Assignments:

1. Perform and execute molecular similarity search of a single molecule (your query) in a library using
    - 2D fingerprint similarity(either MACCS or MORGAN) ,
    - 3D alignment (RD Kit package)
    - 3D similarity (using CDK package)
2. Add a snip or a screenshot of the following results

- Your Knime Workflow
- Heatmap obtained

3.

Molecular Docking

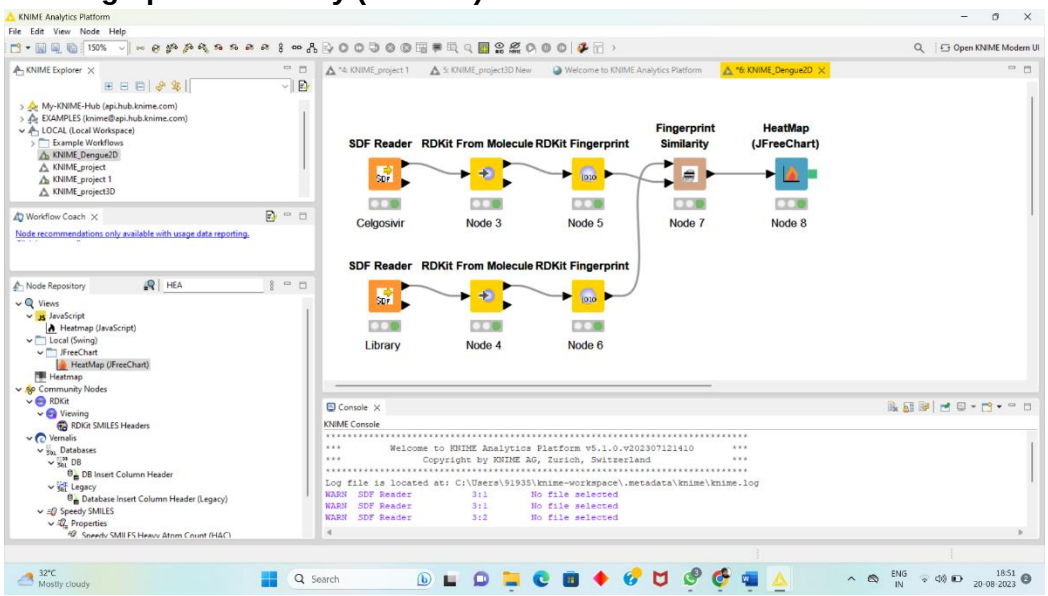
Protein Name:
Protein ID -

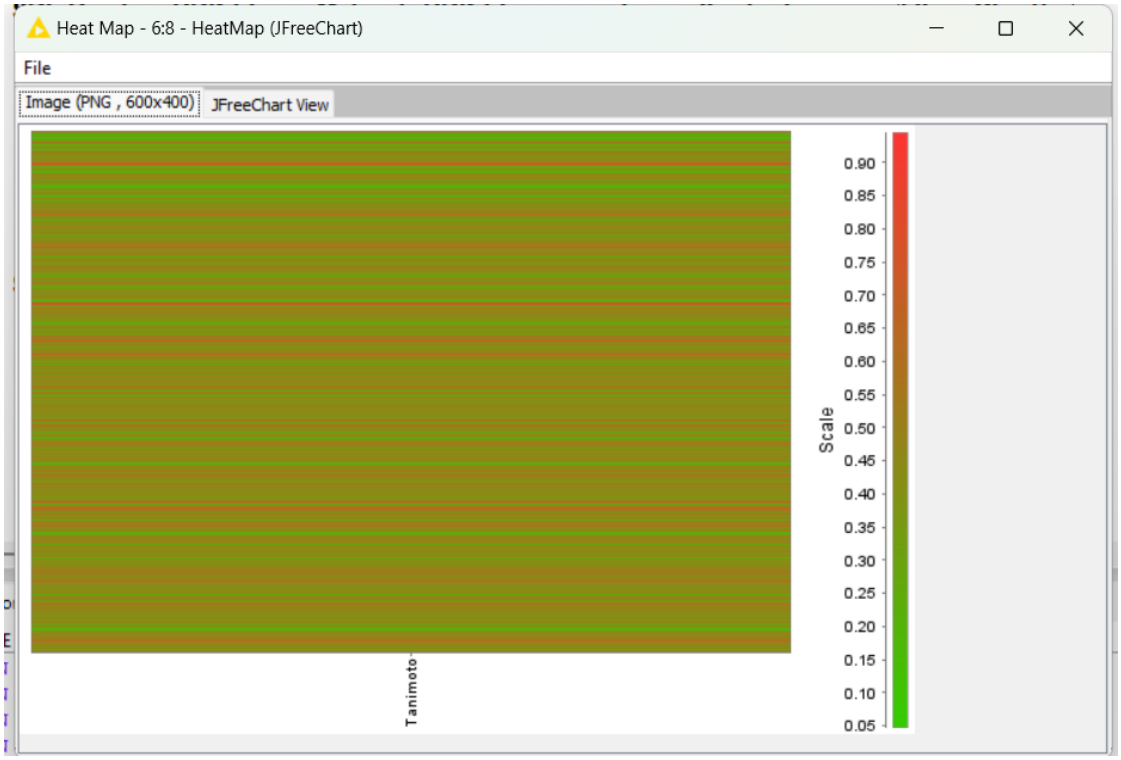
Ligand Name	Ligand ID	Energy value	Dock Image

Solutions

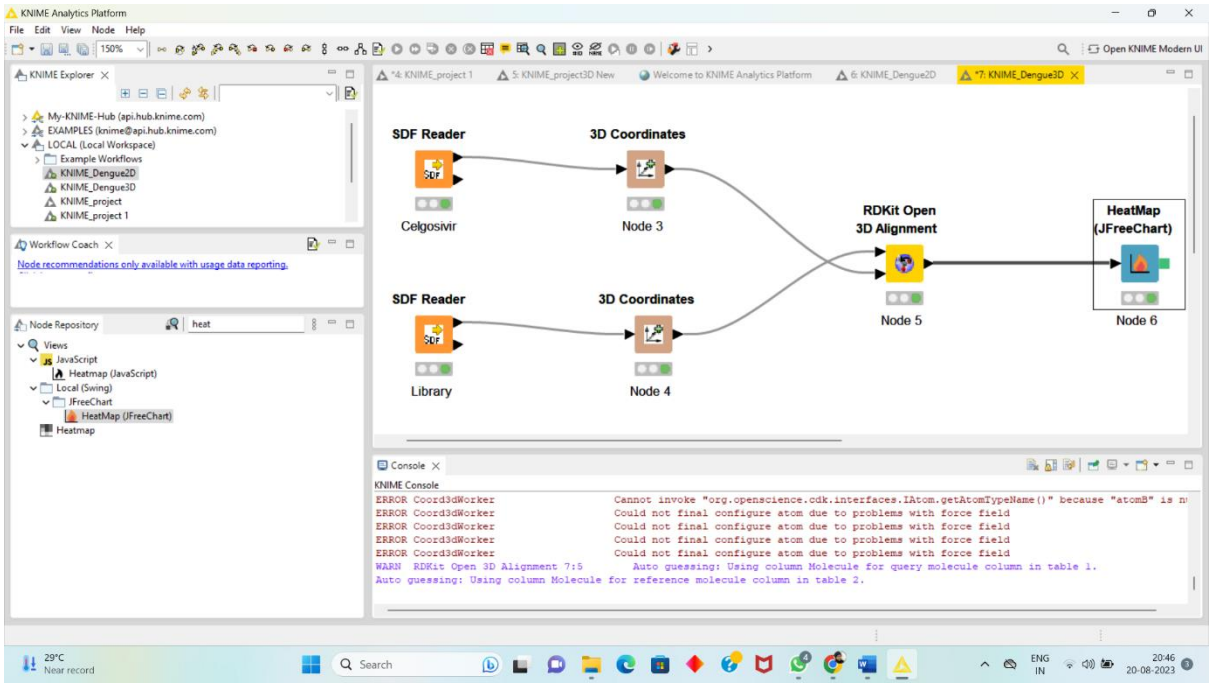
- Query- Celgosivir antiviral drug for Dengue
- Library- Antiviral drugs

