Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Supplementary Information

Dual Functional Quaternary Chitosans with Thermoresponsive Behavior: Structure-Activity Relationships in Antibacterial Activity and Biocompatibility

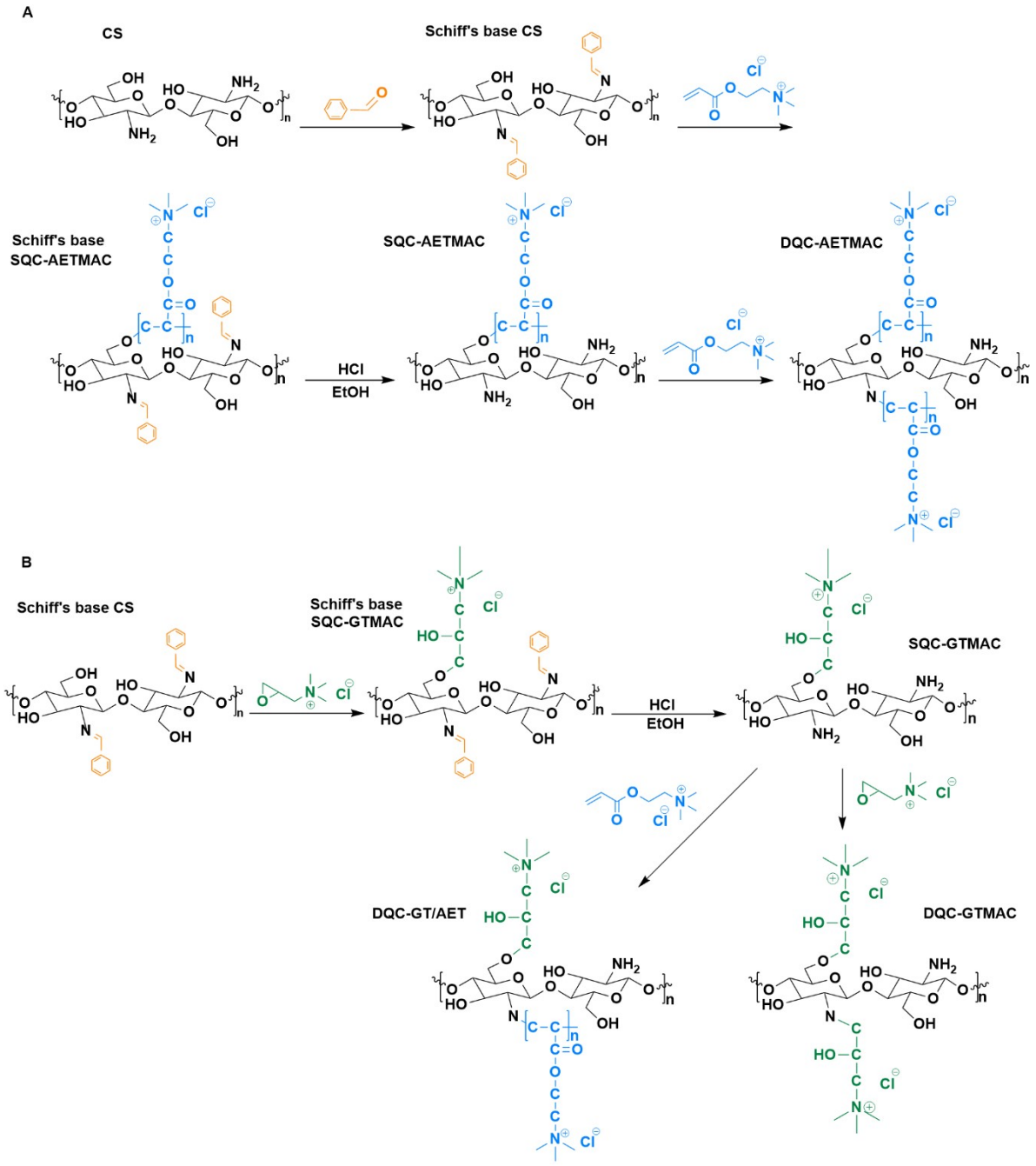
Sedigheh Borandeh[†], Isabella Laurén[†], Arun Teotia, Jukka Niskanen, Jukka Seppälä[*]

Polymer Technology, School of Chemical Engineering, Aalto University, 02150 Espoo, Finland

[†] Equal contribution

[*] Corresponding author: jukka.seppala@aalto.fi

Schemes



Scheme S1. Reaction schemes of the preparation of quaternized chitosan with **(A)** AETMAC and **(B)** GTMAC.

