Electronic Supplementary Material (ESI) for Biomaterials Science.

Electronic Supplementary Information (ESI)

Polymer-antibiotic conjugate as antibacterial additive in dental resin

Runsheng Zhang,[a] Megan M. Jones,[b] Hoda Moussa,[c] Mayuresh Keskar,[a] Ningbo Huo,[a,d] Ziqi Zhang,[a] Michelle B. Visser,[b] Camila Sabatini,[c] Mark T. Swihart [a] and Chong Cheng [a]*

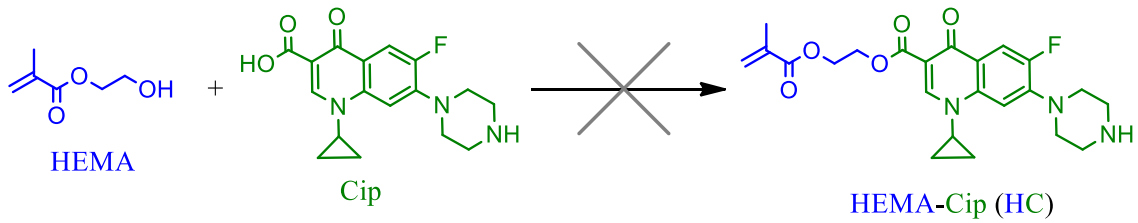
a. Department of Chemical and Biological Engineering, University at Buffalo, The State University of New York, Buffalo, New York 14260, USA. E-Mail: ccheng8@buffalo.edu

b. Department of Oral Biology, University at Buffalo, The State University of New York, Buffalo, New York 14214, USA.

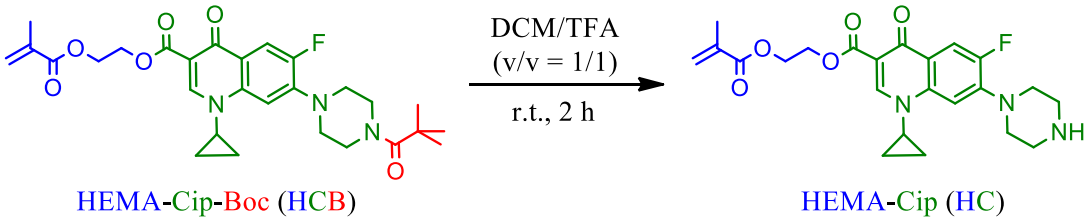
c. Department of Restorative Dentistry, University at Buffalo, The State University of New York, Buffalo, New York 14215, USA.

d. School of Textile and Chemical Engineering, Binzhou Polytechnic College, Binzhou Polytechnic College, Binzhou, Shandong 256600, China.

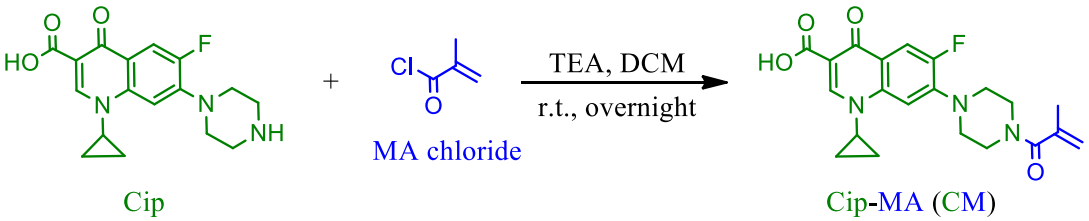
*Corresponding author. E-Mail: ccheng8@buffalo.edu



Scheme S1. Attempts of synthesis of HEMA-Cip by direct esterification of Cip with HEMA



Scheme S2. Synthesis of HEMA-Cip from HEMA-Cip-Boc by deprotection



Scheme S3. Synthesis of Cip-MA.*

***** *Synthesis of Cip-MA*: In a round bottom flask, Cip (1 eq.) and triethylamine (1.3 eq.) was added into DCM under stirring at 0°C. A solution of methacryloyl chloride (2.5 eq.) in DCM was then added dropwise into the stirring system at 0 °C followed with 30 min stirring. Then the resulting system was allowed to warm up to room temperature for an overnight stirring under N_2 protection. The resulting solution was washed with water and brine, and the collected organic phase was concentrated under rotavapor. The product was separated from the concentrated organic phase by a silica gel column chromatography eluted with MeOH/DCM, and collected as a yellow powder (yield: 50%).

