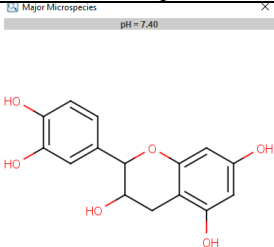
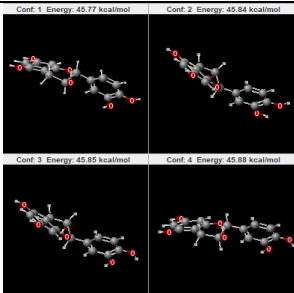
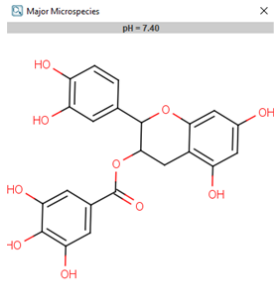
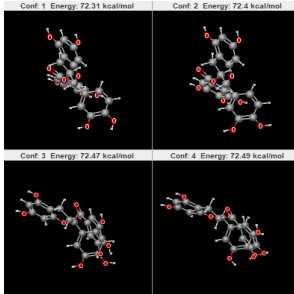
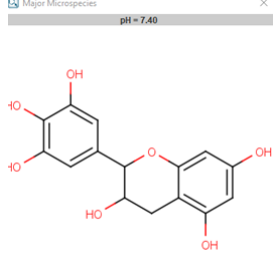
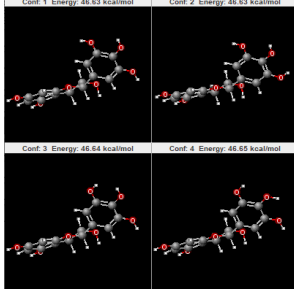
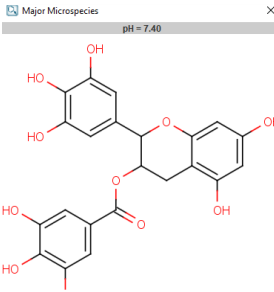
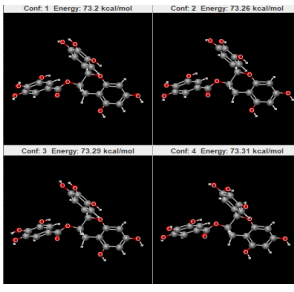
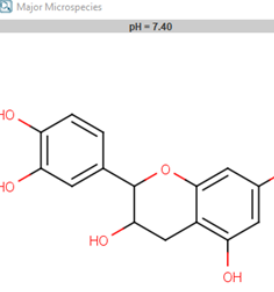
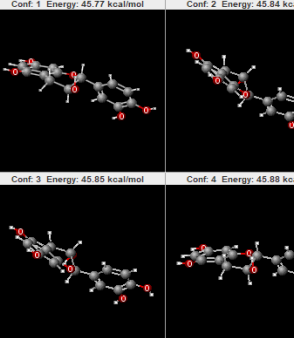
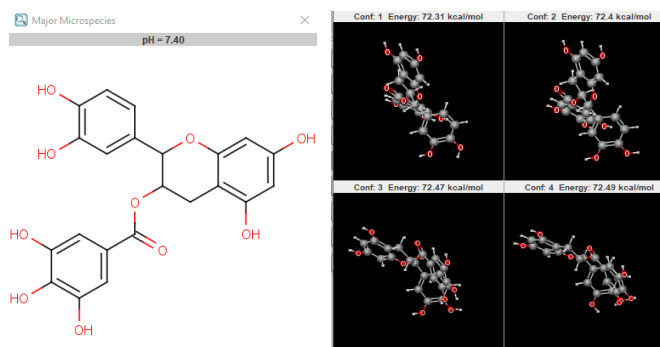


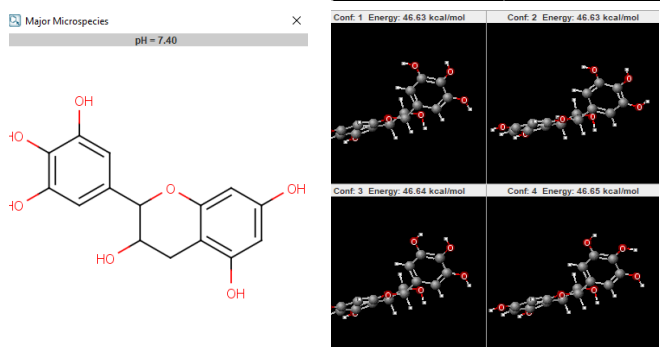
LAMPIRAN 1 PREPARASI LIGAN

No	Senyawa	Protonasi pH 7,4	konformasi
1.	Katekin	 <p>Major Microspecies pH = 7.40</p>	
2.	Katekin galat	 <p>Major Microspecies pH = 7.40</p>	
3.	Galokatekin	 <p>Major Microspecies pH = 7.40</p>	
4.	Galokatekin galat	 <p>Major Microspecies pH = 7.40</p>	
5.	Epikatekin	 <p>Major Microspecies pH = 7.40</p>	