Figures

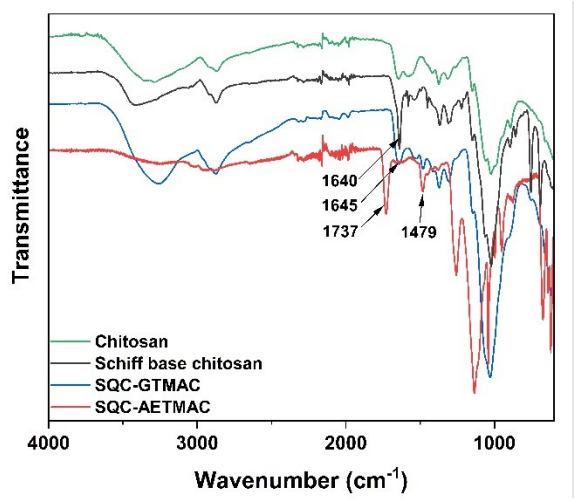


Figure S1. FT-IR spectra of chitosan and derivatives.

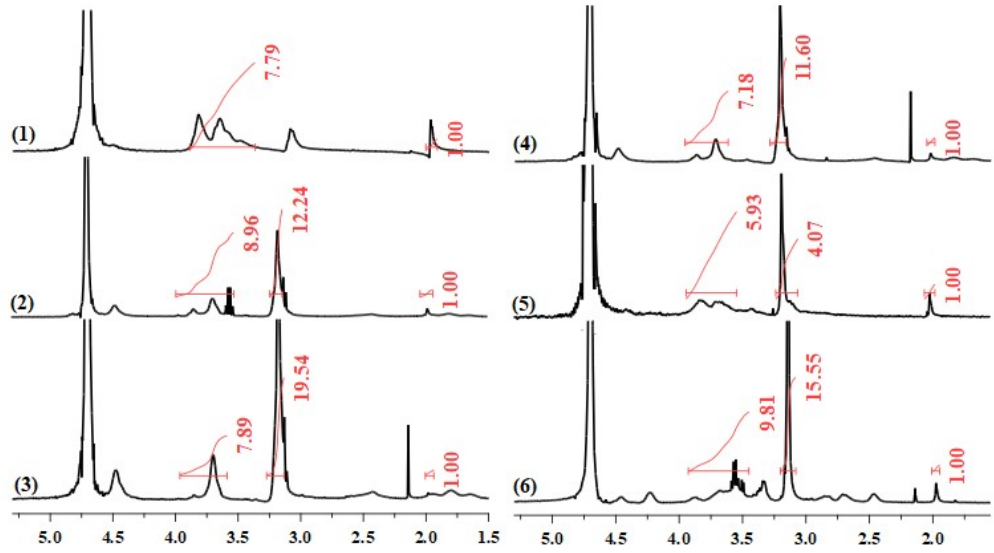


Figure S2. ^{1}H-NMR spectra and integrals used for the determination of the degree of quaternization (dQ) and deacetylation (DDA), where 1-6 is chitosan, SQC-AETMAC, DQC-AETMAC, DQC-GT/AET, SQC-GTMAC, and DQC-GTMAC.