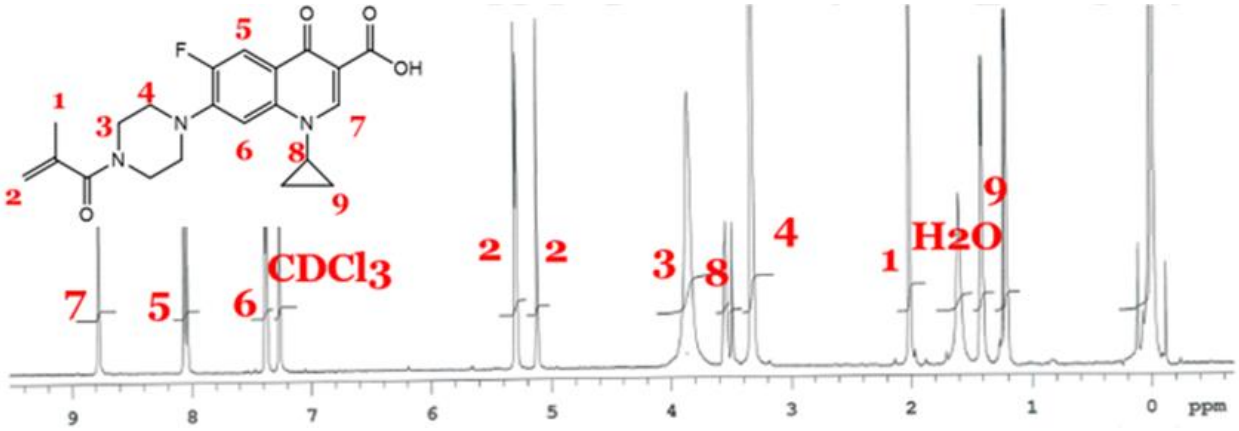


Fig. S1 500 mHz ^{1}H NMR spectrum of Cip-MA in $CDCl_3$

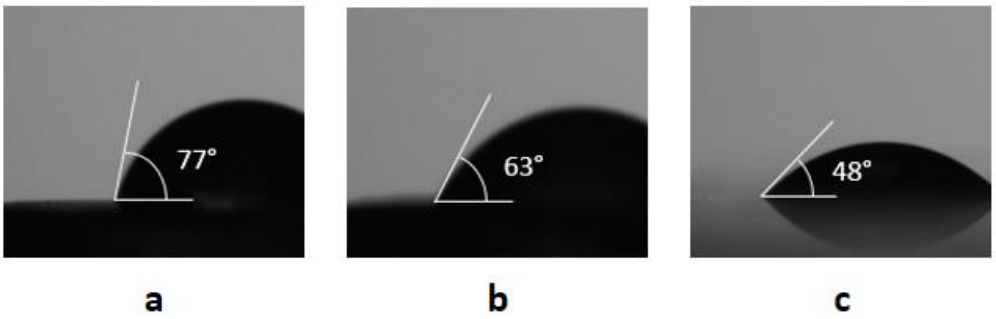


Fig. S2. Water contact angle images of the surfaces of a) SB+ disc; b) UP-PAC-incorporated SB+ disc; c) UP.PAC coated thin film.* The result that the UP-PAC-incorporated resin surface is slight more hydrophilic than the blank resin surface can be ascribed to the remarkable hydrophilicity of UP-PAC, which has 75 mol% of hydrophilic HEMA units.

** Water contact angle measurement*: Water contact angle was measured using a Rame Hart 190-F2 CA Goniometer on both the resin disc surfaces and the p($HC_{0.25}$-*co*-$HEMA_{0.75}$)$_{40}$ thin film surface. Two sets of resin discs were prepared, one with incorporation of p($HC_{0.25}$-*co*-$HEMA_{0.75}$)$_{40}$ and the other without. The PAC thin film surface was prepared by solution casting on a flat glass surface using DMF as solvent followed by gentle evaporation under reduced pressure overnight. The coated surface was further washed with acetone to remove possible remaining DMF and dried three times. The contact angles of both surfaces were measured right after dripping a water droplet (20 µL) onto the surfaces.

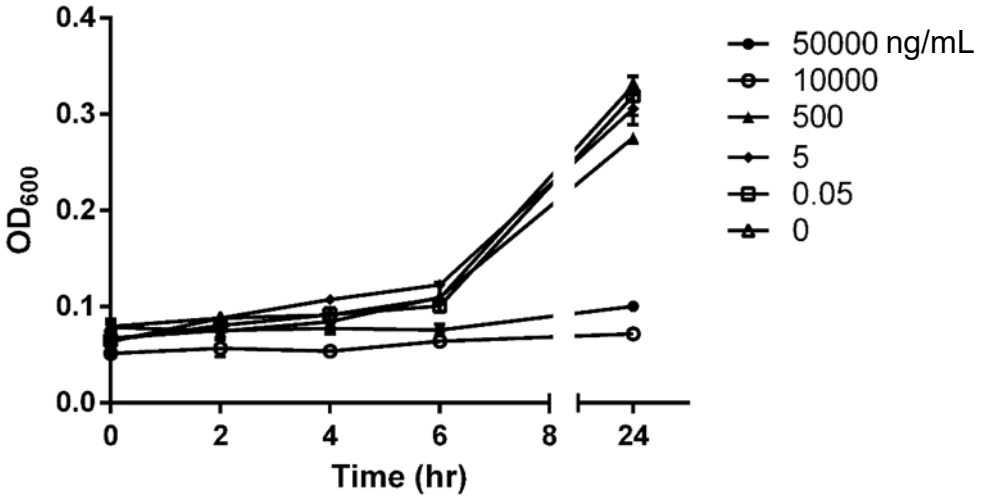


Fig. S3. Growth assays of *S. mutans* (ATCC 25175) in BHI media with varying concentrations of free Cip at 37 °C, assessed through optical density at λ = 600 nm (OD_{600}). The results indicate that Cip has a minimal inhibition concentration (MIC) of Cip between 500 and 10,000 ng/mL against *S. mutans*.