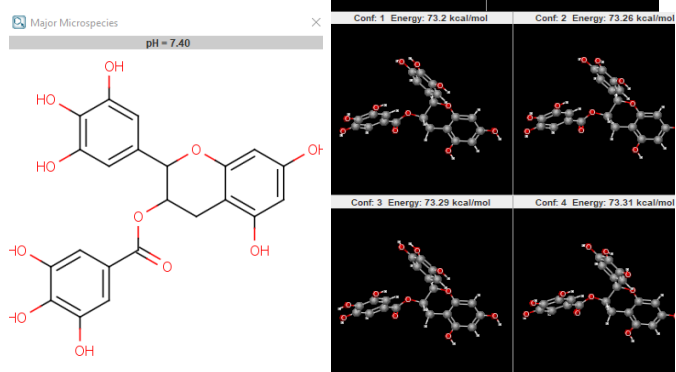
6. Epikatekin galat



7. Epigallocatekin

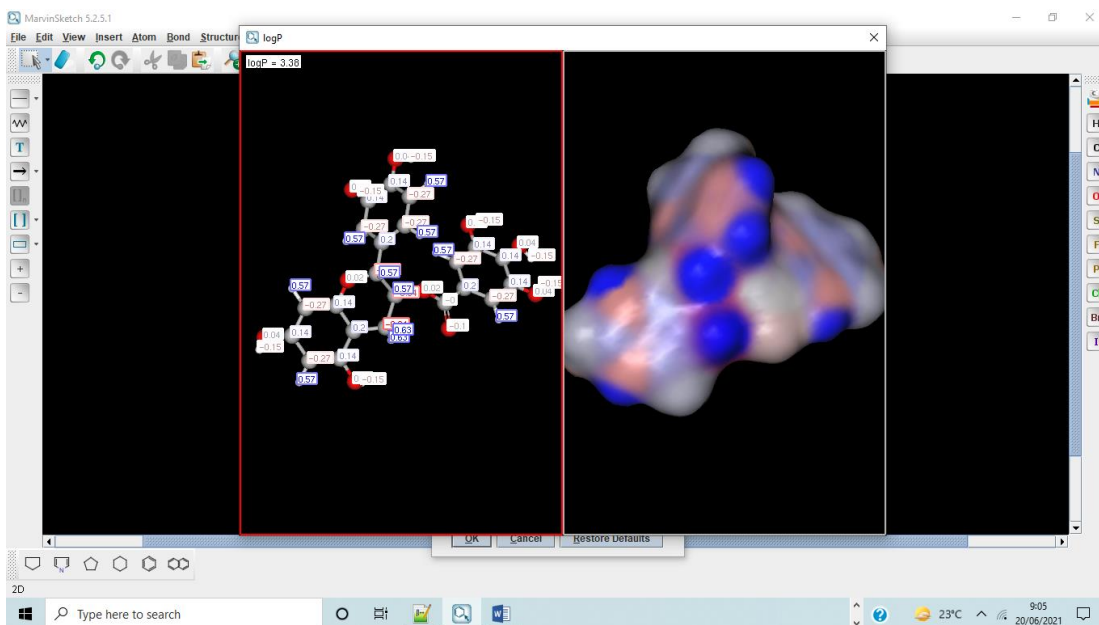
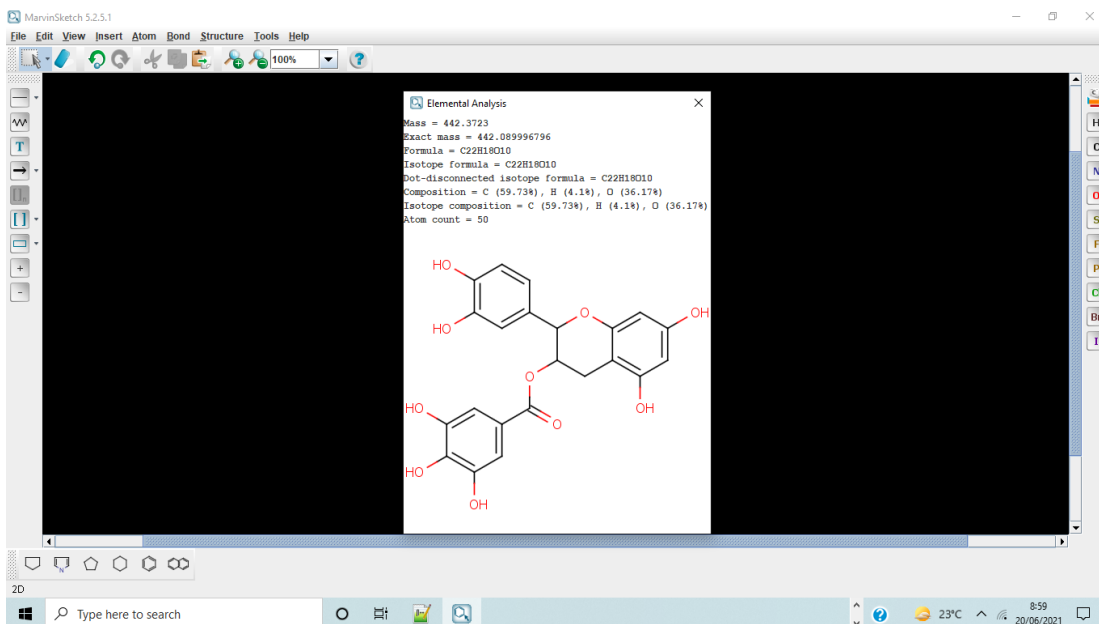