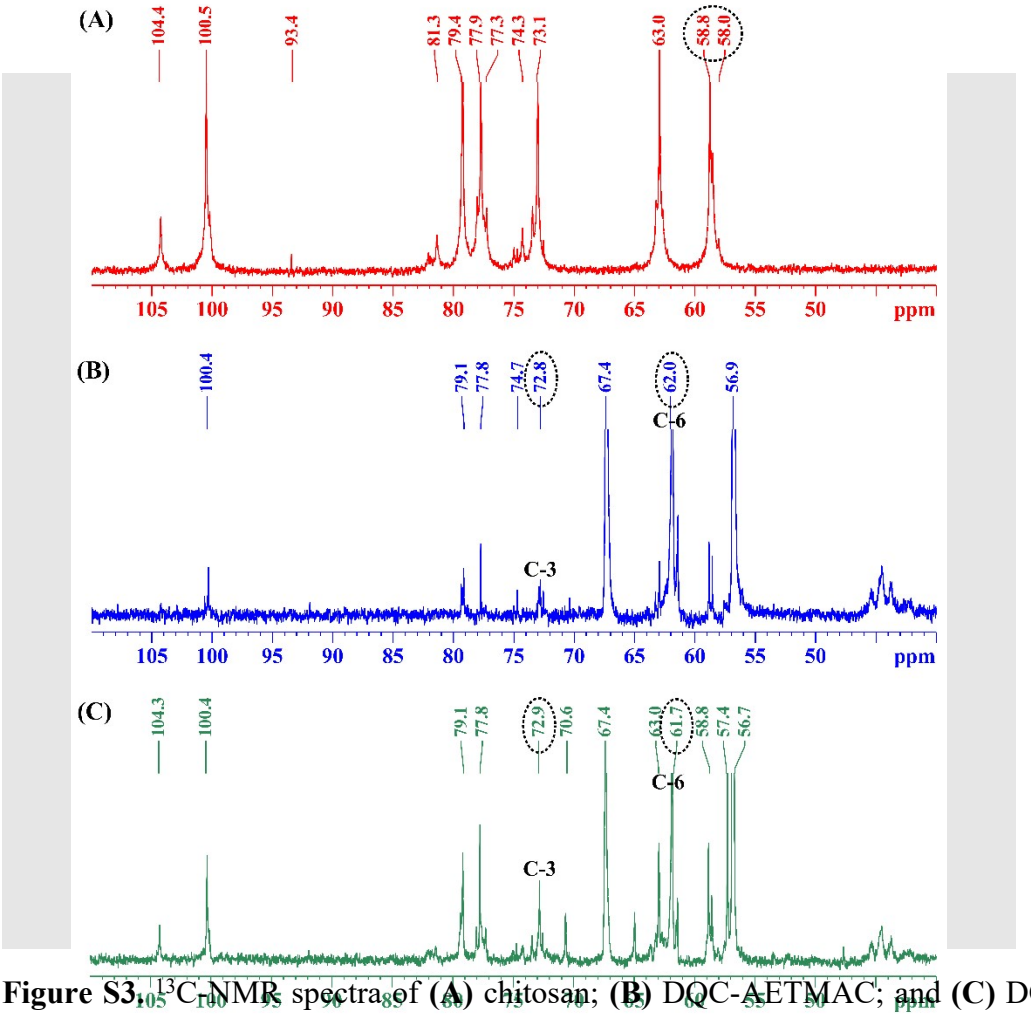


Figure S3. ^{13}C-NMR spectra of **(A)** chitosan; **(B)** DQC-AETMAC; and **(C)** DQC-GT/AET. DQC-GTMAC was excluded due to processing difficulties.

