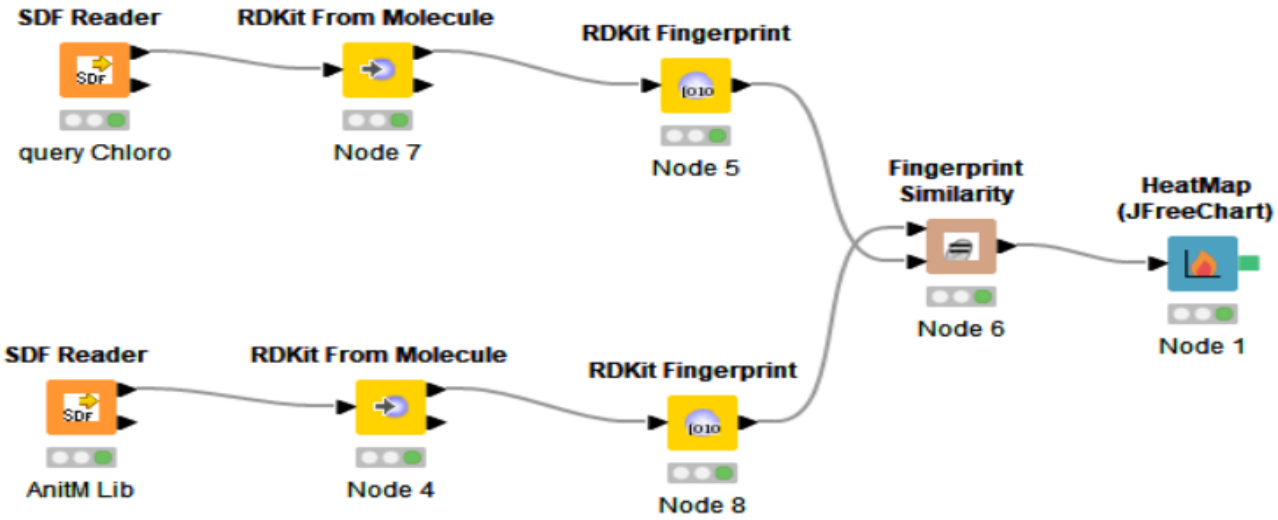
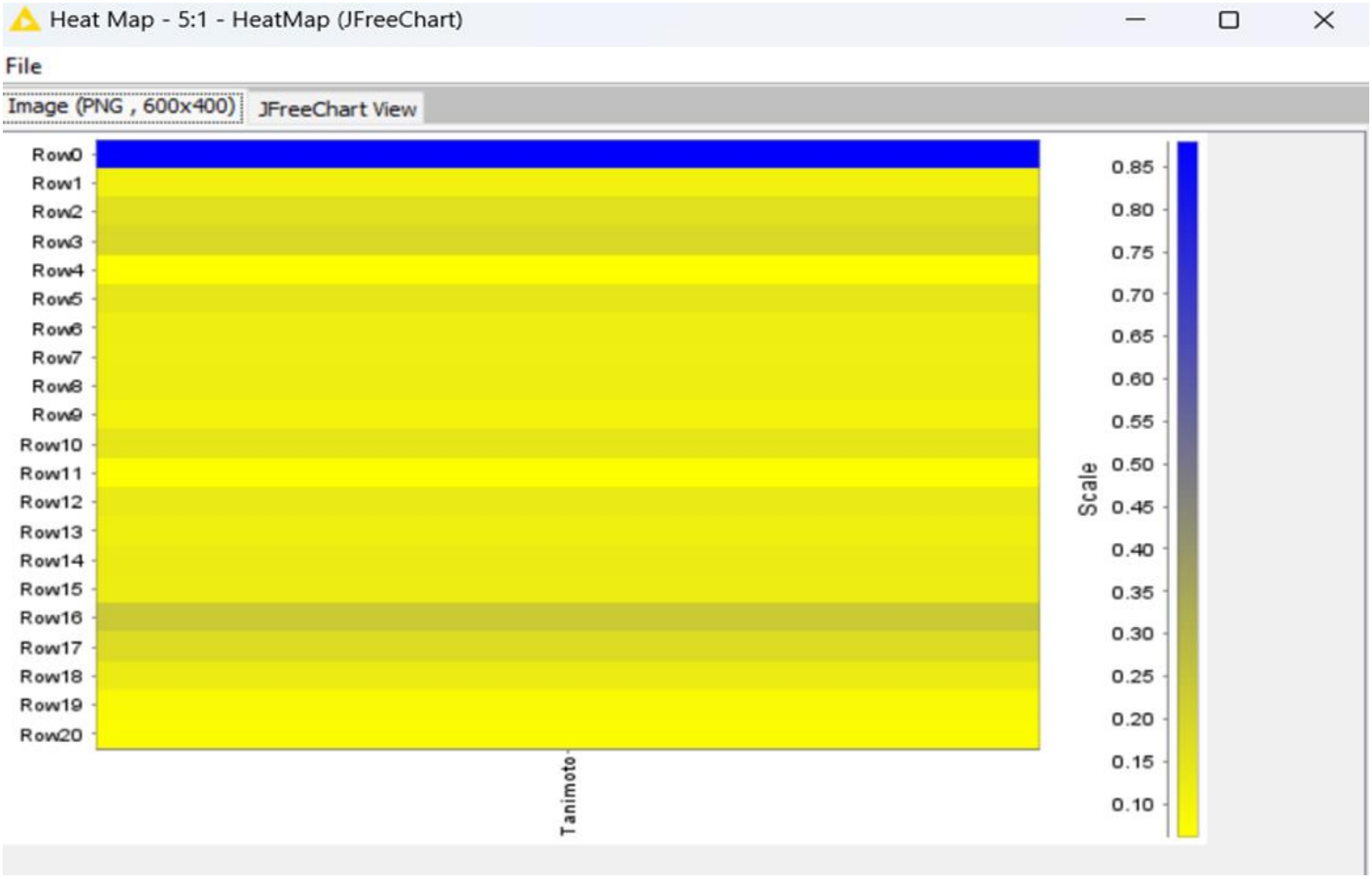