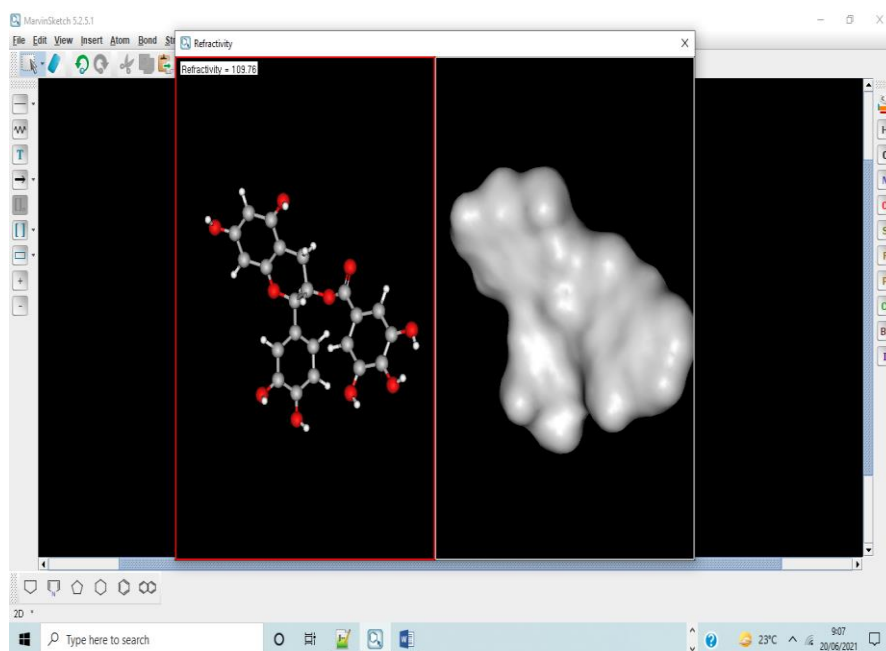
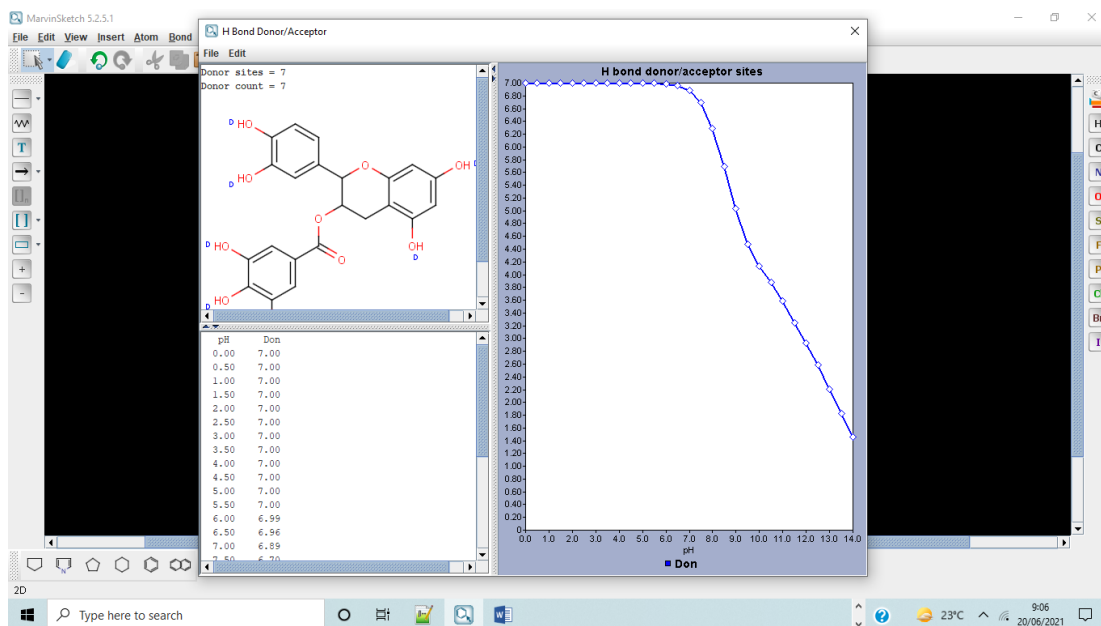
8. Epigallocatekin galat