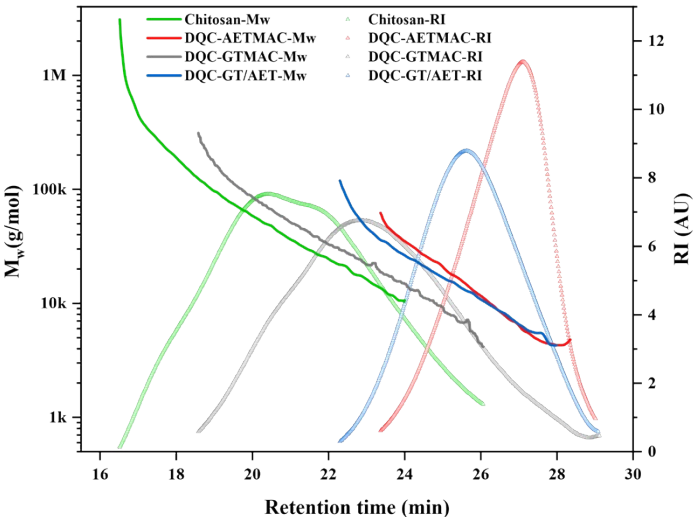


Figure S4. Results of GPC analysis: the obtained molecular weight (M_w) and refractive index (RI) versus their respective elution time of chitosan and DQCs.

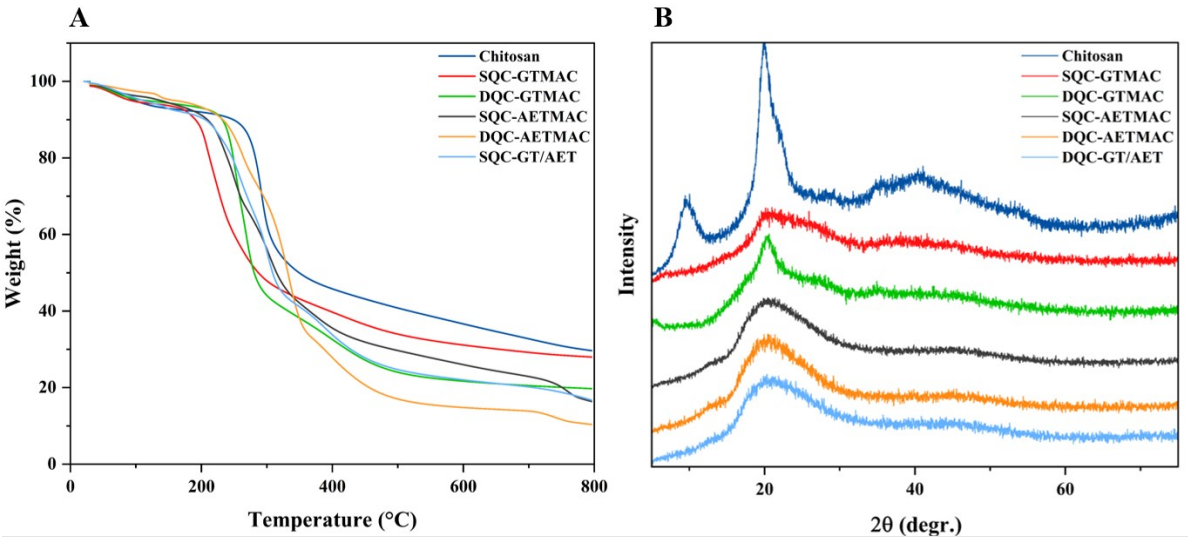


Figure S5. (A) TGA thermogram curves and **(B)** X-ray diffraction patterns of chitosan and its derivatives.

