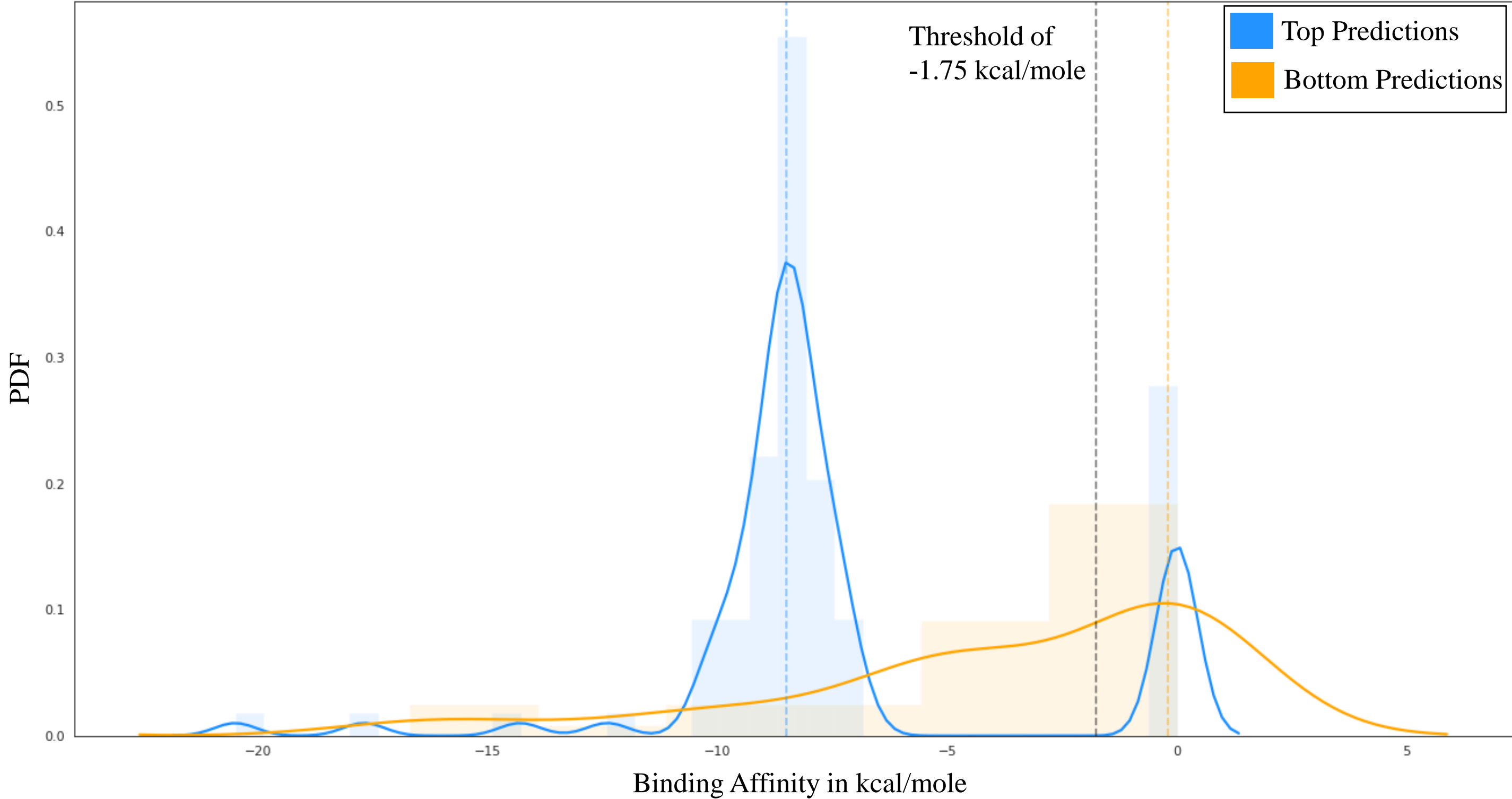
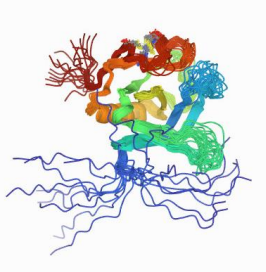
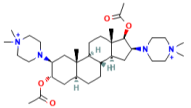
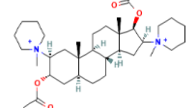
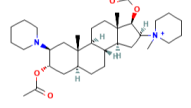
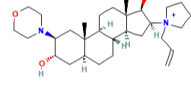
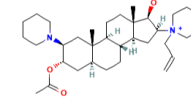
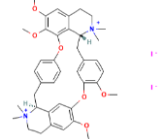
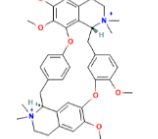