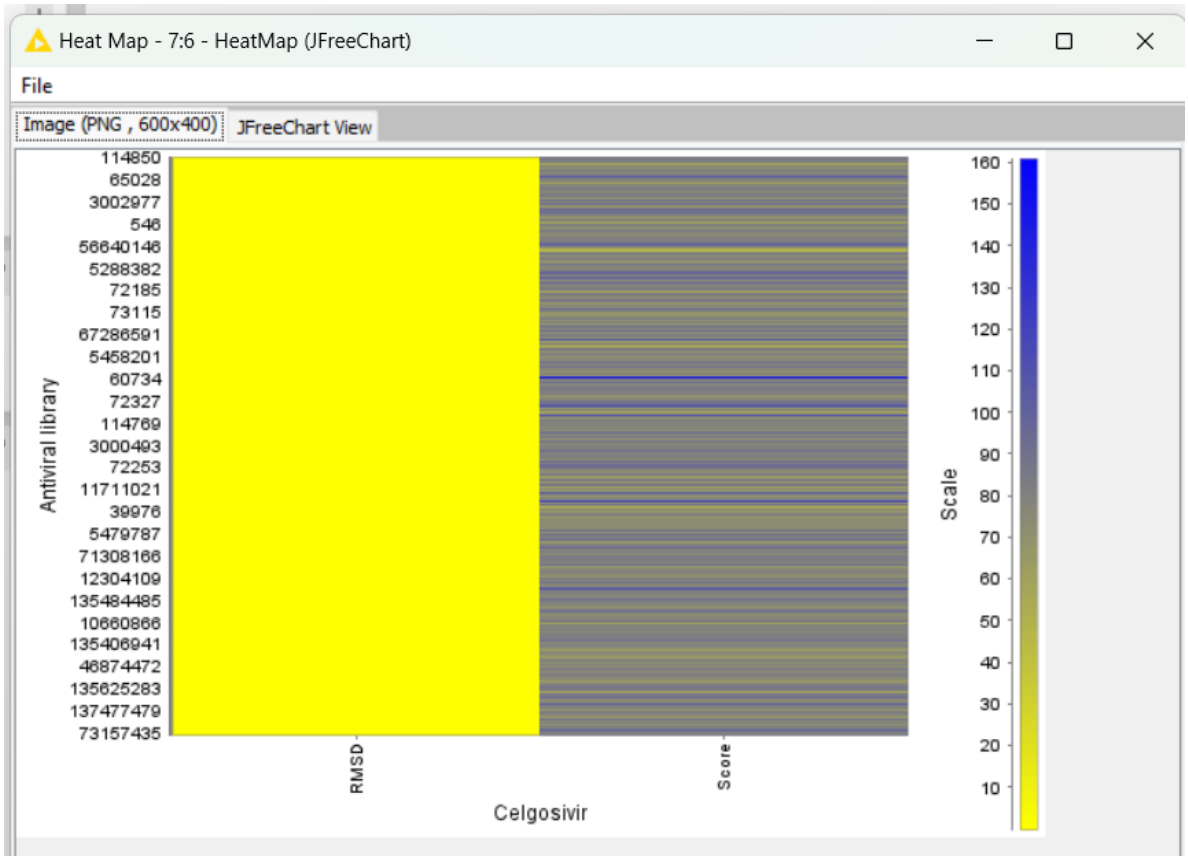
➢ **2D fingerprint similarity (MACCS)**





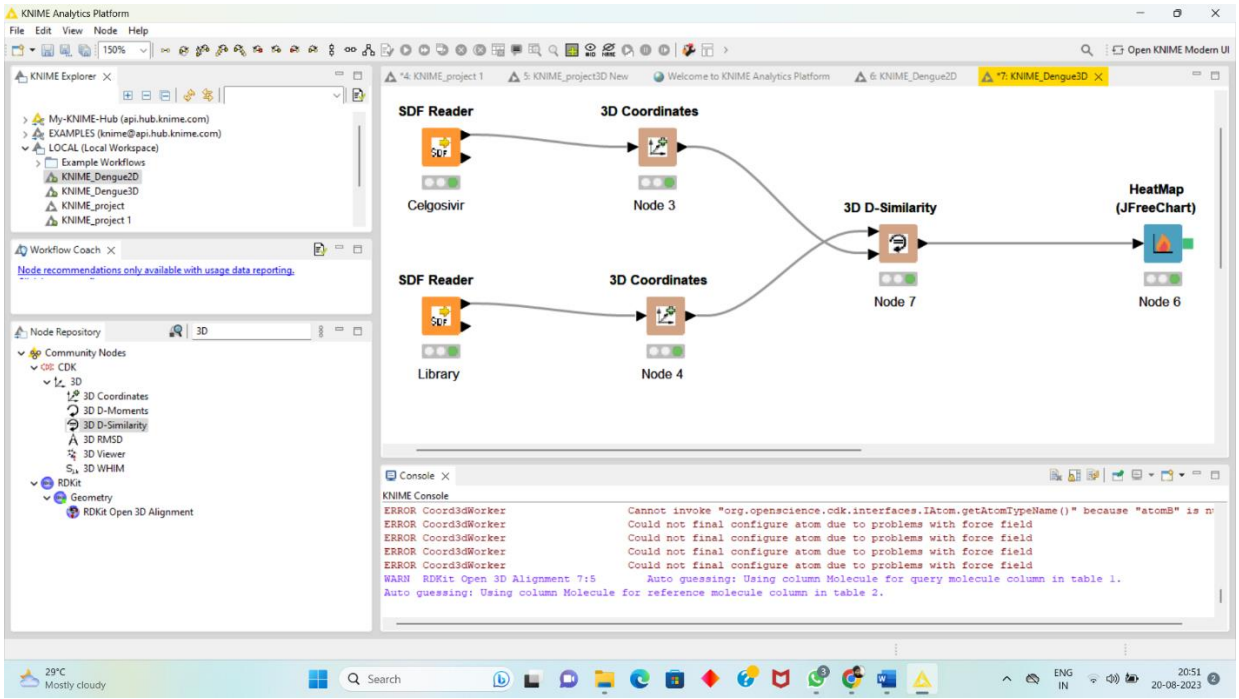
