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Molecular Docking - Final Report

Date: 10/03/2021

Requirement:

1. Molecular docking of SARS CoV-2 with Coronarin E
2. Molecular docking of Human albumin with 1,8 cineole/eucalyptol

Results:

S.no	Protein	Ligand	Binding affinity (kcal/mol)	Interacting amino acids	Interacting bond	Bond length (Å)
1.	SARS CoV-2	Coronarin E	-7.2	ARG B:765	Hydrophobic alkyl bond	5.00024
				ASN A:317	Hydrogen bond	2.72454
2.	Human albumin	1,8 cineole/eucalyptol	-6.0	LEU A: 115	van der Waals	5.22166

Description:

1. The protein structures for analysis were retrieved from Protein Data Bank (PDB):
   - SARS CoV-2 – PDB ID: 6VXX
   - Human albumin – PDB ID: 1AO6
2. AutoDock Vina version 1.5.6 was used for molecular docking
3. Discovery Studio Visualiser v21.1.0.20298 was used to visualise and analyse molecular docking

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