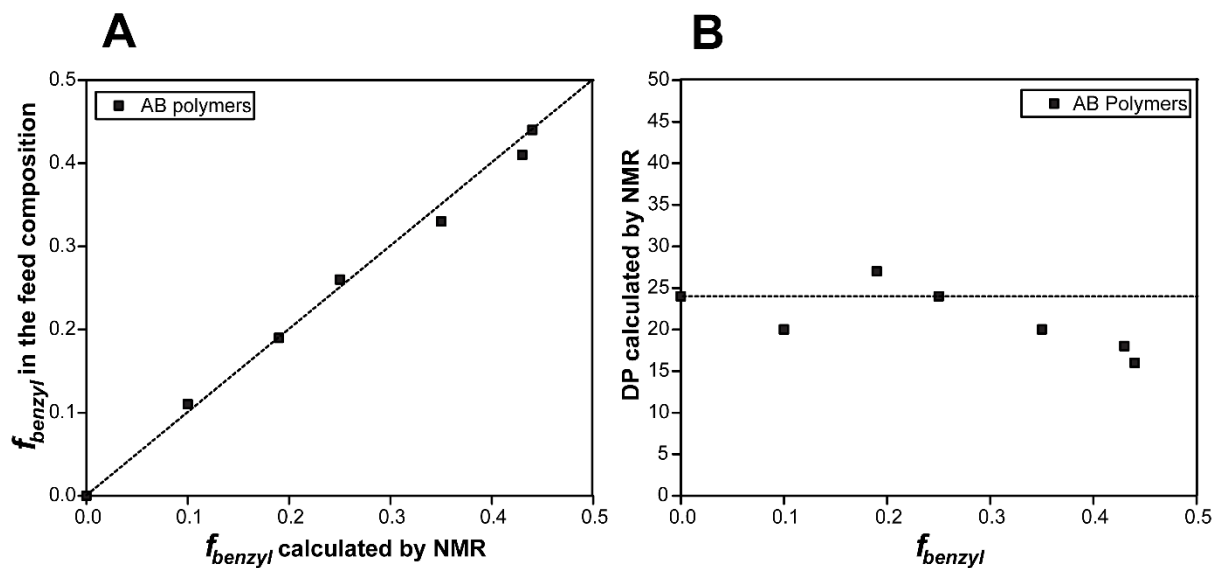


Figure S2. (A) The observed f_{benzyl} values of random copolymers were interpreted by NMR spectra as a measure of f_{benzyl} in feed composition. (B) DP values as a function of f_{benzyl}

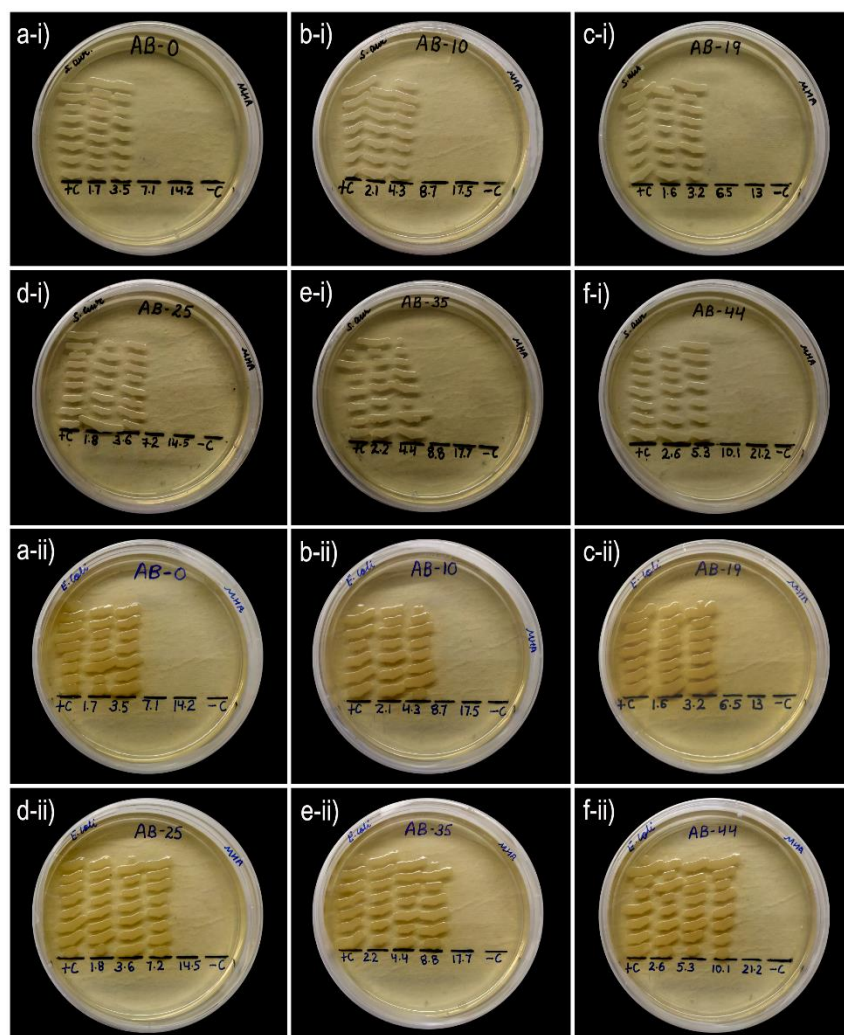


Figure S3. MIC validation check from MH agar plates against *S. aureus* (a-i to f-i), and *E. coli* (a-ii to f-ii). +C is positive control (without polymer in the growth media), and -C is negative control (without bacteria in the growth media). Numbers indicate the final concentration of polymer in μM . Visible colonies of bacteria seen below the MIC level. Each experiment runs in triplicate.