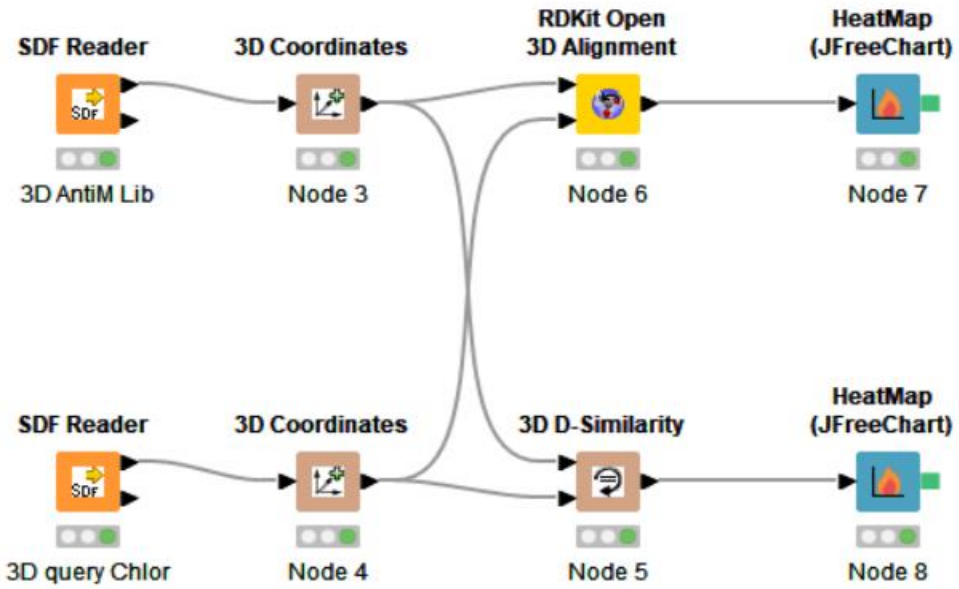
Result

