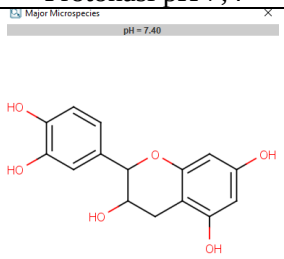
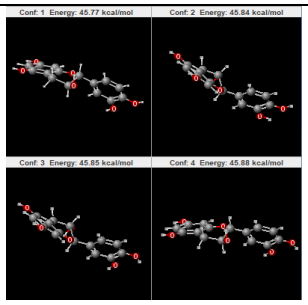
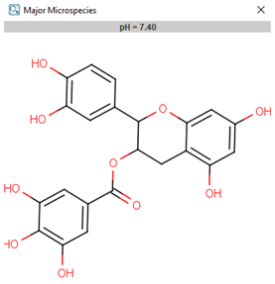
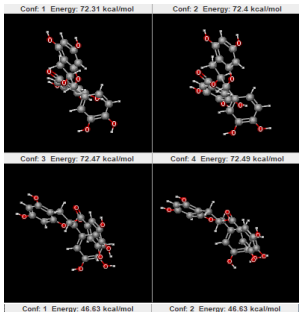
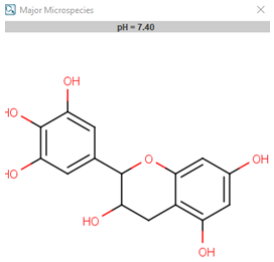
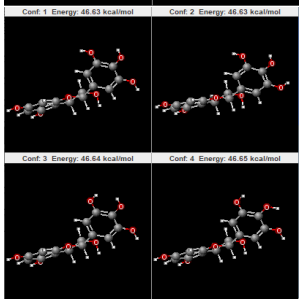
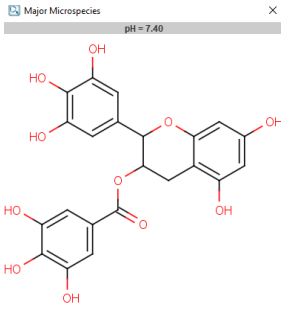
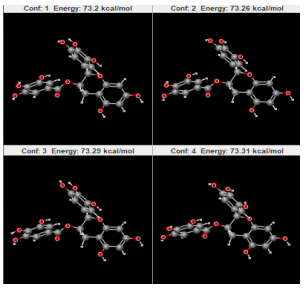
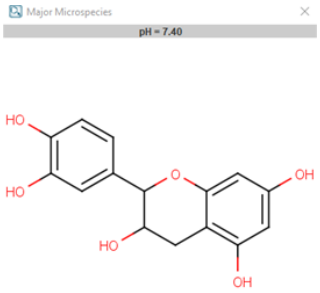
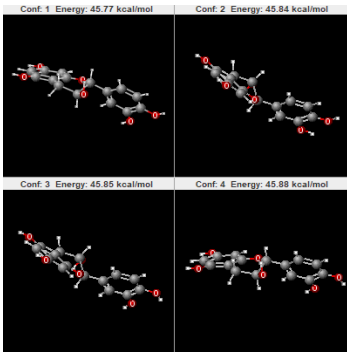
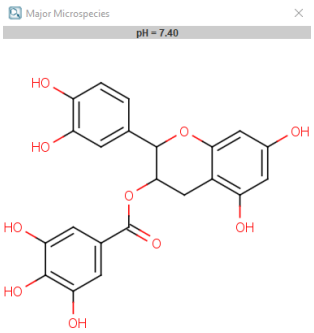
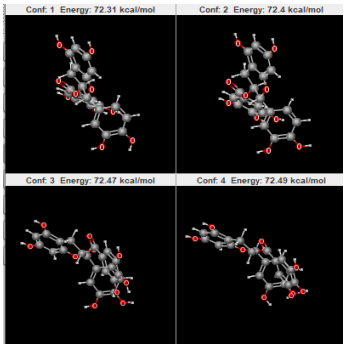
LAMPIRAN 1

PREPARASI LIGAN

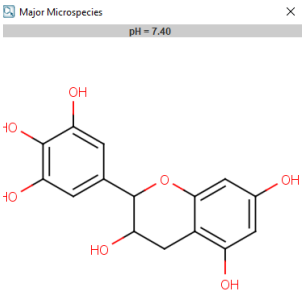
No	Senyawa	Protonasi pH 7,4	konformasi
1.	Katekin		
2.	Katekin galat		
3.	Galokatekin		
4.	Galokatekin galat		
5.	Epikatekin		

