

Electronic Supplementary Information

Smart nanomicelles with bacterial infection-responsive disassembly for selective antimicrobial applications

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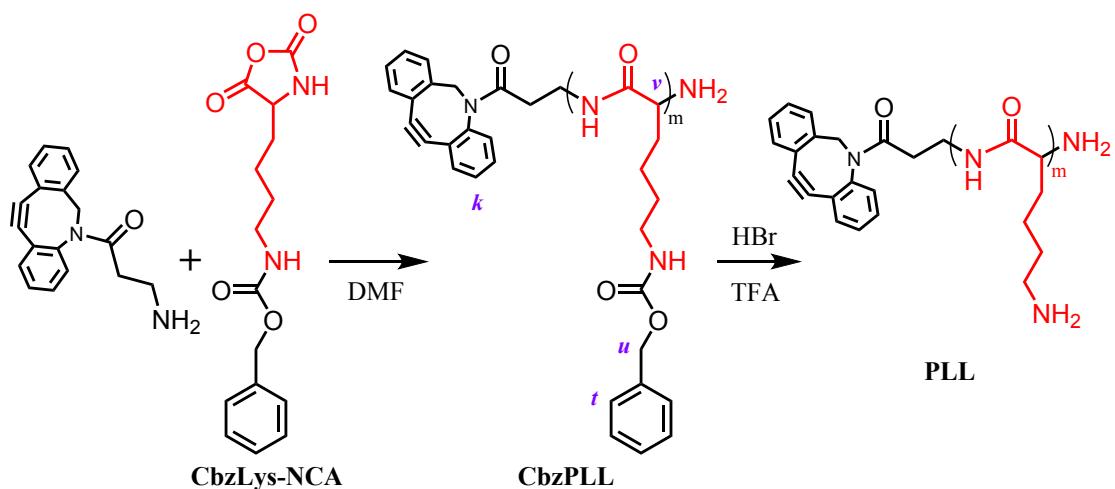


Figure S1. Ring-opening polymerization of CbzLys-NCA and subsequent deprotection to obtain ‘clickable’ cyclooctyne-terminated PLL.

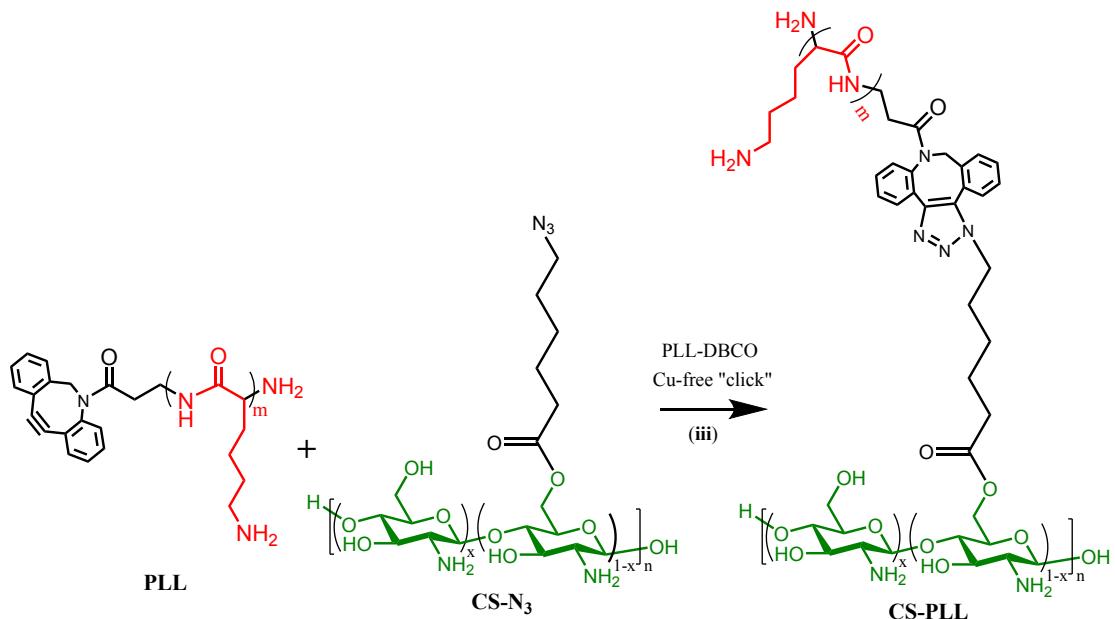


Figure S2. Strain-promoted azide-alkyne cycloaddition between cyclooctyne-terminated PLL and CS-N₃ to obtain CS-PLL conjugate.

