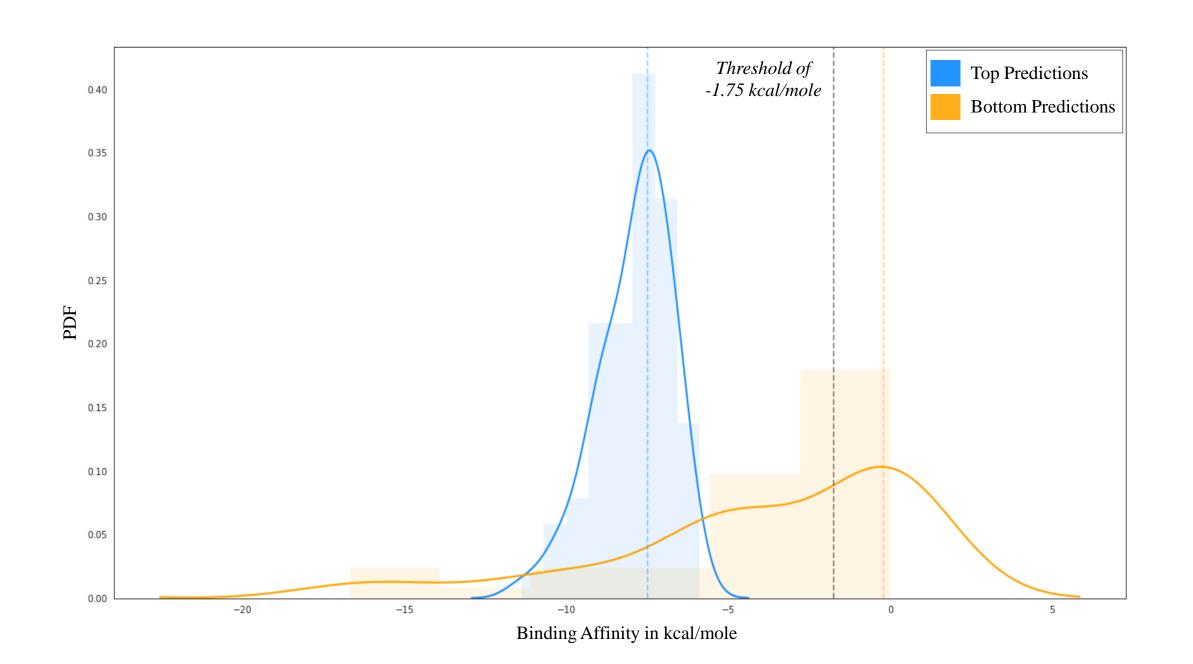
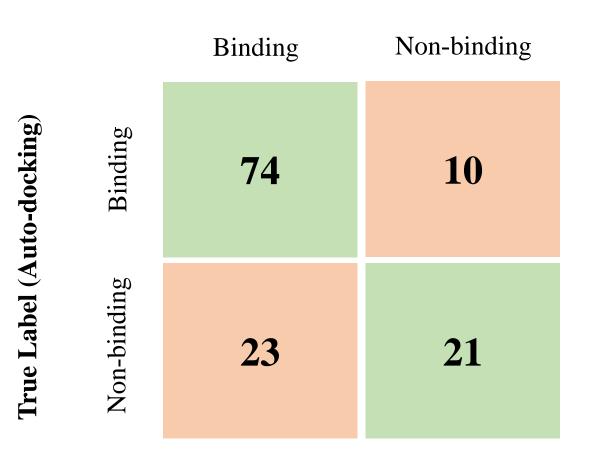
\mathbf{A}

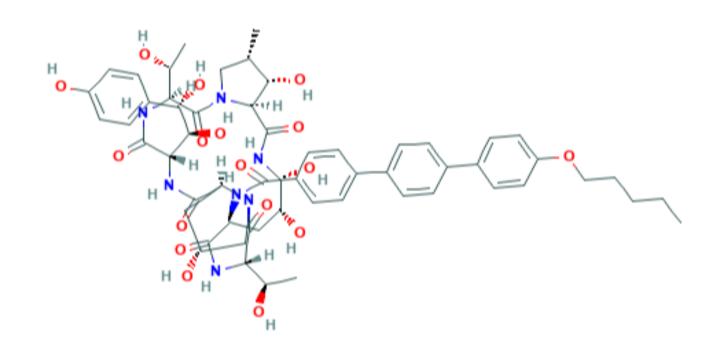


Predicted Label (AI-Bind)



F1-Score = 0.82

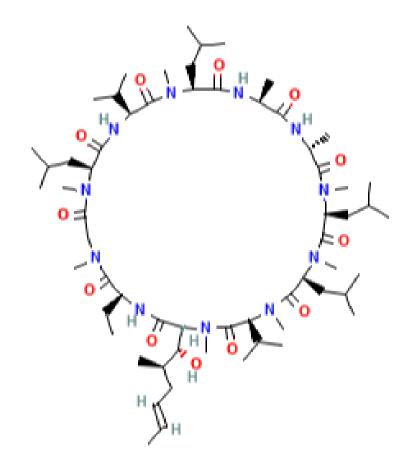
C



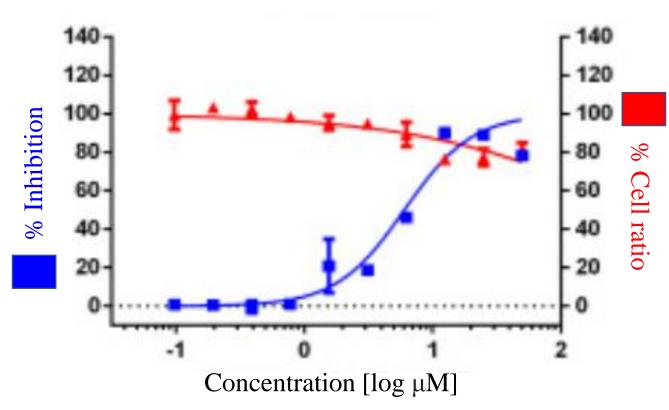
Anidulafungin % Cell ratio wontiquy %

IC₅₀=4.64; CC₅₀>50; SI=10.78

Concentration [log μM]



Cyclosporin



IC₅₀=5.82; CC₅₀>50; SI=8.59

^{*}Adapted from Jeon, S.et al. Identification of antiviral drug candidates against SARS-CoV-2 from FDA-approved drugs. Antimicrobial Agents and Chemotherapy 64 (2020). URL https://doi.org/10.1128/aac.00819-20. Adapted with permission.