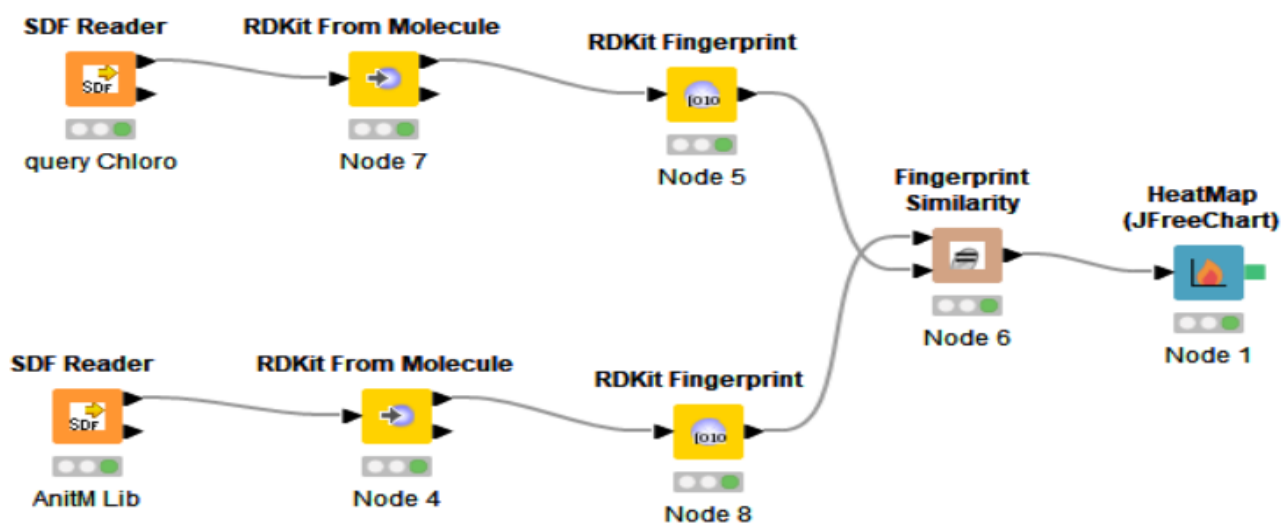


Result

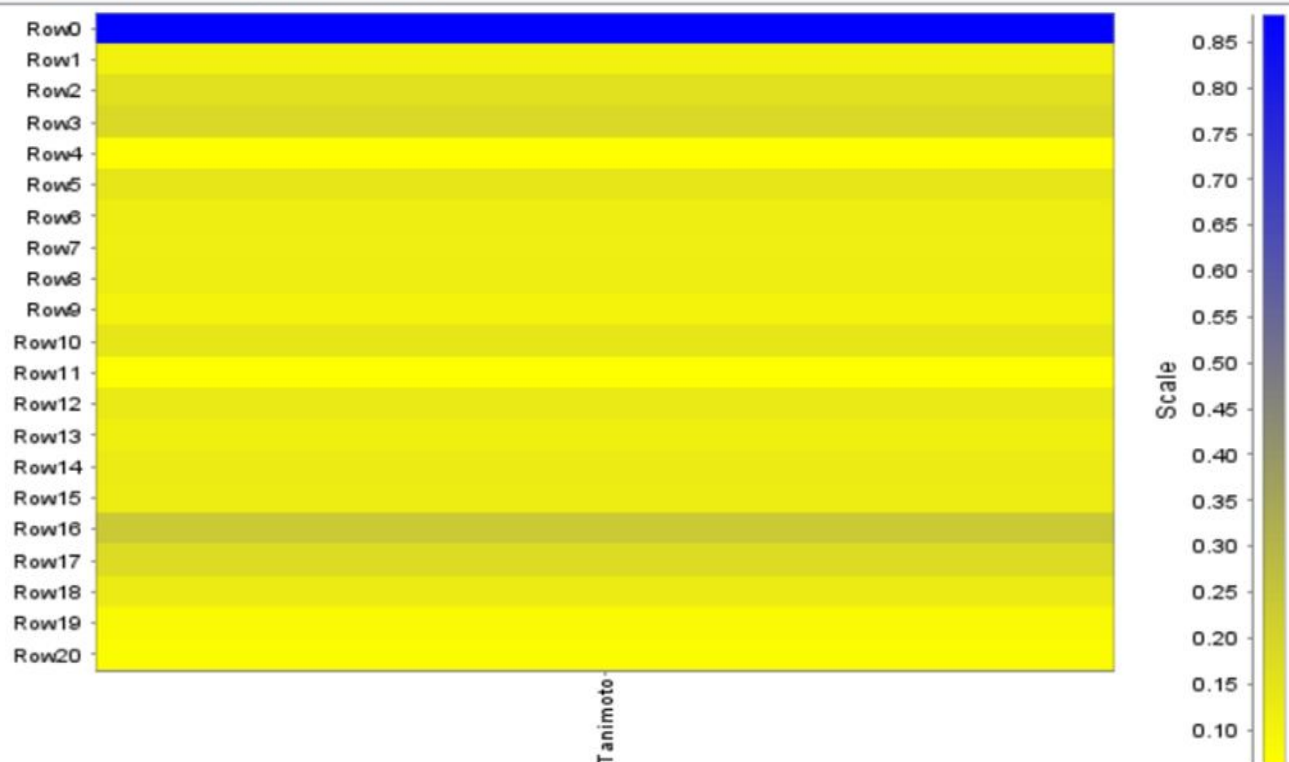
2D workflow and Heatmap



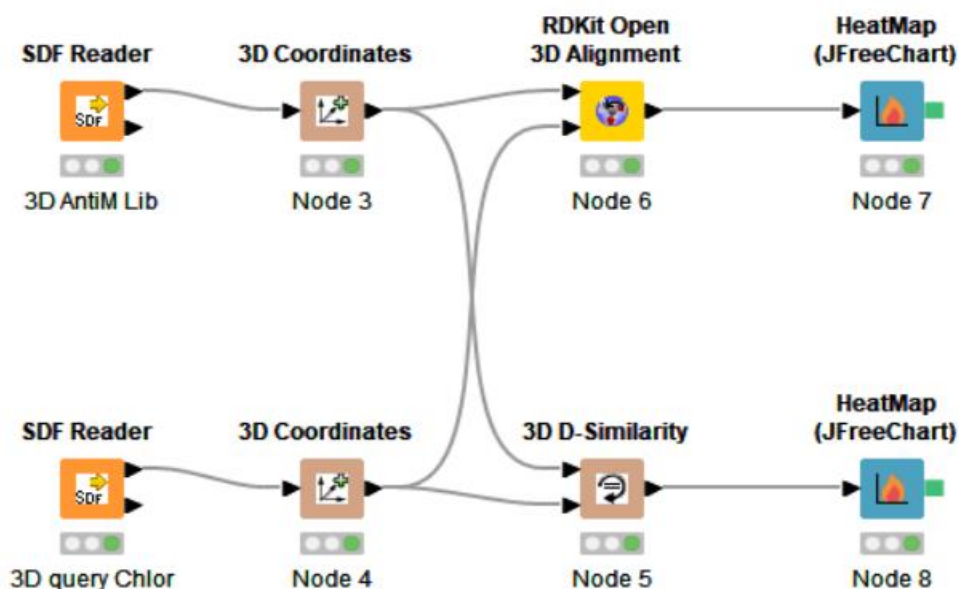
Heat Map - 5:1 - HeatMap (JFreeChart)