- **3D alignment (RD Kit package)**

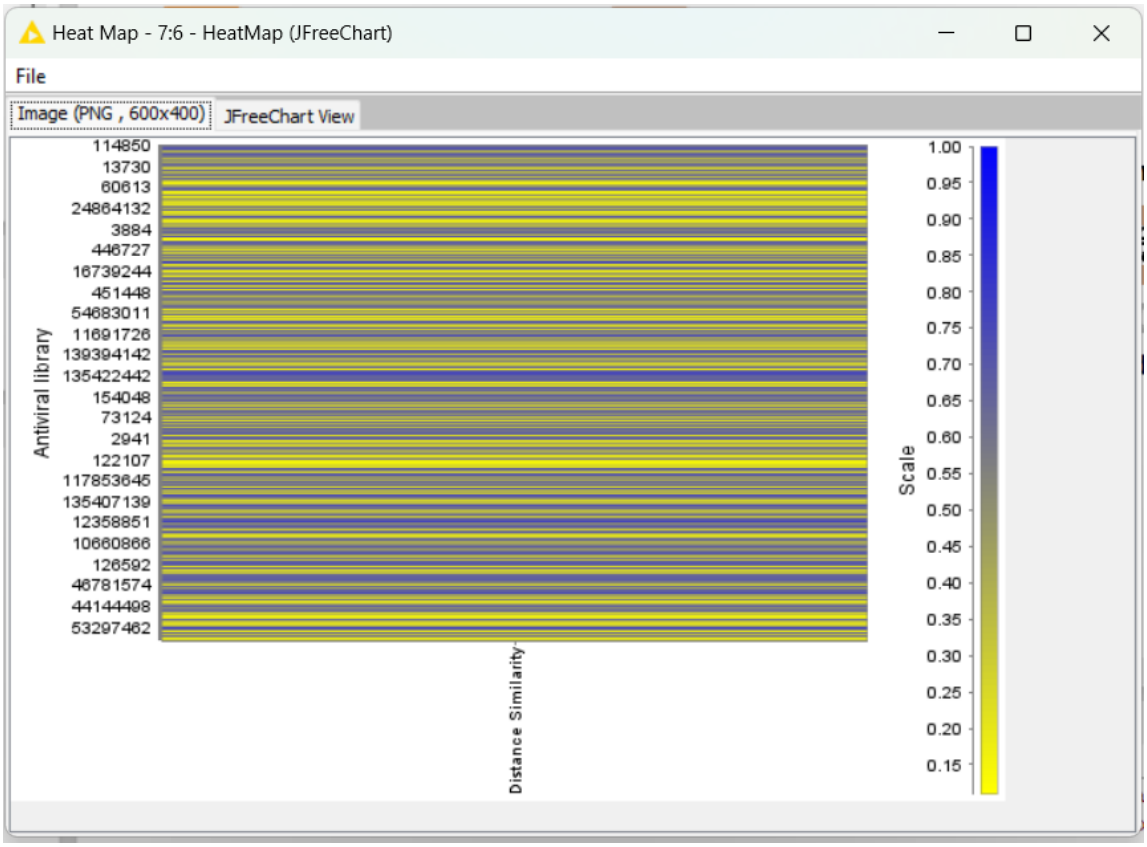




- 3D similarity (using CDK package)