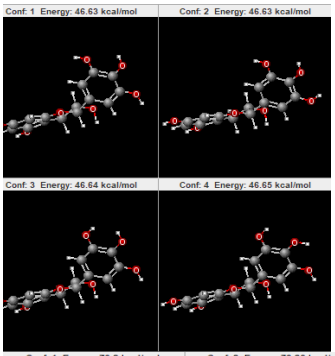
6. Epikatekin galat



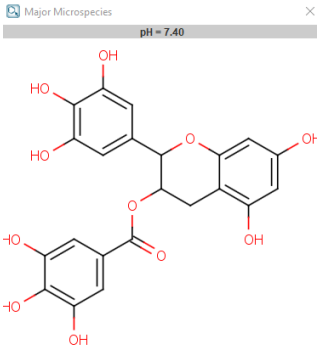


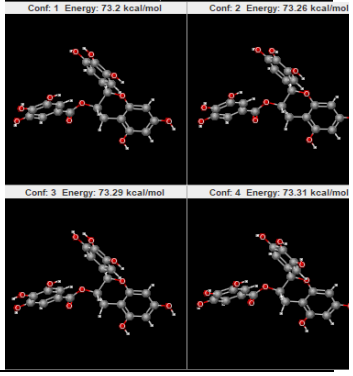
7. Epigalokatekin





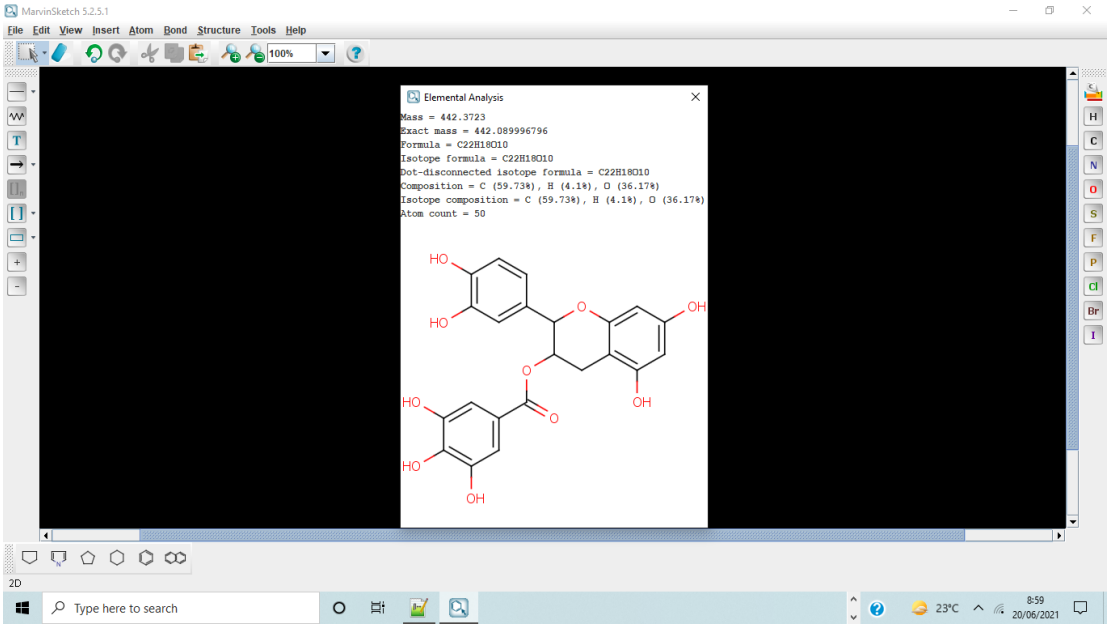
8. Epigalokatekin galat

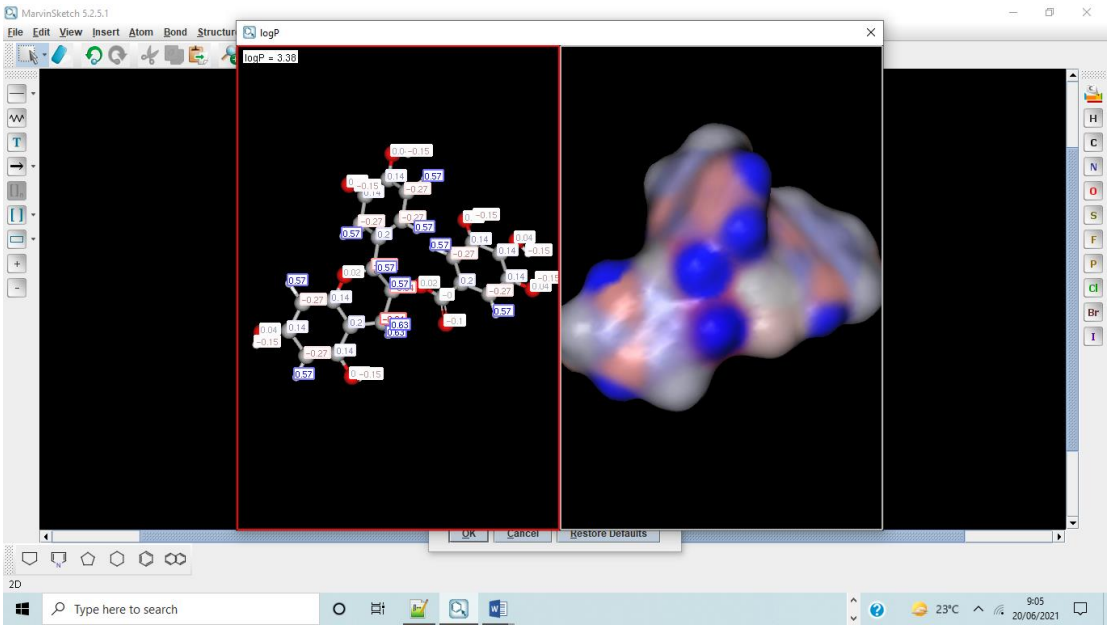


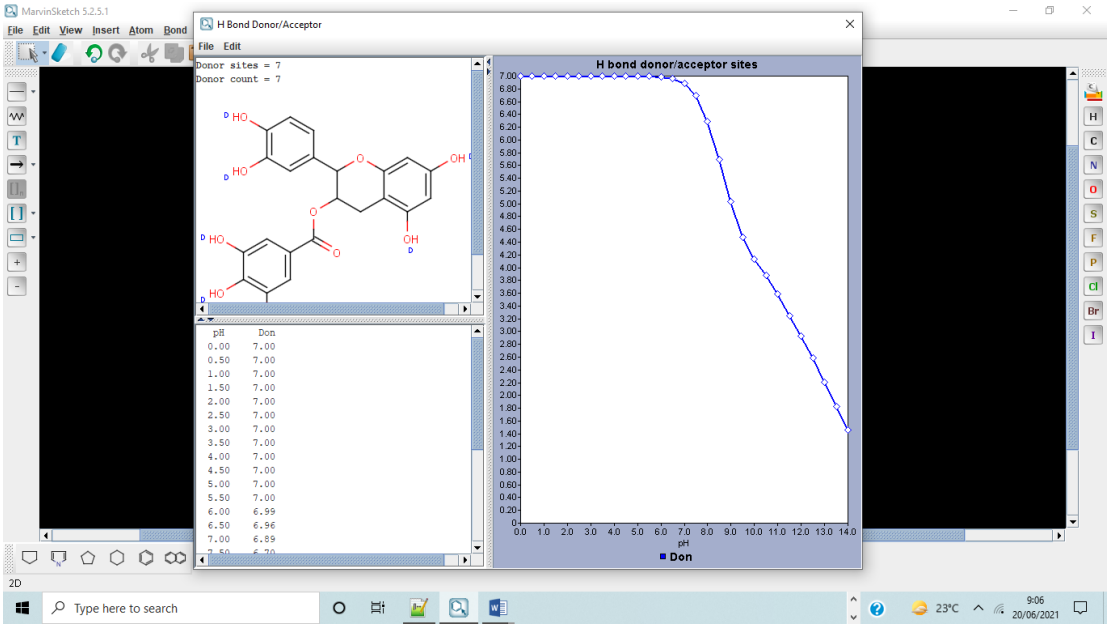


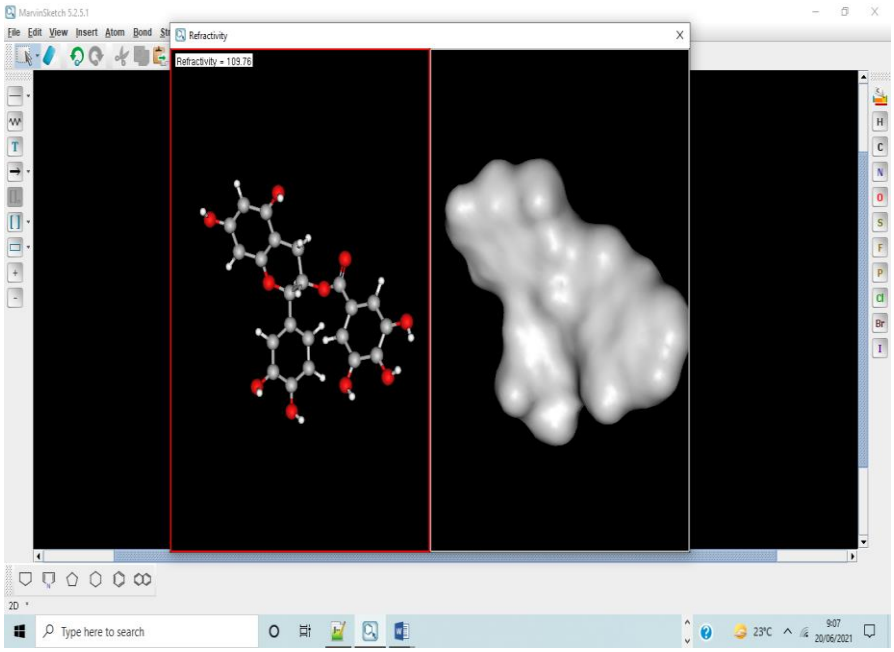
LAMPIRAN 2

DRUGS SCAN