File

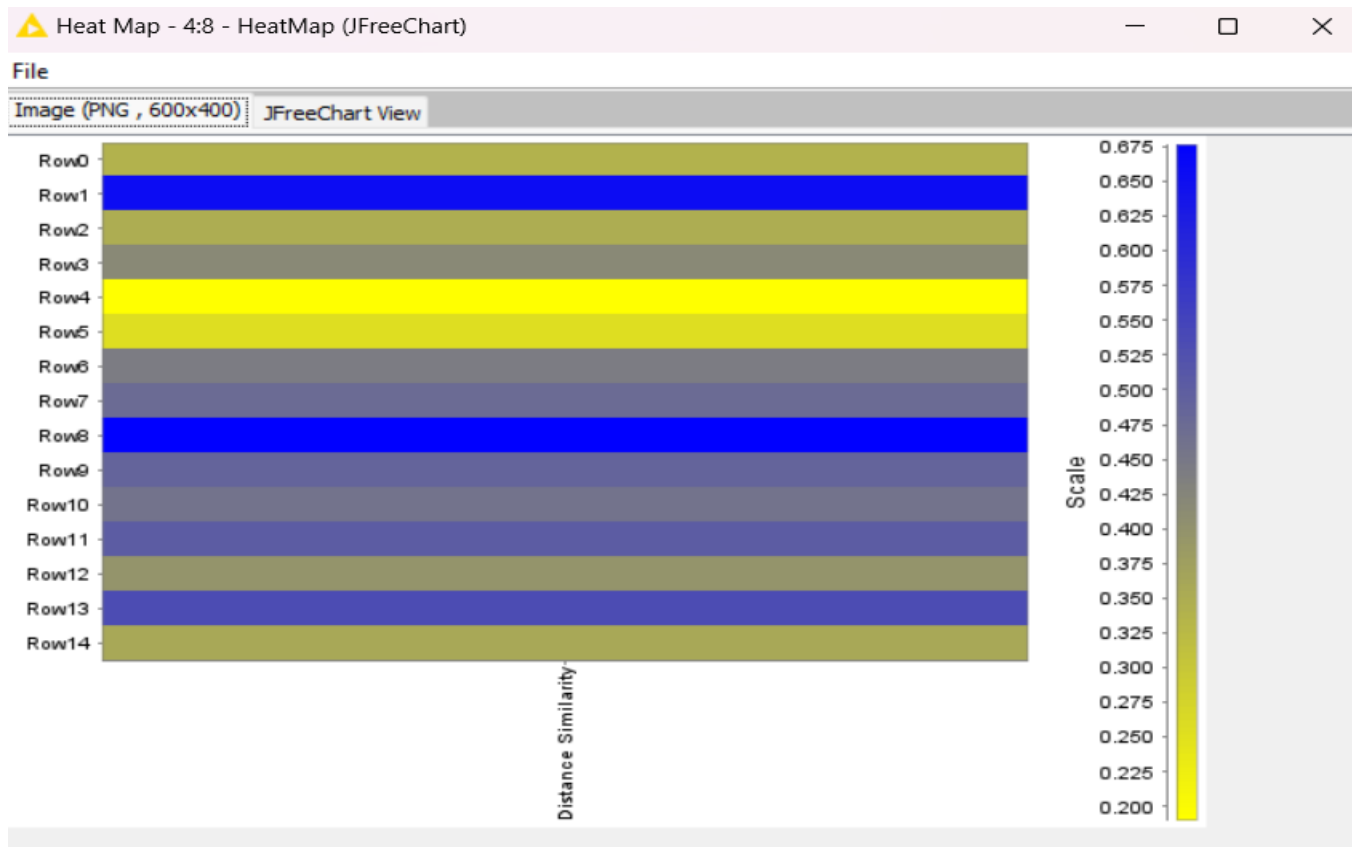
Image (PNG , 600x400) JFreeChart View