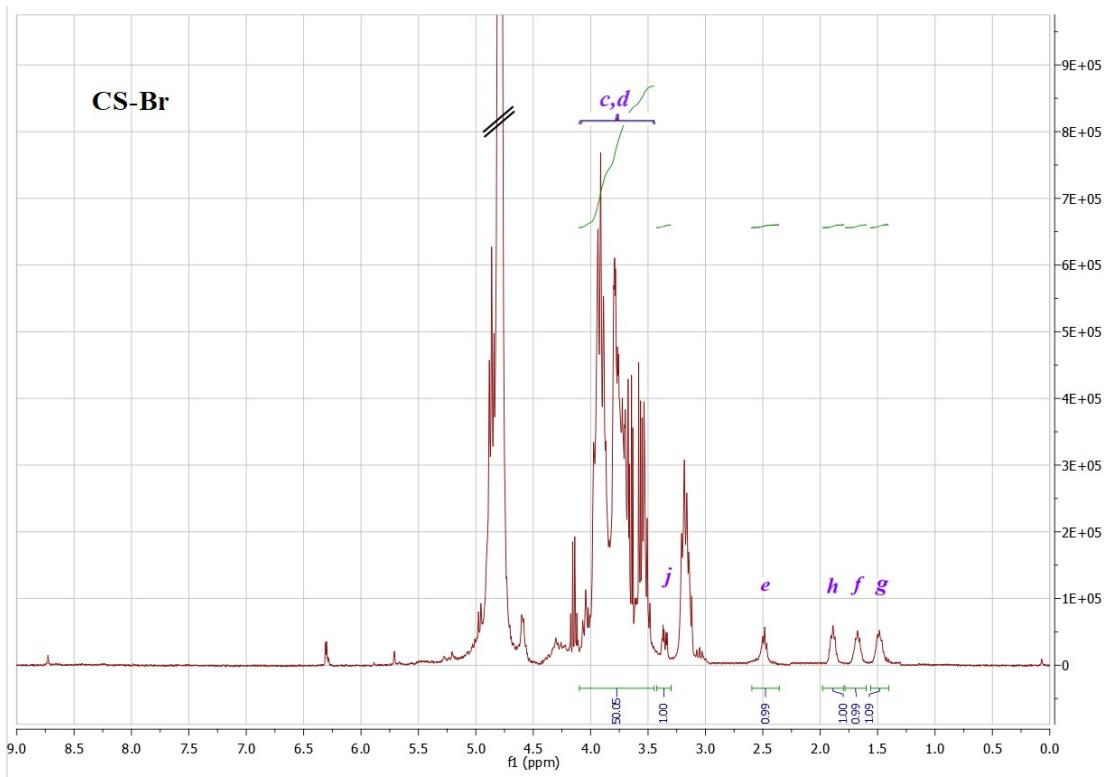


Figure S3. Peak integration ratio on the ^1H NMR spectra of the CS-Br.