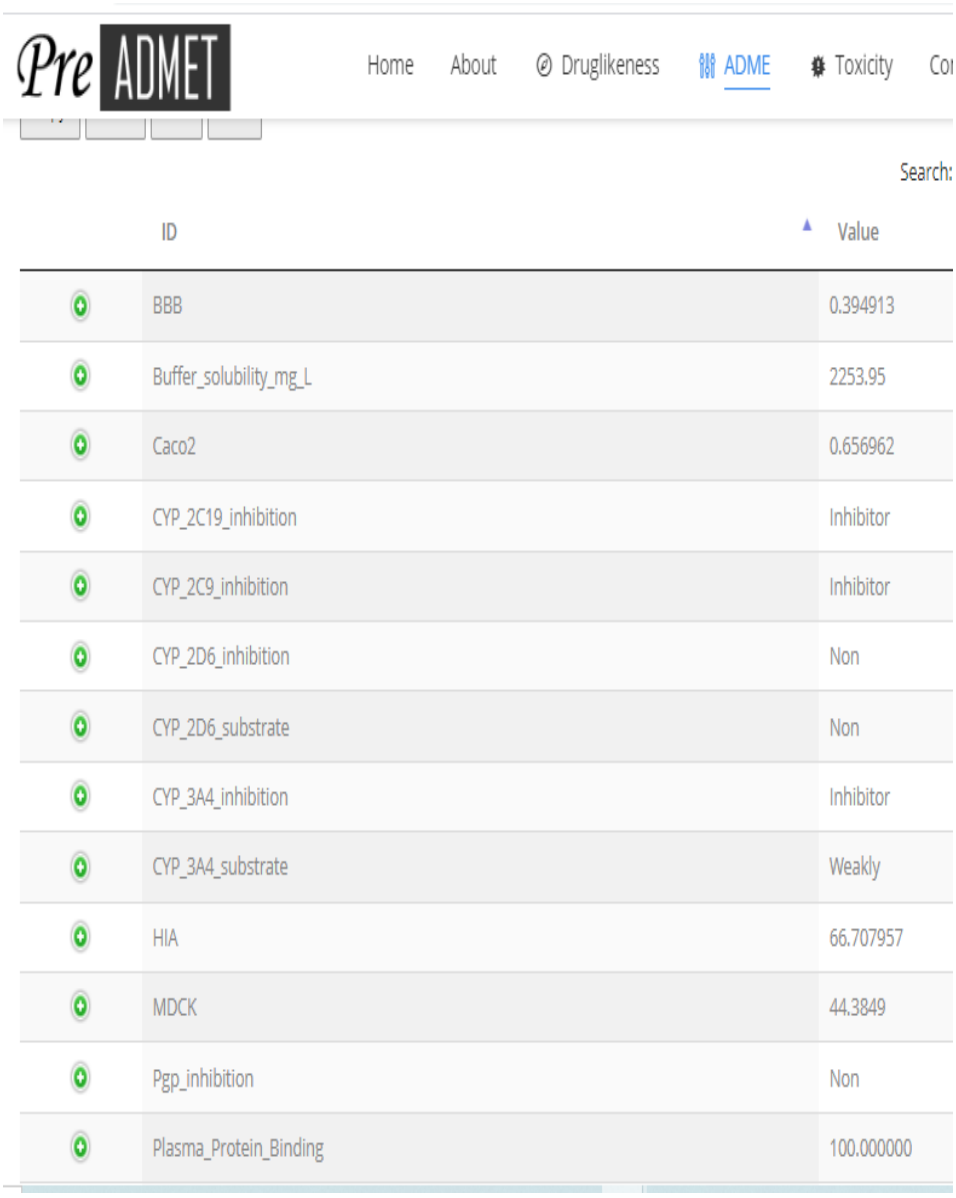



MarvinSketch 5.2.5.1
File Edit View Insert Atom Bond
H Bond Donor/Acceptor
File Edit
Donor sites = 7
Donor count = 7
H bond donor/acceptor sites
pH Don
0.00 7.00
0.50 7.00
1.00 7.00
1.50 7.00
2.00 7.00
2.50 7.00
3.00 7.00
3.50 7.00
4.00 7.00
4.50 7.00
5.00 7.00
5.50 7.00
6.00 6.99
6.50 6.96
7.00 6.89
pH
Don
2D
Type here to search
23°C
9:06