LAMPIRAN 2

DRUGS SCAN





LAMPIRAN 3

STUDI ADME DAN TOKSISITAS

Pre ADMET Home About Druglikeness **ADME** Toxicity CoM

Search:

	ID	Value
	BBB	0.394913
	Buffer_solubility_mg_L	2253.95
	Caco2	0.656962
	CYP_2C19_inhibition	Inhibitor
	CYP_2C9_inhibition	Inhibitor
	CYP_2D6_inhibition	Non
	CYP_2D6_substrate	Non
	CYP_3A4_inhibition	Inhibitor
	CYP_3A4_substrate	Weakly
	HIA	66.707957
	MDCK	44.3849
	Pgp_inhibition	Non
	Plasma_Protein_Binding	100.000000

LAMPIRAN 4

PREPARASI RESEPTOR

RSB PDB Deposit Search Visualize Analyze Download Learn More Documentation MyPDB

DB-101 PDB EMDataResource Worldwide Protein Data Bank Celebrating 50 YEARS OF Protein Data Bank

Structure Summary 3D View Annotations Experiment Sequence Genome Versions

Biological Assembly 1

6XR3

X-ray Structure of SARS-CoV-2 main protease bound to GRL-024-20 at 1.45 Å

DOI: 10.2210/pdb6XR3/pdb

Classification: **HYDROLASE**

Organism(s): Severe acute respiratory syndrome coronavirus 2

Expression System: Escherichia coli BL21(DE3)

Mutation(s): No

Deposited: 2020-07-10 Released: 2020-08-19

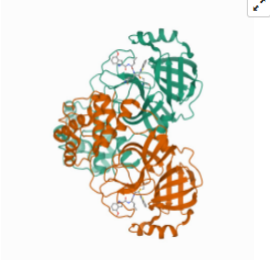
Deposition Author(s): Anson, B., Ghosh, A.K., Mesecar, A., Center for Structural Genomics of Infectious Diseases (CSGID)

Funding Organization(s): National Institutes of Health/National Institute Of Allergy and Infectious Diseases (NIH/NIAD)

3D View: Structure | Electron Density | Ligand Interaction

Display Files Download Files


Contact Us



Pengunduhan reseptor 6XR3 melalui website <https://www.rcsb.org/>

RCSB PDB Deposit Search Visualize Analyze Download Learn More Documentation

Ligands (1 Unique)

ID	Chains	Name / Formula / InChI Key	2D Diagram	3D Interactions
V7G (Subject of Investigation/LOI) Query on V7G	B [auth A]	N-[(2S)-1-[[[(1S,2S)-1-(1,3-benzothiazol-2-yl)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl]amino]-4-methyl-1-oxopentan-2-yl]-4-methoxy-1H-indole-2-carboxamide C ₃₀ H ₃₅ N ₅ O ₅ S DHQWCSZTRDSRP-XIBGDNMGSA-N		Ligand Interaction

