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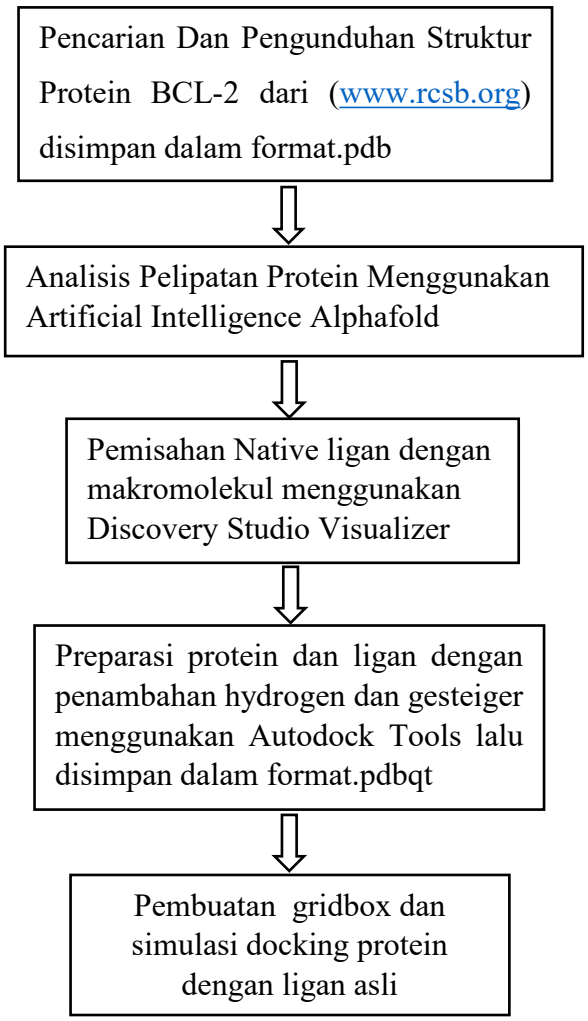
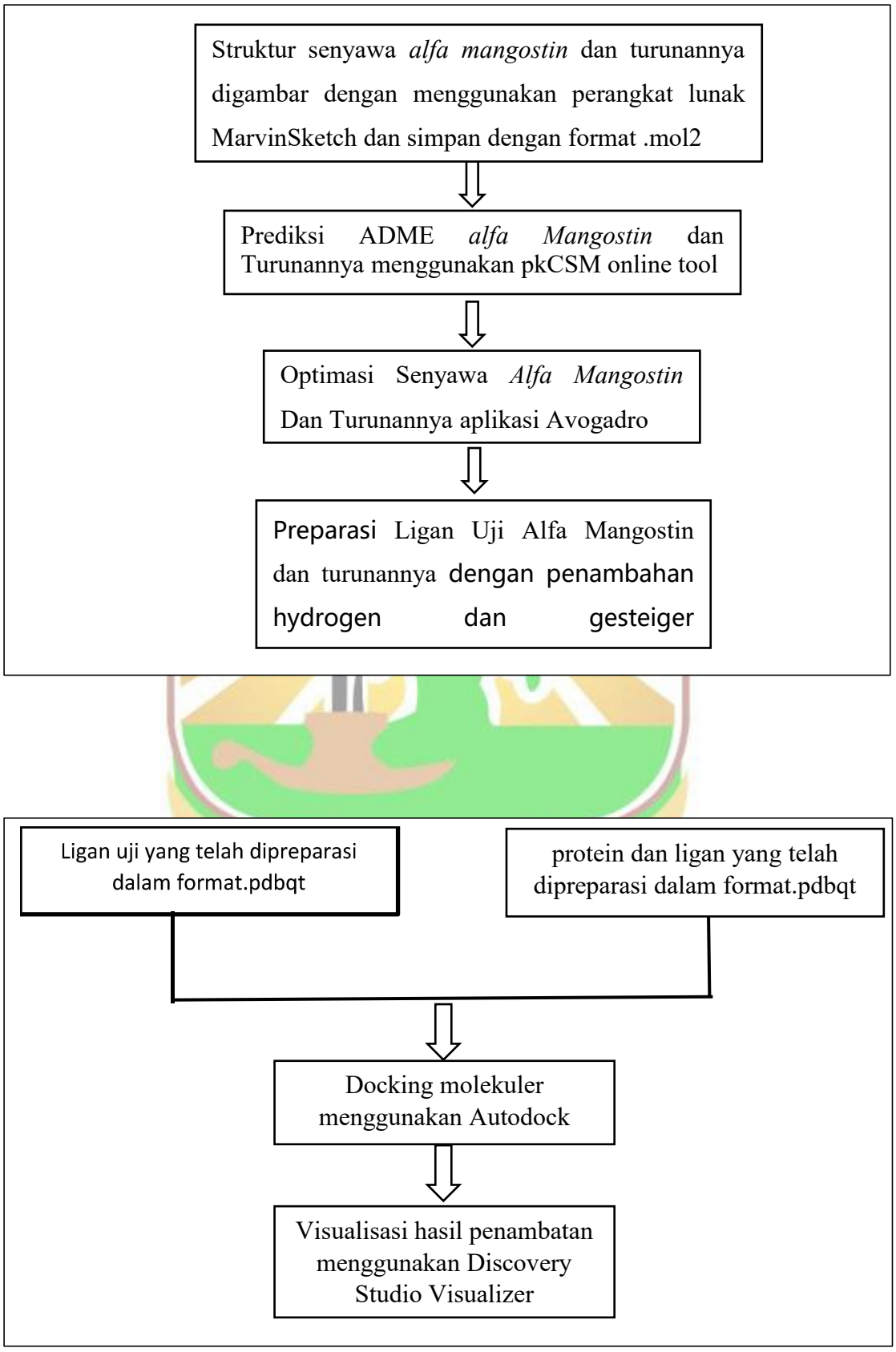
LAMPIRAN