20/06/2021


MarvinSketch 5.2.5.1
File Edit View Insert Atom Bond
Refractivity
Refractivity = 109.76
2D
Type here to search
23°C
9:07
20/06/2021

LAMPIRAN 3

STUDI ADME DAN TOKSISITAS

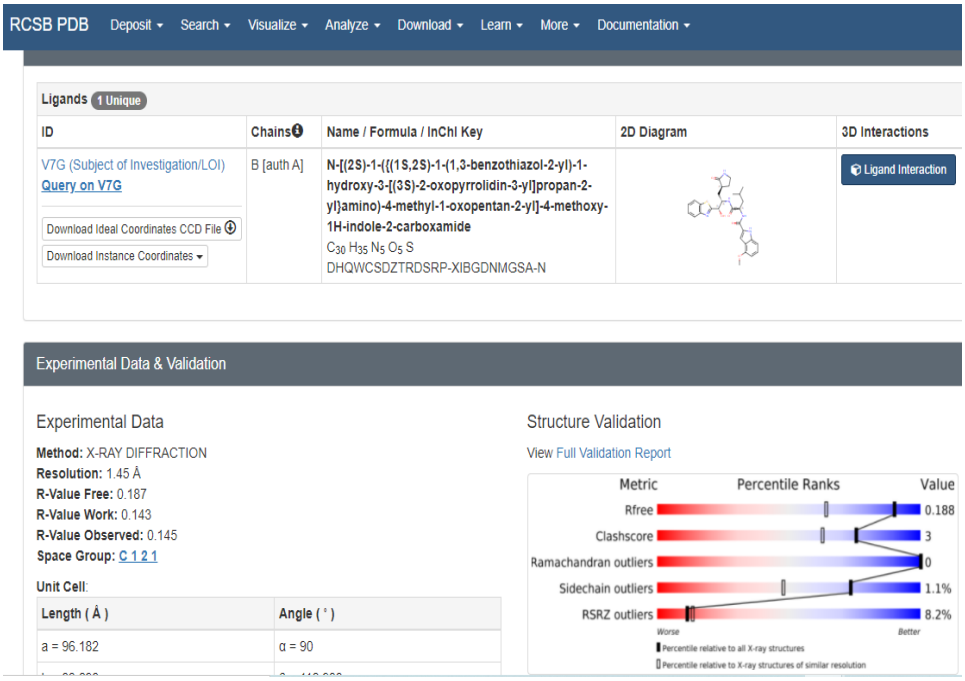


ID	Value
BBB	0.394913
Buffer_solubility_mg_L	2253.95
Caco2	0.656962
CYP_2C19_inhibition	Inhibitor
CYP_2C9_inhibition	Inhibitor
CYP_2D6_inhibition	Non
CYP_2D6_substrate	Non
CYP_3A4_inhibition	Inhibitor
CYP_3A4_substrate	Weakly
HIA	66.707957
MDCK	44.3849
Pgp_inhibition	Non
Plasma_Protein_Binding	100.000000

LAMPIRAN 4

PREPARASI RESEPTOR

Pengunduhan reseptor 6XR3 melalui website https://www.rscb.org/



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 affnity* hasil *docking* senyawa katekin galat dan epikatekin galat

LAMPIRAN 7

MOLECULAR DYNAMIC