Computational Insights into the Linker-Dependent Binding of Trehalose–Porphyrin Conjugates to Antigen 85B of *Mycobacterium tuberculosis*

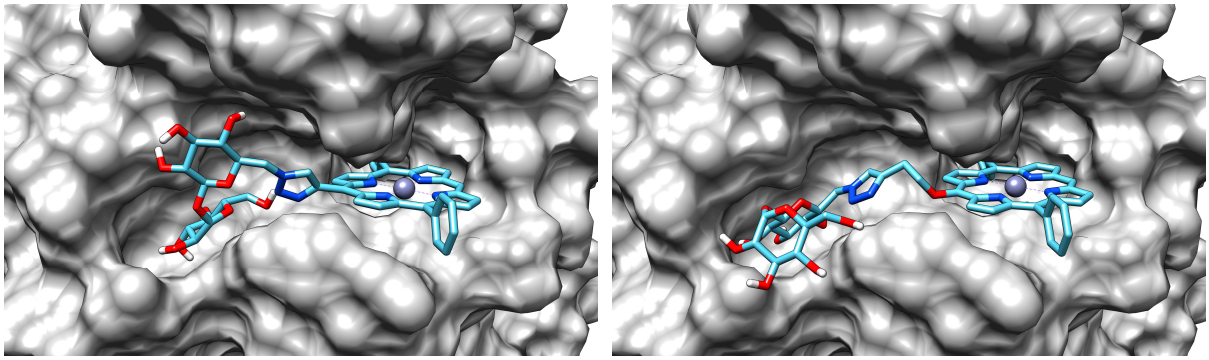
Supporting Information

Christopher T. Piatnichouk [1], Joshua V. Ruppel [2] and Nicole L. Snyder [1,*]

[1] Department of Chemistry, Davidson College, Davidson, NC 28035, USA; chpiatnichouk@davidson.edu

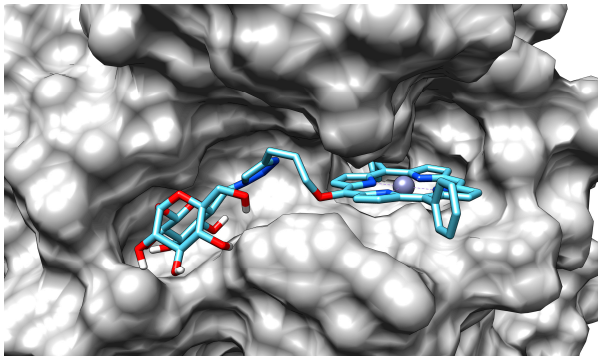
[2] Department of Natural Sciences and Engineering, University of South Carolina Upstate, Spartanburg, SC 29303, USA; ruppelj@uscupstate.edu

* Correspondence: nisnyder@davidson.edu

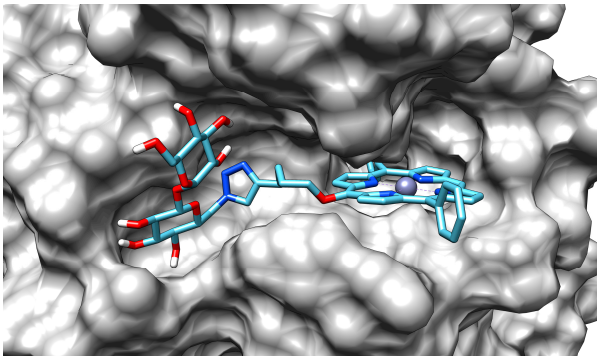


(**a**)

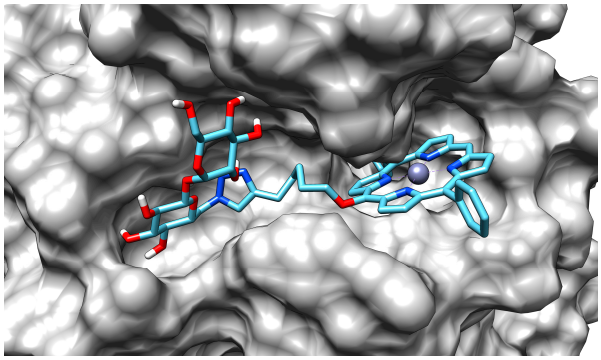
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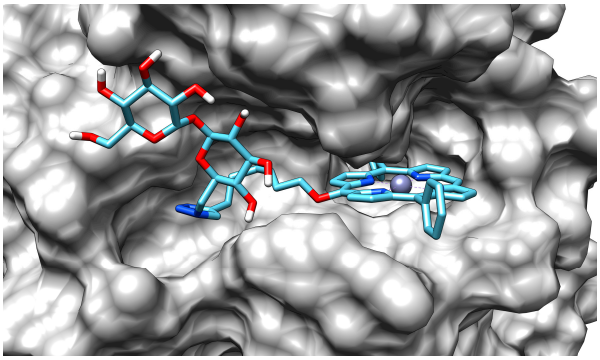
(c)



(d)



(e)



(f)

Figure S1. Highest-affinity binding poses for each docked linker variant. The zero-carbon linker is shown in **(a)**, the two-carbon linker in **(b)**, the three-carbon linker in **(c)**, the four-carbon linker in **(d)**, the five-carbon linker in **(e)**, and the six-carbon linker in **(f)**.