S

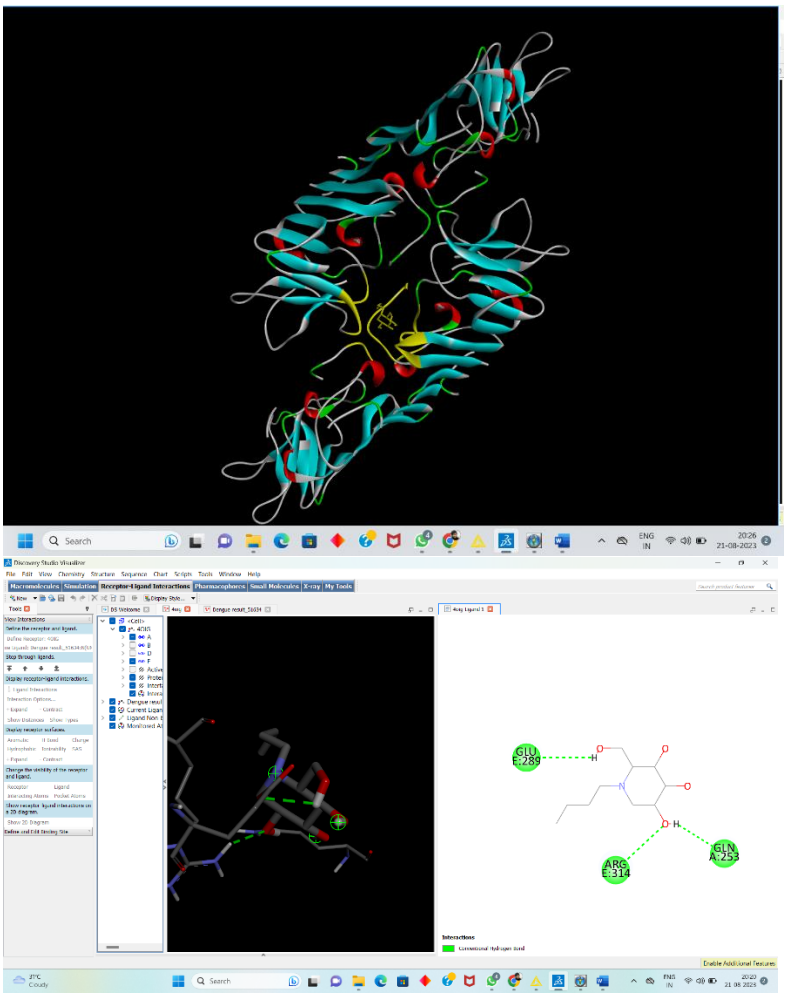