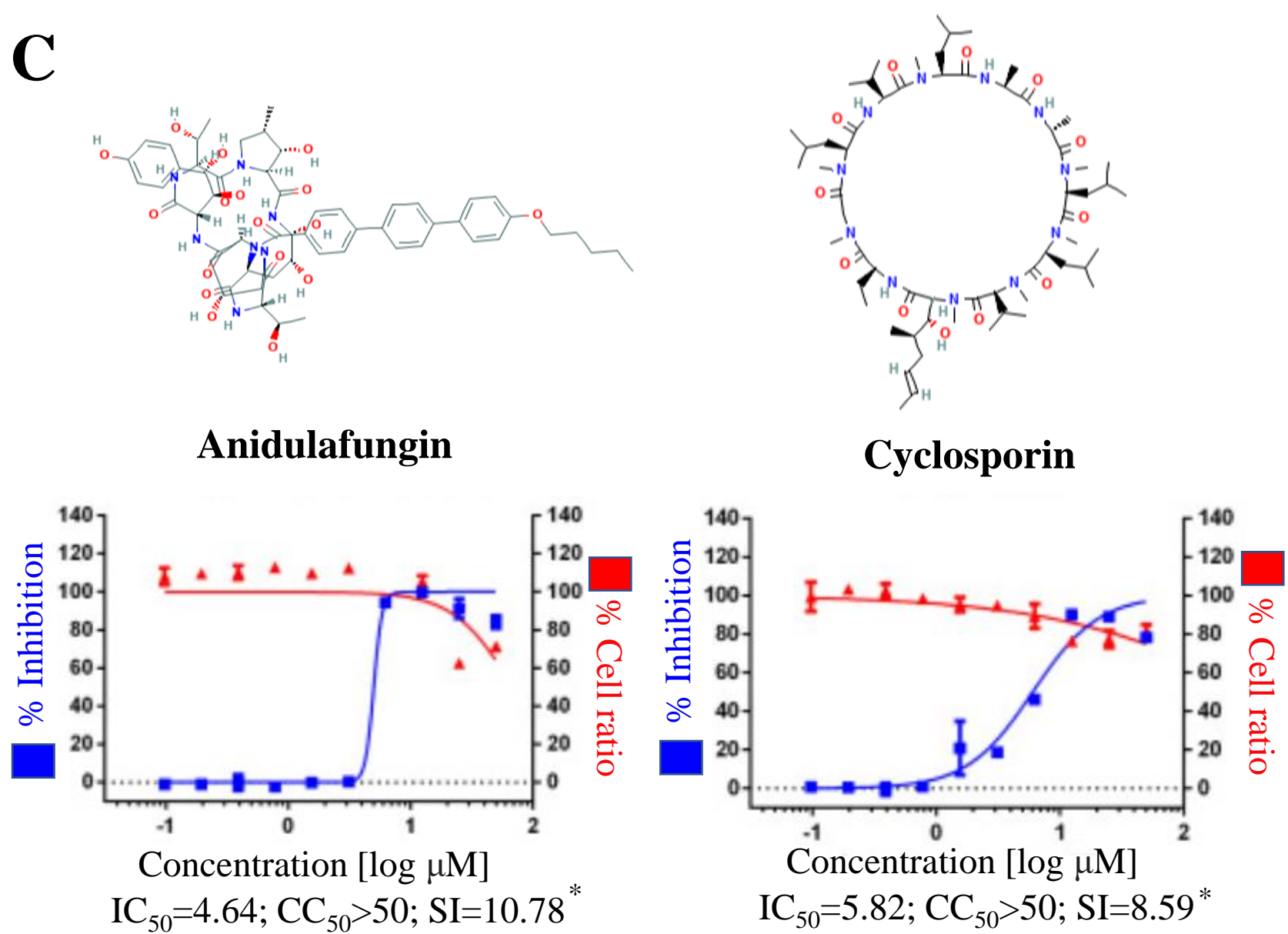
A



B

		$c_{\text{Spearman}}(p_{ij}^{\text{VecNet}}, \Delta G) = -0.40$			
	Tyrosine-protein kinase Tec	Prediction Percentile	Binding Affinity (kcal/mole)	Change in Rank	
Pipecuronium		99.99976	-7.6	0	
Pancuronium		99.99955	-7.6	0	
Vecuronium		99.99901	-7.5	-3	
Rocuronium		99.99701	-7.5	-1	
Rapacuronium		99.99691	-7.3	-2	
Metocurine iodide		99.99687	-7.1	+3	
Metocurine		99.99671	-6.9	+3	

C



*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.