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Supplemental Information

Molecular State of the Membrane-Active Antibiotic Daptomycin

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for **Molecular state of the membrane-active antibiotic daptomycin**

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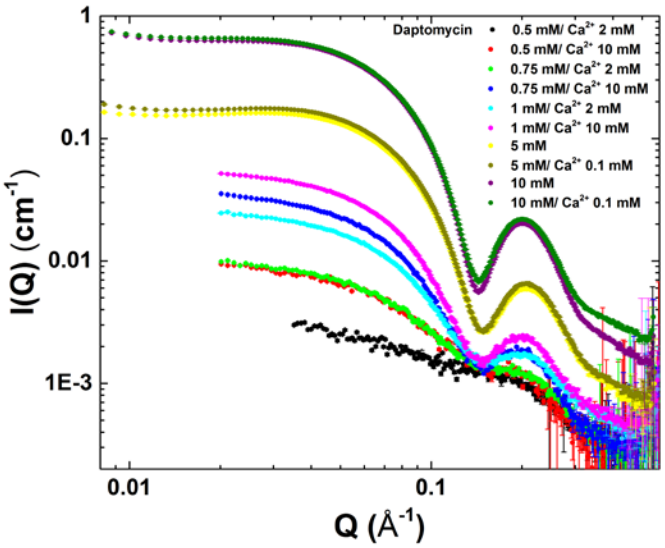


Fig. S1 More small-angle X-ray scattering curves of daptomycin in solution, supplemental to Fig. 2a. The SAXS intensity profiles *I(Q)* at five different concentrations of daptomycin in 10 mM Tris buffer at pH 7.4 with Ca^{2+} from 0.1 to 10 mM.

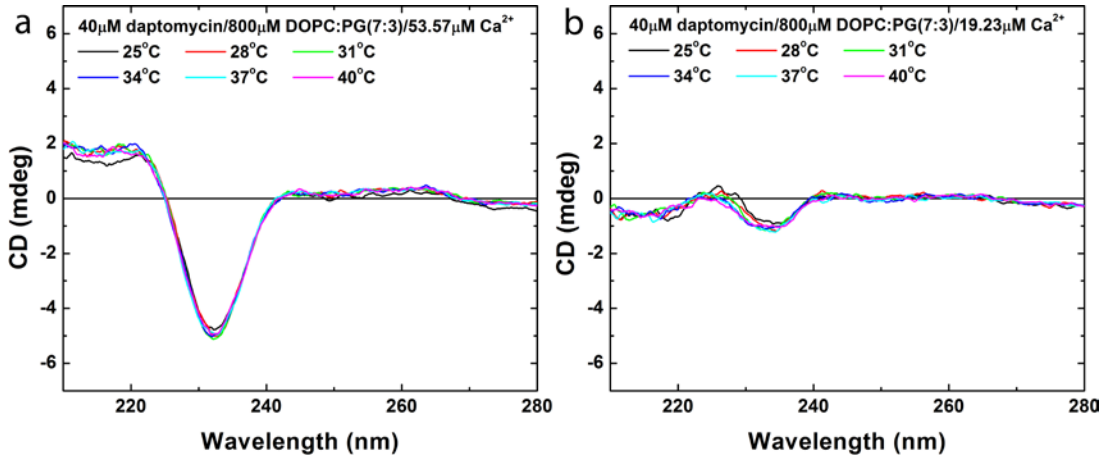


Fig. S2 Temperature dependence of daptomycin CD spectra. (a) The sample is in 13% A and 87% B mixture, shown in Fig. 3b. (b) The sample is in 67% A and 33% B mixture, shown in Fig. 3b. We allowed 20 min for sample to reach equilibrium at each temperature. There is no detectable temperature dependence from 25° C to 40° C.

SAXS comparison

Our SAXS measurement at NSSRC vs. Kirkham et al. (2016) at Diamond Light Source (DLS)

	NSRRC (BL23A beamline)	DLS (B21 beamline)
Flux (photons/s)	10^{11}	10^{11}
Photon energy (keV)	15	12.4
Detector	Pilatus 1M	Pilatus 2M
Sample to detector distance	1.83 m	4.01 m
Sample cell	Quartz cuvette with 30 μm window	Capillary with 100 μm wall

SAXS model fittings

The SAXS data were modeled by using the software SasView (http://www.sasview.org/ originally developed by the DANSE project under NSF award DMR-0520547). Solid sphere, core shell and RaspBerry models were used in the low, medium and high daptomycin concentrations respectively. The main parameters are listed in the following table: the fittings are shown in Fig. 1a.

(a) Sphere model

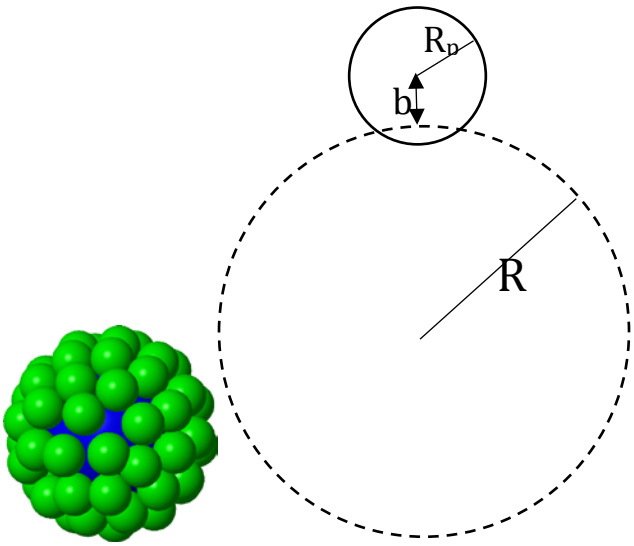
Daptomycin (mM)	Ca^{2+} (mM)	R (Å)
0.5	0	10.35
0.5	1	10.60
0.75	0	10.28

(b) Core shell model

Daptomycin (mM)	Ca^{2+} (mM)	R_{in} (Å)	R_{out} (Å)
0.75	1	9.98	39.59
1	0	10.41	37.86

(c) RaspBerry model

Daptomycin (mM)	Ca^{2+} (mM)	R_o (Å)	R_p (Å)	b (Å)	N
1	1	19.27	10.67	9.07	28
2	0	20.47	10.26	6.77	28
2	1	19.96	10.15	7.00	28



Cartoon for the RaspBerry model.