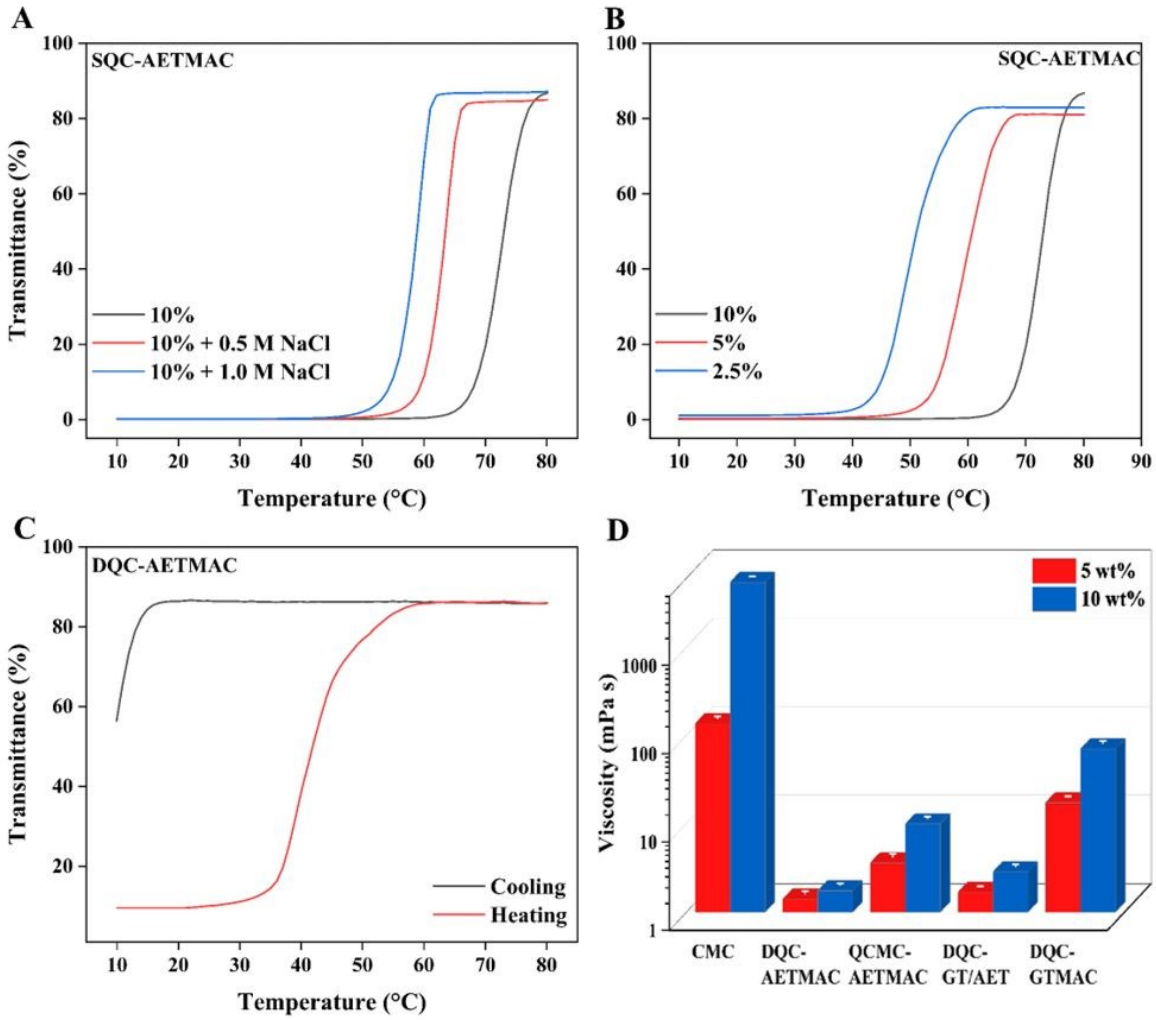


Figure S6. (A, B) UCST behavior of SQC-AETMAC during heating 10-80 °C, at different concentrations and with the addition of NaCl. **(C)** UCST behavior of DQC-AETMAC at a concentration of 10 % (w/v). **(D)** viscosity (log_{10}) of CMC and DQCs at 5 and 10 % (w/v) concentrations. Chitosan and QCMC-GTMAC were excluded due to too high viscosities.

