

Supplementary Materials: Mycolactone A vs. B: Multiscale Simulations Reveal the Roles of Localization and Association in Isomer-Specific Toxicity

John D. M. Nguyen, Gabriel C. A. da Hora and Jessica M. J. Swanson

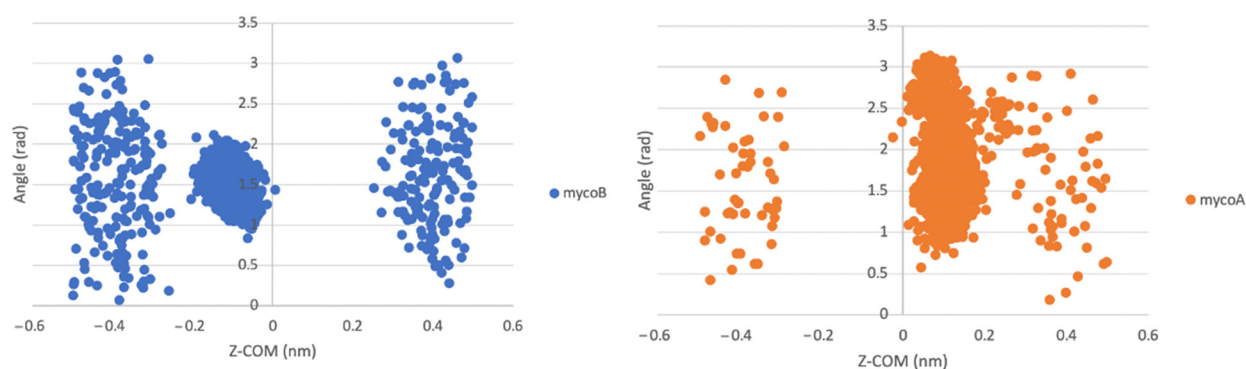


Figure S1. Distribution of the two CVs in unbiased simulations of mycolactone A/B with the ER membrane.