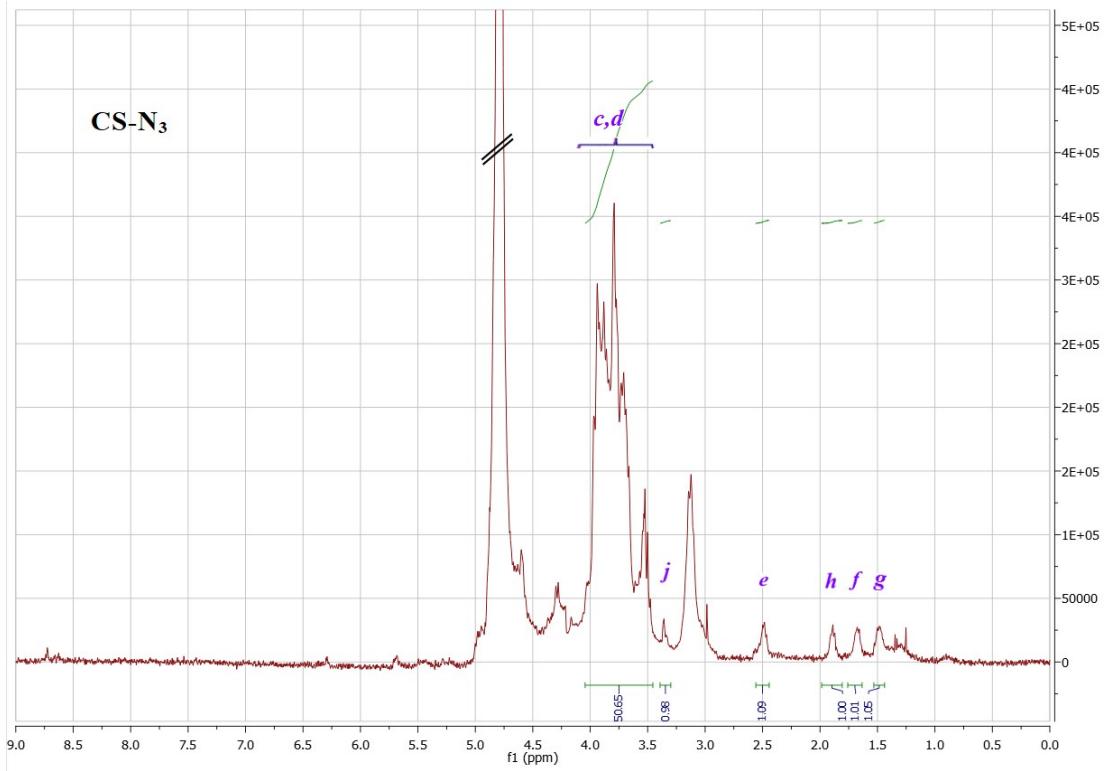


Figure S4. Peak integration ratio on the ^1H NMR spectra of the CS-N₃.