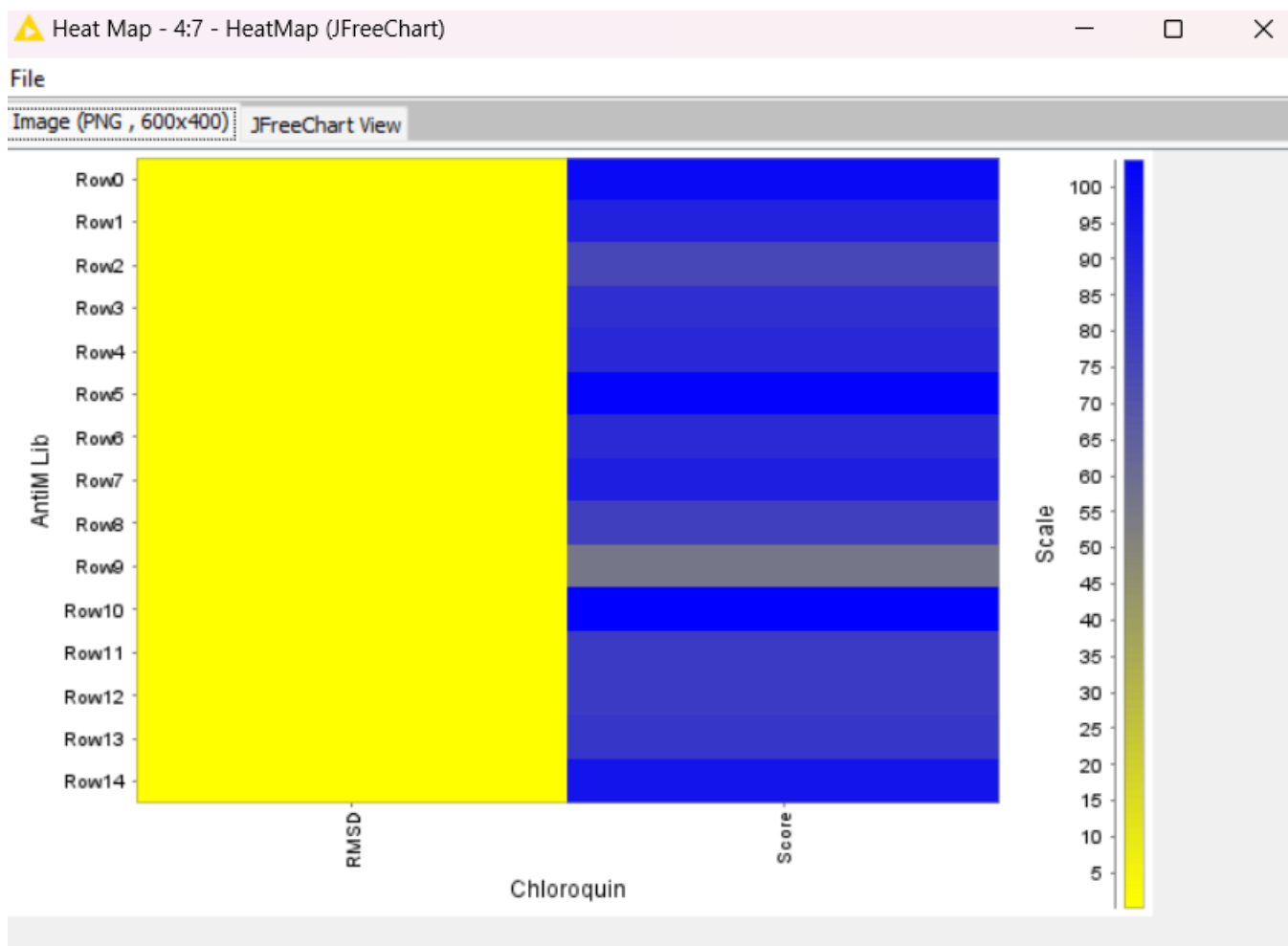
3D Workflow (Using CDK and RDkit Packages)



