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Figure S1. Optimized structure of N-acetylglucosamine-N-acetylsalicylic acid β-1,4 Glucoside (β-1,4 Glucoside)



Forcite Geometry Optimization - Energy

Figure S2. the energy and convergence of β -1,4 Glucoside



Figure S3. Optimized structure of Ce6

Z-Y



Figure S4. the energy and convergence of Ce6

Energy Change (kcal/mol) 🗹 Grad. Norm (kcal/mol/Angstrom)

240 270 Optimization Step -1.5 -2 -2.5 -3



Figure S5. Optimized structure of Ce6-IL

Z L Y



Energy (kcal/mol)







Figure S7. Optimized structure of Ce6 with β -1,4 Glucoside



Forcite Geometry Optimization - Energy

et z

Figure S8. The energy and convergence of Ce6-ILwith $\beta\text{-}1,4$ Glucoside



Figure S9. Optimized structure of Ce6-IL with $\beta\text{-}1,4$ Glucoside

zt.



Forcite Geometry Optimization - Energy

Figure S10. The energy and convergence of Ce6-IL with $\beta\text{-}1,4$ Glucoside



Figure S11. Optimized structure of IL and β -1,4 Glucoside



Forcite Geometry Optimization - Energy





Figure S13. UV absorption spectroscopy of Ce6-IL



Figure S14. Wide scan of XPS (a) and FT-IR of Ce6-IL (b) $\,$







m/z: 342.1677, required m/z: 342.1671







m/z: 596.2602, required m/z: 597.2635

1.39e4

Channel name: 2: Average Time 1.0554 min : TOF MSe (50-2000) 6eV ESI+ : Centroided : Combined



Figure S17. Ce6-IL mass spectrometry

m/z: 1382.9815, required m/z:1382.9862

Channel name: 2: Average Time 0.3781 min : TOF MSe (50-2000) -6eV ESI- : Centroided : Combined





1.08e4



m/z: 263.2484, required m/z: 263.2482



Channel name: 2: Average Time 0.8010 min : TOF MSe (50-2000) -6eV ESI- : Centroided : Combined

1.63e3



Figure S21. Cation 1-vinyl-3-dodecyl imidazole in Ce6-IL at pH 4.5 mass spectrometry m/z: 263.2446, required m/z: 263.2482

Channel name: 2: Average Time 0.3781 min : TOF MSe (50-2000) -6eV ESI- : Centroided : Combined



m/z: 858.5066, required m/z:858.5044



Figure S23. Fluorescence microscope images of Ce6-IL and Ce6 with E.Coli and S.aureus after 30 min irradiation with 660 nm light. Green staining indicates live bacteria, and red staining indicates dead bacteria, the

magnification is 40 times.



Figure S24. The dual-mode antibacterial mechanism of Ce6-IL