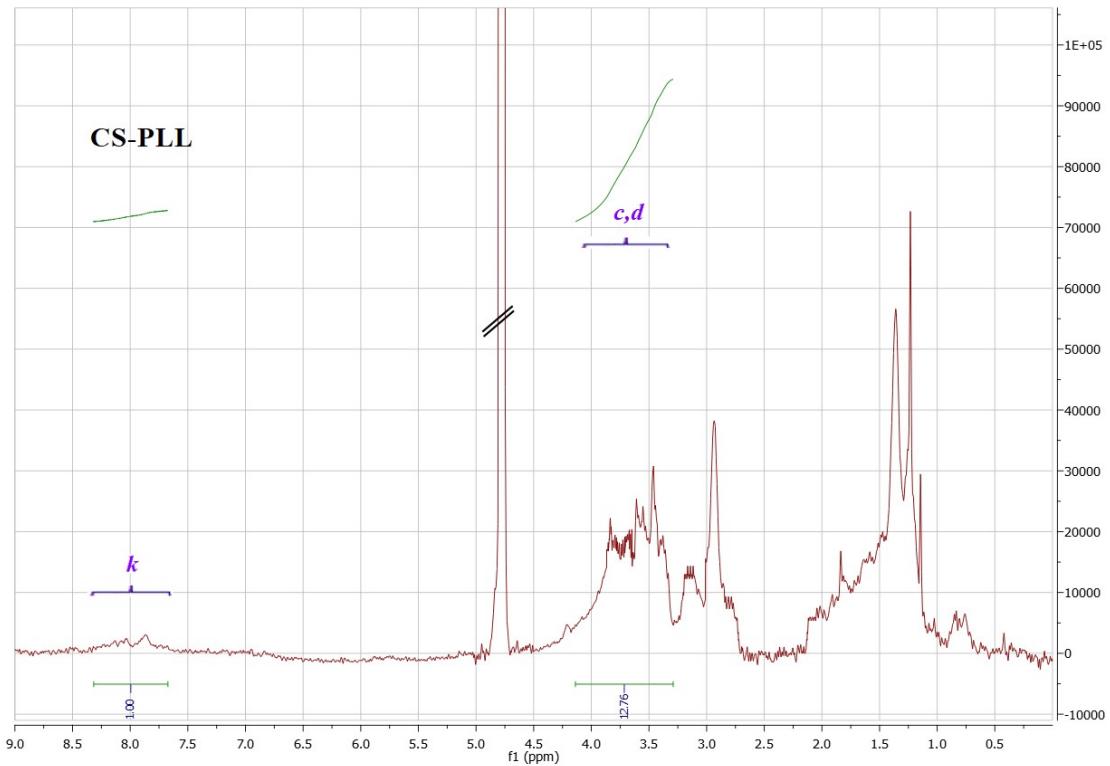


Figure S5. Peak integration ratio on the ^1H NMR spectra of the CS-PLL.

Calculations for degree of modification of the chitosan derivatives

CS-Br

$$= \frac{1}{50.05} \div \frac{2}{5} = 0.04995$$

CS-N₃

$$= \frac{1}{50.65} \div \frac{2}{5} = 0.04936$$

CS-PLL

$$= \frac{1}{12.76} \div \frac{8}{5} = 0.04898$$

Table S1. Molecular weight and polydispersity index of the functionalized chitosan and chitosan-polylysine, and percentage modification of the chitosan derivatives.

Sample	M_w^a (g/mol)	M_n^a (g/mol)	M_w/M_n^a	Modification degree of CS ^b
CS	3,572	2,251	1.58	-
CS-Br	3,791	2,384	1.59	5%
CS-N ₃	3,621	2,270	1.60	5%
CS-PLL	8,763	4,596	1.90	5%

^a Molecular weight and polydispersity index were determined from GPC analysis.

^b Modification degree was determined from peak integration ratio of ¹H NMR spectra.

Table S2. Zeta potential values and particle diameters of the polymers and nanomicelles.

Sample	Particle diameter ^a (nm)		Zeta potential, ζ (mV)
	TEM	DLS	
PLL	-	-	30.8 ± 3.2
CS-PLL	-	-	30.3 ± 4.1
CS-PLL-CA	-	-	-23.2 ± 4.9
CS-PLL/CA NMs, pH 7.4	55.2 ± 3.7	76.4 ± 7.1	21.4 ± 5.2
CS-PLL/CA NMs, pH 5.0	35.1 ± 25.3	22.9 ± 9.5	29.7 ± 6.2

^a Dry-state and hydrodynamic diameters of the NCs were determined from TEM image and DLS measurement, respectively.

Table S3. Bactericidal activity of the PLL, CS-PLL, CS-PLL-CA, CS-PLL/CA NMs at pH 7.4, and CS-PLL/CA NMs at pH 5.0.

Sample	MBC, $\mu\text{g/mL}$				
	<i>E. coli</i>	<i>P. aeruginosa</i>	<i>S. aureus</i>	<i>S. epidermidis</i>	<i>MRSA</i>
PLL	32	64	32	16	32
CS-PLL	64	128	64	16	64
CS-PLL-CA	> 1024 ^a	> 1024 ^a	> 1024 ^a	> 1024 ^a	> 1024 ^a
CS-PLL/CA NMs, pH 7.4	> 1024 ^a	> 1024 ^a	> 1024 ^a	> 1024 ^a	> 1024 ^a
CS-PLL/CA NMs, pH 5.0	64	128	64	16	64

^a The values were not observed up to the highest concentrations of compound tested (1024 $\mu\text{g/mL}$).