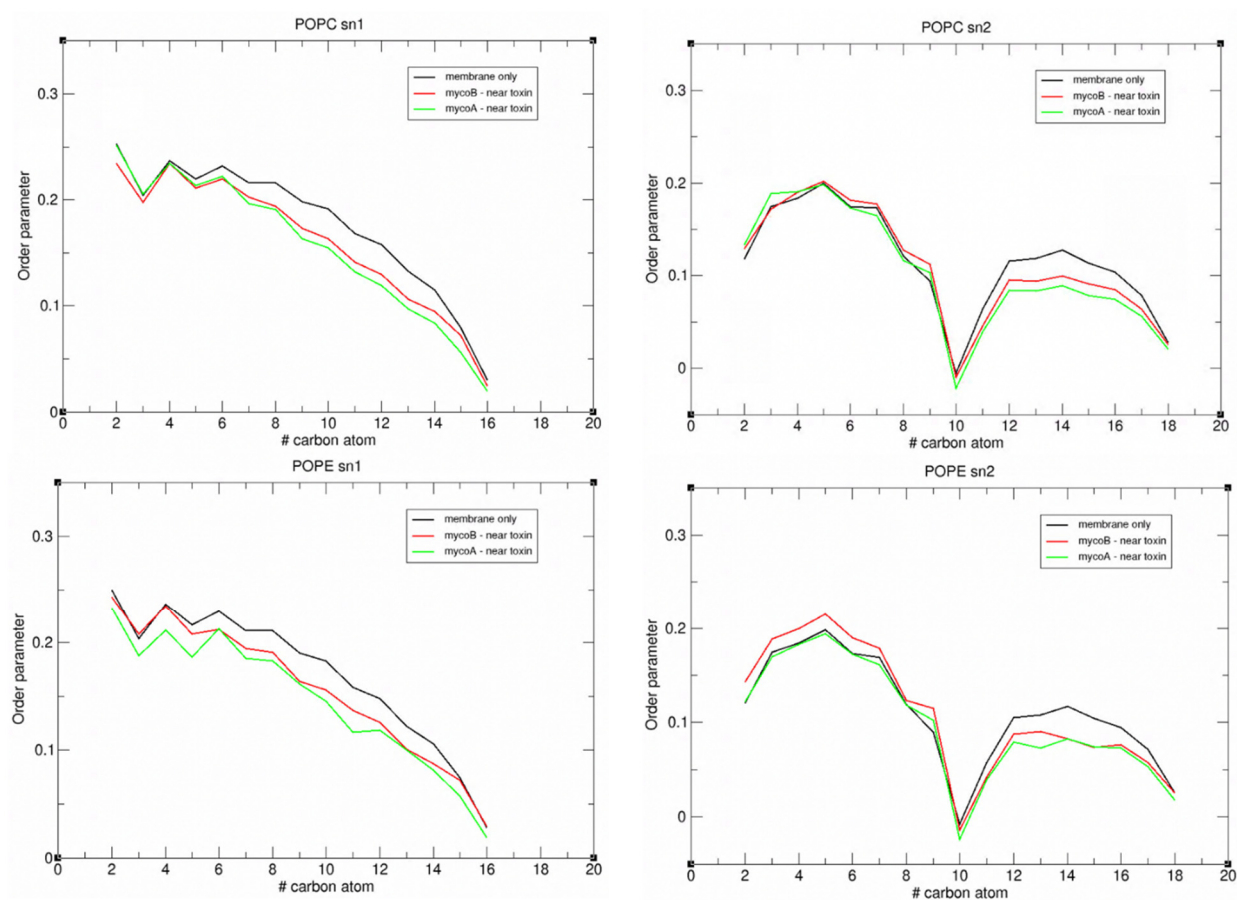


Figure S2. Tail order parameters of lipids near mycolactone and lipids of an ER membrane with-out the toxin.

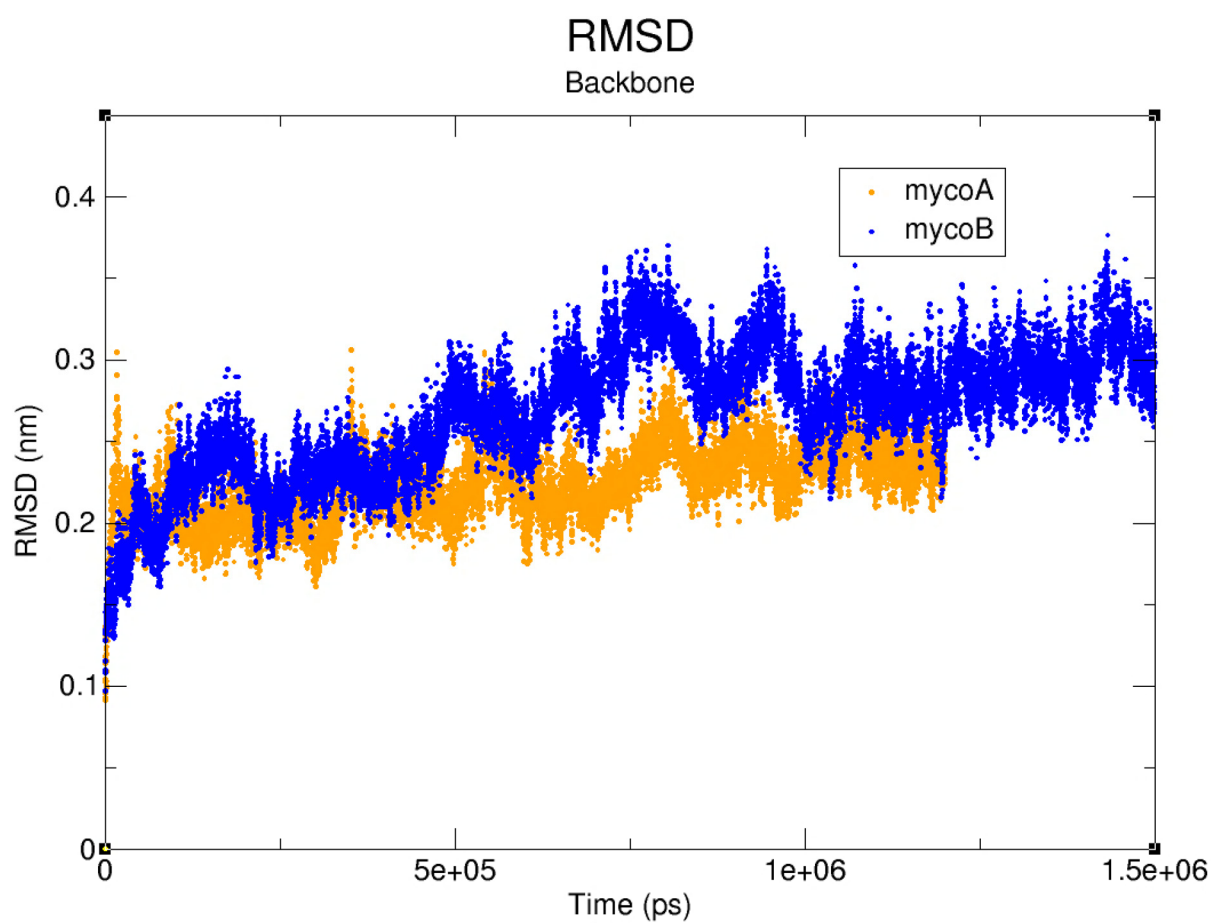


Figure S3. Root mean square deviation of mycolactone-Sec61 complexes.