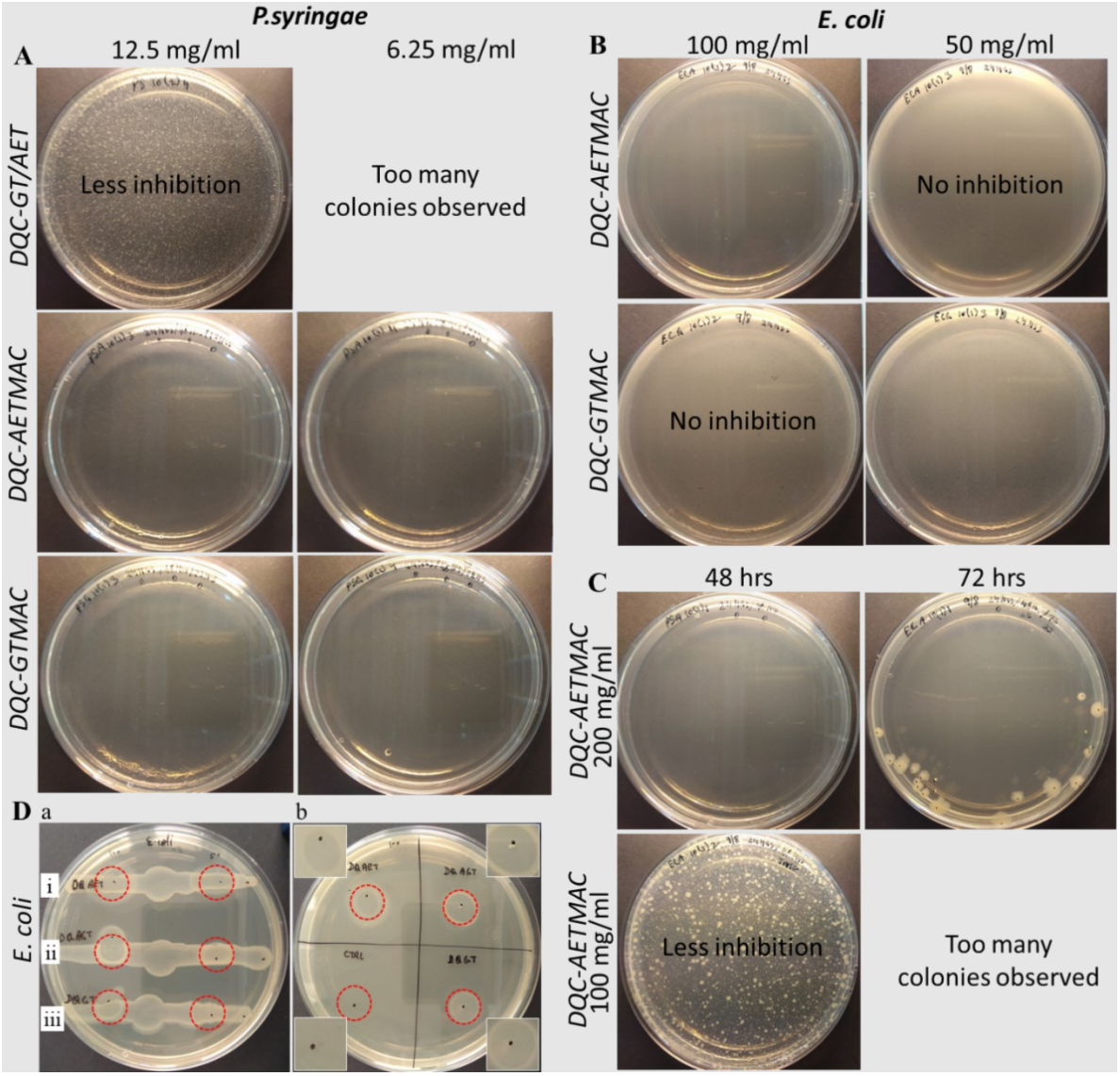


Figure S7. Antimicrobial activity analysis of representative chitosan derivatives on *P. syringae* and *E. coli* after 10 minutes of contact time. **(A)** Photograph showing antimicrobial activity of **(i)** DQC-GT/AET; **(ii)** DQC-AETMAC; and **(iii)** DQC-GTMAC, on *P. syringae* at 6.25 and 12.5 mg/mL of bioactive molecules, after 72 hours of incubation. **(B)** Photograph showing antimicrobial activity of **(i)** DQC-AETMAC; and **(ii)** DQC-GTMAC, on *E. coli*, at 100 and 50 mg/mL, after 24 hours of incubation. **(C)** Photograph showing antimicrobial activity of **(i)** DQC-AETMAC on *E. coli*, at 200 and 100 mg/mL, showing the number of CFUs observed after 48 and 72 hours of incubation. **(D)** Photograph showing zone of inhibition of different QCs for **(a)** streak, and **(b)** spread-plated *E. coli*, showing positive antimicrobial properties of QCs. (Inset 4x zoomed image).