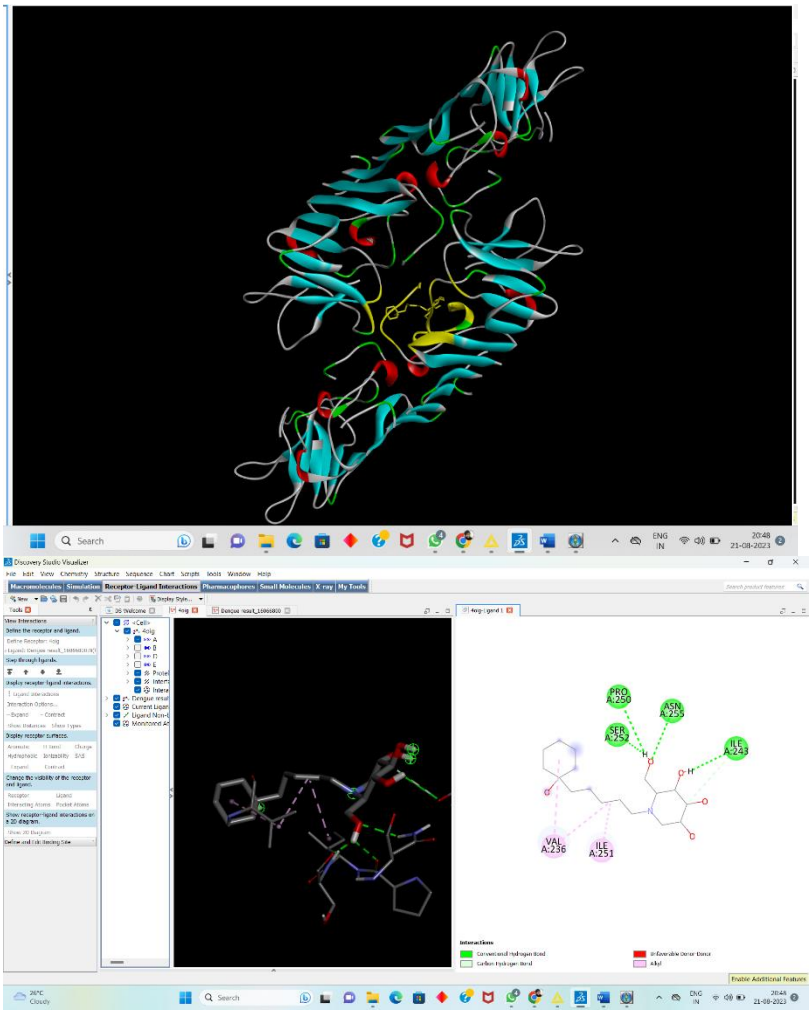
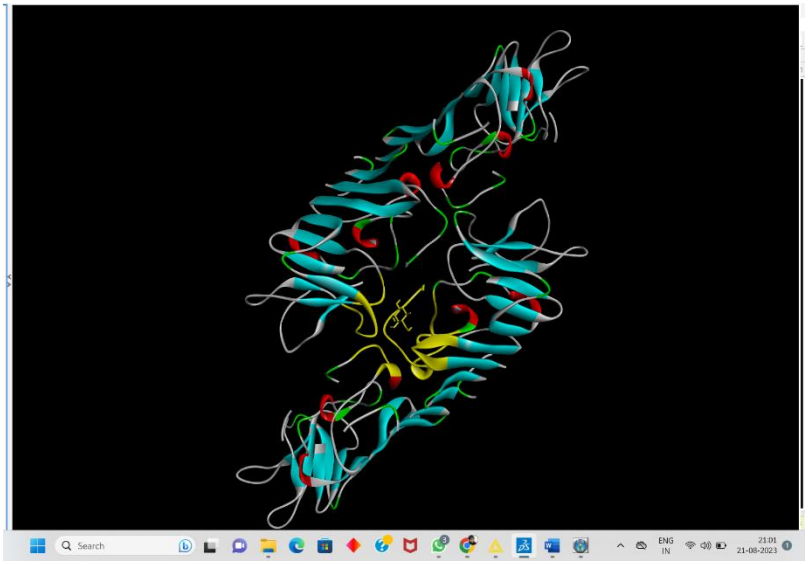