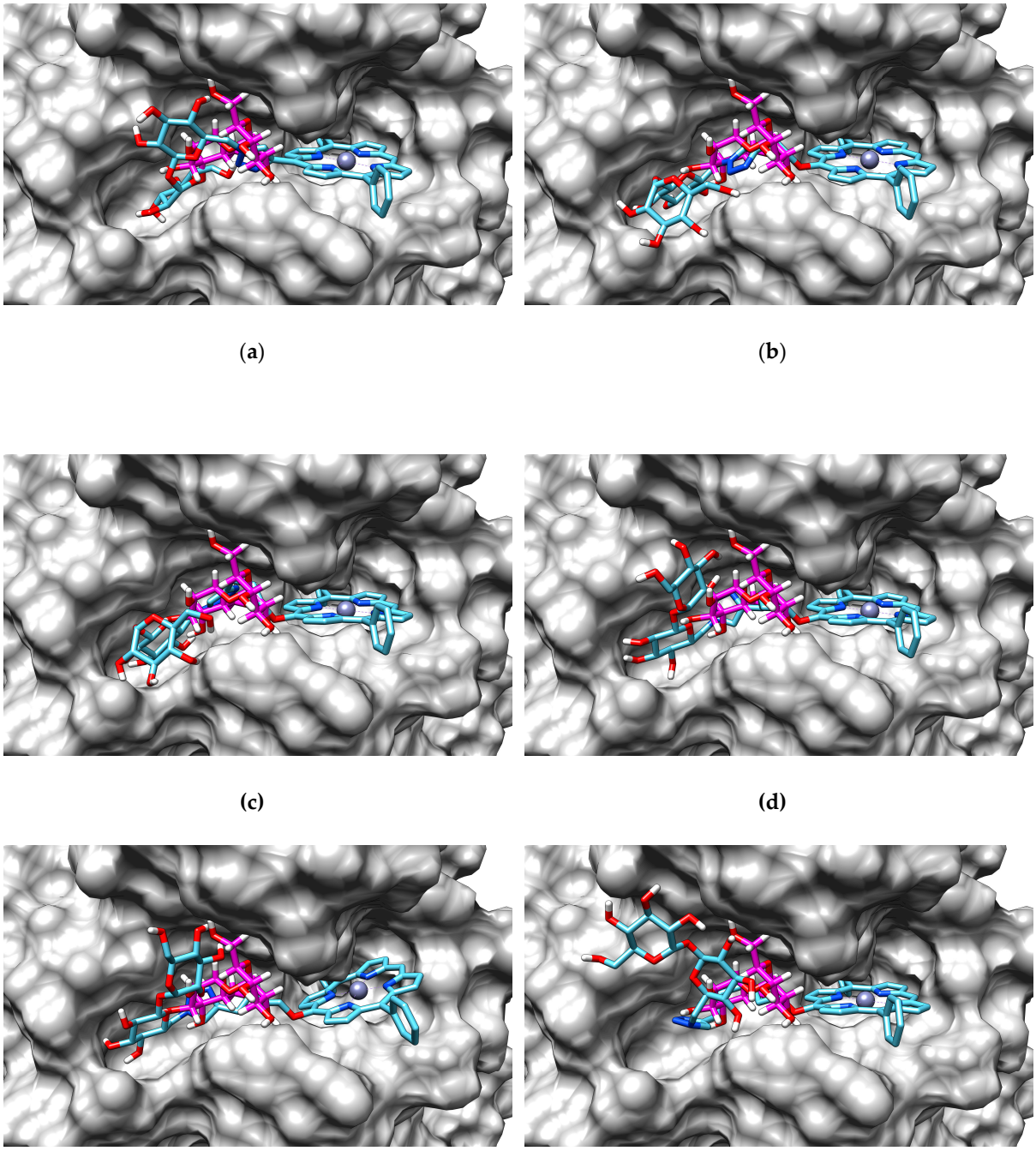


Figure S2. Highest-affinity binding poses for each docked linker variant (blue) relative to trehalose cocrystal structure (magenta). The zero-carbon linker is shown in **(a)**, the two-carbon linker in **(b)**, the three-carbon linker in **(c)**, the four-carbon linker in **(d)**, the five-carbon linker in **(e)**, and the six-carbon linker in **(f)**.