2D workflow and Heatmap

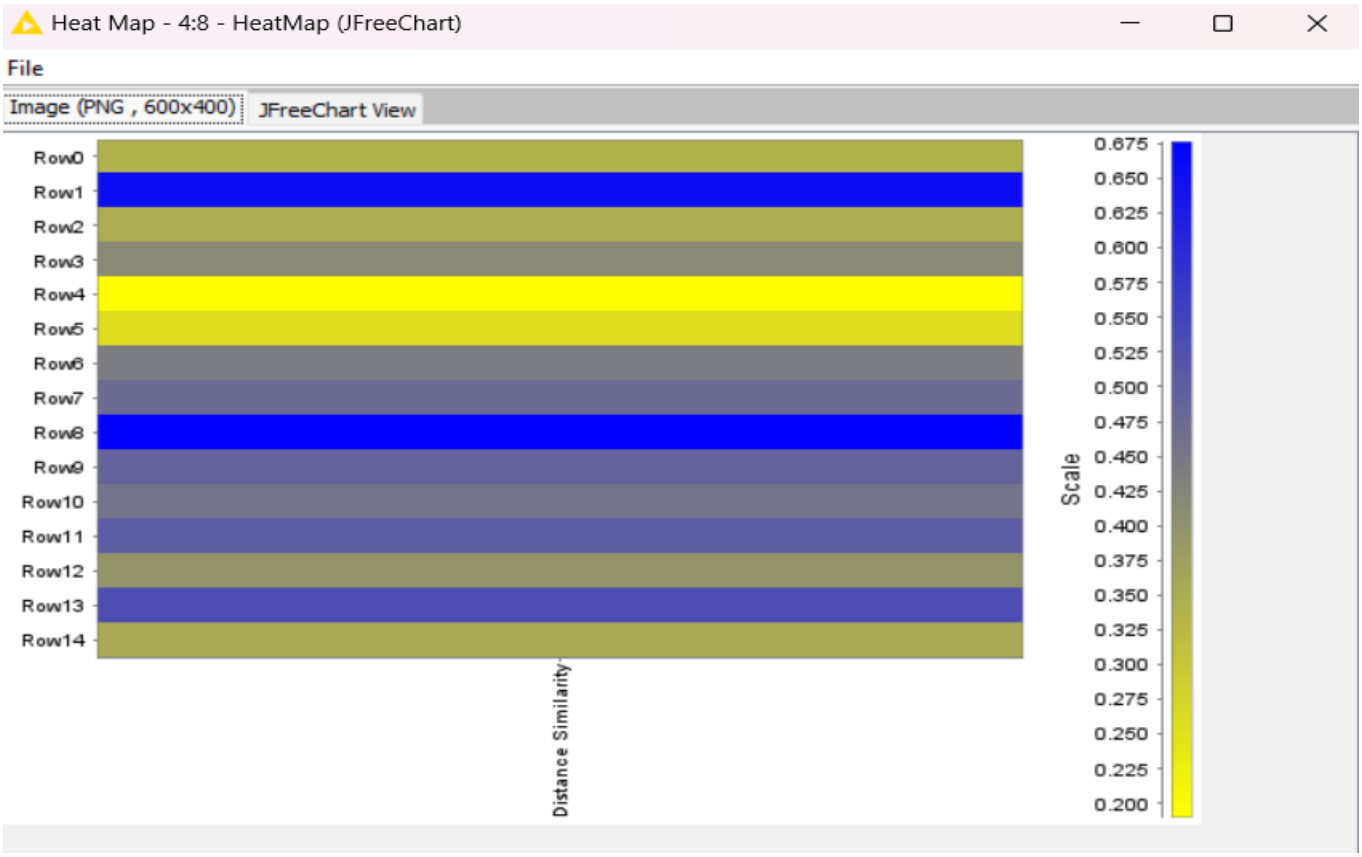




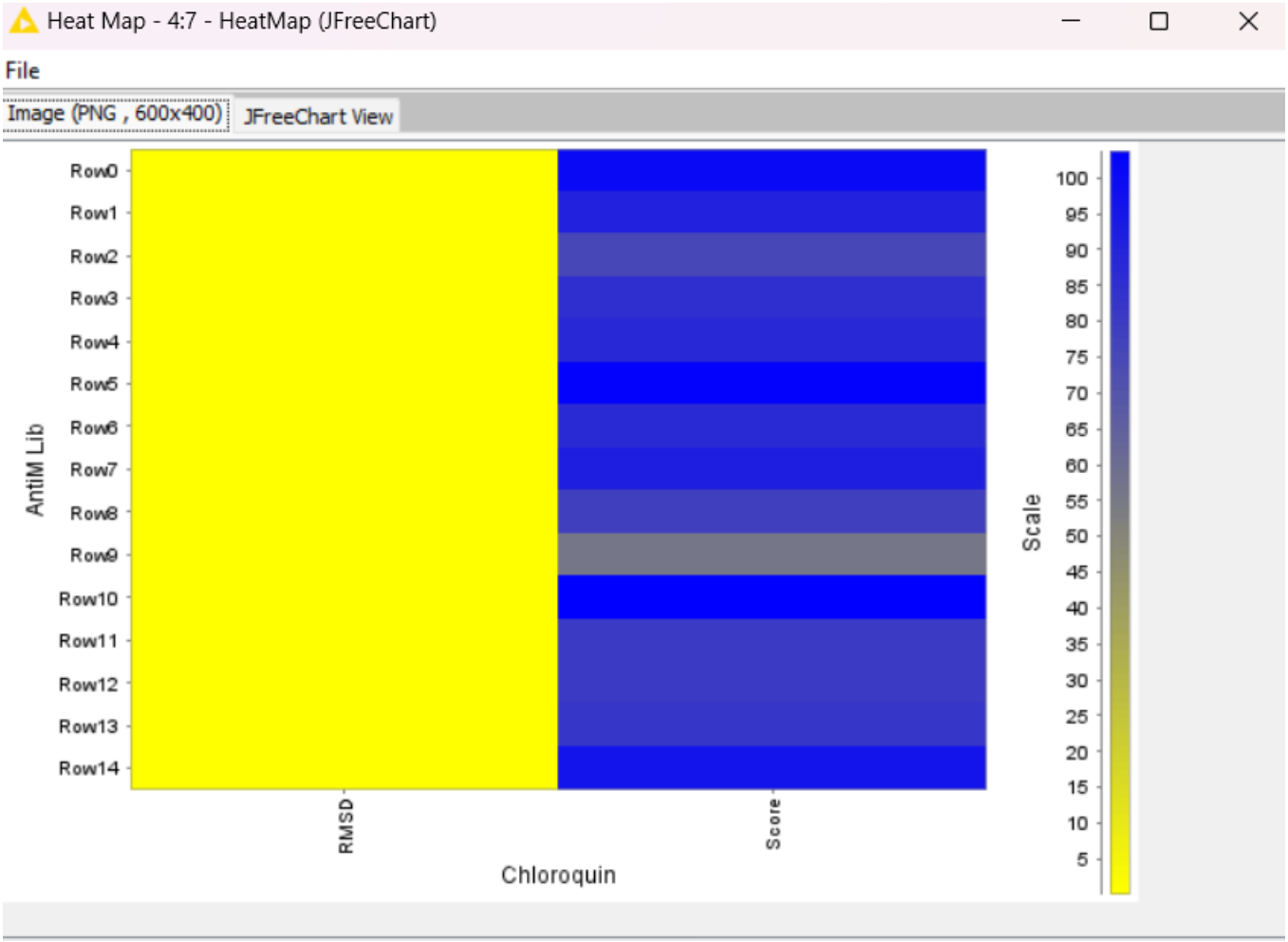
3D Workflow (Using CDK and RDkit Packages)