Heat Map - 7:6 - HeatMap (JFreeChart)
File
Image (PNG , 600x400)
JFreeChart View
Antiviral library
114850
13730
60613
24864132
3884
446727
16739244
451448
54683011
11691726
139394142
135422442
154048
73124
2941
122107
117853645
135407139
12358851
10660866
126592
46781574
44144498
53297462
Distance Similarity
Scale
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
0.55
0.50
0.45
0.40
0.35
0.30
0.25
0.20
0.15

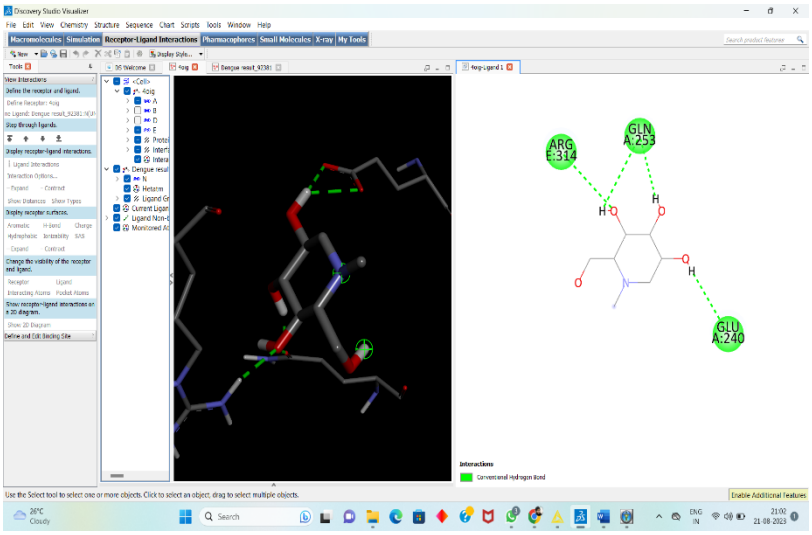
Molecular Docking

Protein Name: Dengue Virus Non-structural Protein NS1

Protein ID – 4OIG

Ligand Name	Ligand ID	Energy value (kcal/mol)	Dock Image
Miglustat	51634	-5.8	

OSL-95II	16066800	-6.5	
N-Methyldeoxynojirimycin	92381	-5.5	

			 Discovery Studio Visualizer File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools ARG F:314 GLN A:253 GLU A:240 Interactions Conventional Hydrogen Bond Use the Select tool to select one or more objects. Click to select an object, drag to select multiple objects. Enable Additional Features