Download Ideal Coordinates CCD File

Download Instance Coordinates

Experimental Data & Validation

Experimental Data

Method: X-RAY DIFFRACTION

Resolution: 1.45 Å

R-Value Free: 0.187

R-Value Work: 0.143

R-Value Observed: 0.145






Space Group: [C 1 2 1](#)

Unit Cell:

Length (Å)	Angle (°)
a = 96.182	α = 90
b = 100.000	β = 90
c = 100.000	γ = 90

Structure Validation

View Full Validation Report

Metric	Percentile Ranks	Value
Rfree		0.188
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.1%
RSRZ outliers		8.2%

Worse Better

■ Percentile relative to all X-ray structures

□ Percentile relative to X-ray structures of similar resolution

LAMPIRAN 5

VALIDASI DOCKING

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	8	-15.79	0.00	0.76	RANKING
1	2	73	-15.77	0.31	0.80	RANKING
1	3	5	-15.76	0.30	0.78	RANKING
1	4	17	-15.75	0.28	0.75	RANKING
1	5	78	-15.75	0.29	0.78	RANKING
1	6	14	-15.75	0.29	0.74	RANKING
1	7	99	-15.74	0.28	0.76	RANKING
1	8	7	-15.74	0.29	0.74	RANKING
1	9	54	-15.74	0.32	0.77	RANKING
1	10	26	-15.73	0.36	0.80	RANKING
1	11	44	-15.73	0.33	0.80	RANKING
1	12	53	-15.72	0.30	0.77	RANKING
1	13	61	-15.72	0.36	0.80	RANKING
1	14	74	-15.72	0.31	0.75	RANKING
1	15	66	-15.71	0.30	0.74	RANKING
1	16	33	-15.71	0.34	0.79	RANKING
1	17	85	-15.70	0.27	0.72	RANKING
1	18	24	-15.70	0.32	0.81	RANKING
1	19	18	-15.69	0.31	0.75	RANKING

Perolehan nilai *binding affinity* dan RMSD (*Root mean Square Deviation*) Ligan alami

LAMPIRAN 6

DOCKING LIGAN UJI

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	17	-12.44	0.00	33.46	RANKING
1	2	83	-12.43	0.01	33.45	RANKING
1	3	9	-12.43	0.01	33.46	RANKING
1	4	21	-12.43	0.02	33.46	RANKING
1	5	71	-12.43	0.02	33.46	RANKING
1	6	19	-12.43	0.04	33.46	RANKING
1	7	24	-12.42	0.01	33.45	RANKING
1	8	44	-12.42	0.02	33.46	RANKING
1	9	32	-12.42	0.03	33.45	RANKING
1	10	89	-12.42	0.04	33.46	RANKING
1	11	5	-12.42	0.01	33.46	RANKING
1	12	65	-12.42	0.04	33.47	RANKING
1	13	67	-12.42	0.02	33.45	RANKING
1	14	80	-12.41	0.02	33.46	RANKING
1	15	25	-12.41	0.02	33.45	RANKING
1	16	58	-12.41	0.02	33.45	RANKING
1	17	72	-12.41	0.06	33.47	RANKING
1	18	54	-12.41	0.03	33.45	RANKING
1	19	70	-12.41	0.02	33.45	RANKING
1	20	11	-12.41	0.04	33.47	RANKING

Perolehan nilai *binding affinity* hasil *docking* senyawa katekin galat dan epikatekin galat

LAMPIRAN 7

MOLECULAR DYNAMIC

The screenshot displays a Windows desktop environment. The primary window is a molecular dynamics simulation interface, likely GROMACS, showing a 3D visualization of a protein-ligand complex. The simulation parameters are visible at the top: [MD:NPA] t: 0.261, H: 2.650430, T: 58, P: 30510, V: 79461, U: -11517.369. The simulation box is labeled MMFF94x PBC. To the right, a Database Viewer window is open, displaying a table with the following data:

	mol	stage	t	H	U
1	gab_best	heat	0.0000	0.0000	-11975.

The status bar at the bottom of the Database Viewer indicates: 1 entry, 0 selected, all visible. 17 fields, 0 selected, all visible. The Windows taskbar at the bottom shows the search bar, taskbar icons, and system tray with a temperature of 29°C Hujan and the date 04/07/2021.