Heatmap (3D similarity using CDK Package)



Heatmap (3D alignment Using RDkit package)

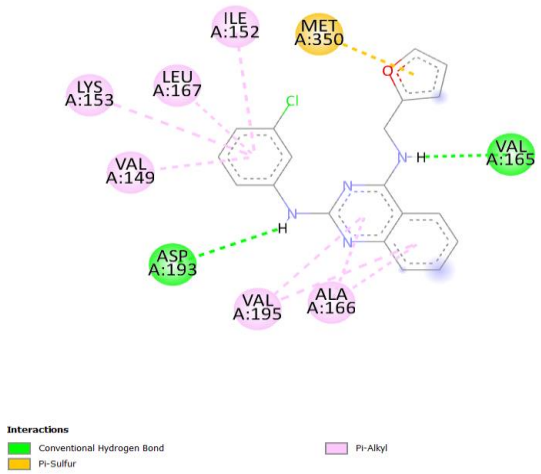


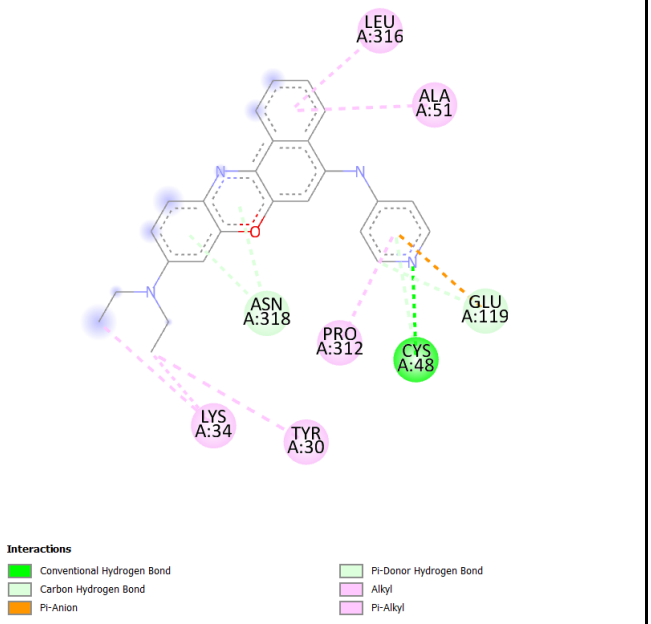
1.

Molecular Docking

Protein Name: Adenosine deaminase (plasmodial vivax)

Protein ID – 3EWC PDB DOI: https://doi.org/10.2210/pdb3ewc/pdb

Ligand Name	Ligand ID	Energy value	Dock Image
2-N-(3-chlorophenyl)-4-N-(furan-2-ylmethyl)quinazoline-2,4-diamine	1285085	-8.2	

N,N-diethyl-5-pyridin-4-yliminobenzo[a]phenoxazin-9-amine	44226912	-8.4	
1-(3,4-dichlorophenyl)-8-methyl-N-[2-(methylamino)ethyl]-9H-pyrido[3,4-b]indole-3-carboxamide	156869265	-7.5