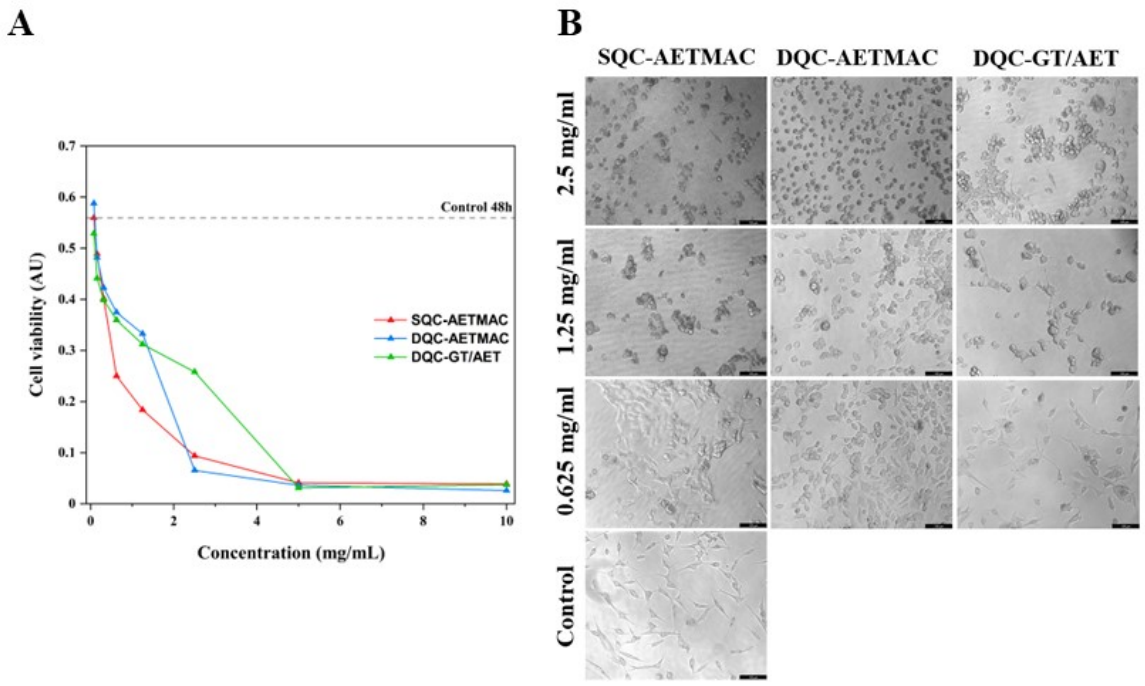


Figure S8. (A) Quantitative data of the cytotoxic behavior of quaternized chitosan on NIH-3T3 cells at different concentrations after 48h of incubation. **(B)** Microscopic images on NIH-3T3 cells after 24 h of incubation.

Tables

Table S1. Concentration dependency of QCs on NIH-3T3 cell viability after 48 h of incubation (live/dead staining).

Conc. [mg/mL]	SQC-AETMAC **%-Live**	SQC-AETMAC **%-Dead**	DQC-AETMAC **%-Live**	DQC-AETMAC **%-Dead**	DQC-GT/AET **%-Live**	DQC-GT/AET **%-Dead**
0.25	17.7	82.29	73.54	26.19	76.3	23.7
0.50	19.0	80.96	26.0	73.0	57.8	42.1
1.00	2.0	98.0	0.67	99	76.3	23.7