Heatmap (3D similarity using CDK Package)



Heatmap (3D alignment Using RDkit package)



1.

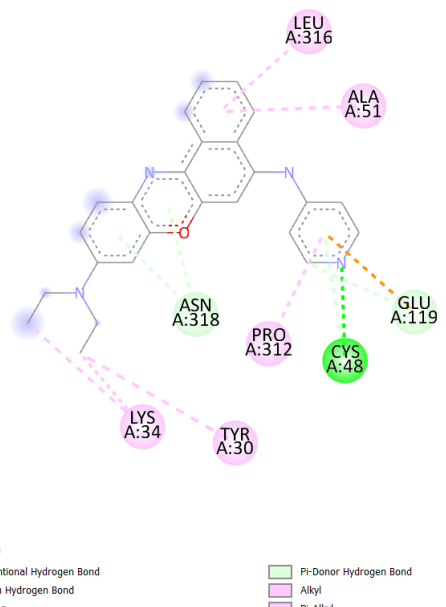
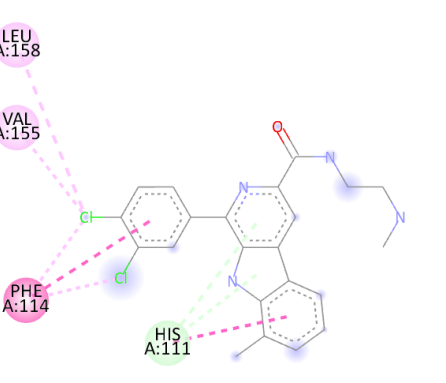
Molecular Docking

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	<p>Interactions</p> <p>Conventional Hydrogen Bond</p> <p>Pi-Sulfur</p> <p>Pi-Alkyl</p>

<p>N,N-diethyl-5-pyridin-4-yliminobenzo[a]phenoxazin-9-amine</p>	<p>44226912</p>	<p>-8.4</p>	 <p>Interactions</p> <ul style="list-style-type: none"> Conventional Hydrogen Bond Carbon Hydrogen Bond Pi-Anion Pi-Donor Hydrogen Bond Alkyl Pi-Alkyl
<p>1-(3,4-dichlorophenyl)-8-methyl-N-[2-(methylamino)ethyl]-9H-pyrido[3,4-b]indole-3-carboxamide</p>	<p>156869265</p>	<p>-7.5</p>	 <p>Interactions</p> <ul style="list-style-type: none"> Pi-Donor Hydrogen Bond Pi-Pi Stacked Pi-Pi T-shaped Pi-Donor Hydrogen Bond Alkyl Pi-Alkyl