Lampiran 1. Skema Alur Penelitian




Struktur senyawa *alfa mangostin* dan turunannya digambar dengan menggunakan perangkat lunak MarvinSketch dan simpan dengan format .mol2
Prediksi ADME *alfa Mangostin* dan Turunannya menggunakan pkCSM online tool
Optimasi Senyawa *Alfa Mangostin* Dan Turunannya aplikasi Avogadro
Preparasi Ligan Uji Alfa Mangostin dan turunannya dengan penambahan hydrogen dan gesteiger
Ligan uji yang telah dipreparasi dalam format.pdbqt
protein dan ligan yang telah dipreparasi dalam format.pdbqt
Docking molekuler menggunakan Autodock
Visualisasi hasil penambatan menggunakan Discovery Studio Visualizer

Lampiran 2. Hasil Prediksi ADMET Senyawa Alfa Mangostin Dan Derivate-Derivatnya Menggunakan Aplikasi Pkcsm Online Tool

Absorbsi

Senyawa	Water Solubility	Caco2 Permeability (nm/detik)	Human Intestinal absorbtion (%)	P glycoprotein
Alfa Mangostin	-3,805	32,0495	94,512077	Iya
Derivate 1	-3,345	19,5148	92,154716	Iya
Derivate 2	-3,299	18,0842	75,578992	Iya
Derivate 3	-3,664	15,6292	75,578994	Iya
Derivate 4	-3,482	19,2653	90,526822	Iya
Derivate 5	-3,531	16,6669	65,352246	Iya
Derivate 6	-3,457	19,289	89,902085	Iya

Distribusi

Senyawa	Vd (log L/kg)	BBB Permeability	Plasma Protein Binding
Alfa Mangostin	0,224	5,34046	97,422116
Derivate 1	0,175	4,06151	96,119689
Derivate 2	-0,01	0,27538	92,760335
Derivate 3	-0,044	0,346757	91,738860
Derivate 4	-0,046	0,485304	91,288943
Derivate 5	0,319	0,0549358	73,215917
Derivate 6	-0,255	0,663653	95,680779

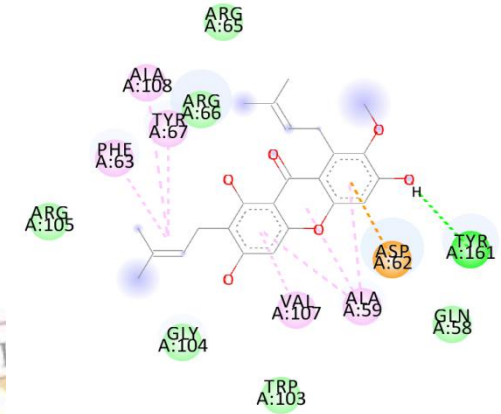
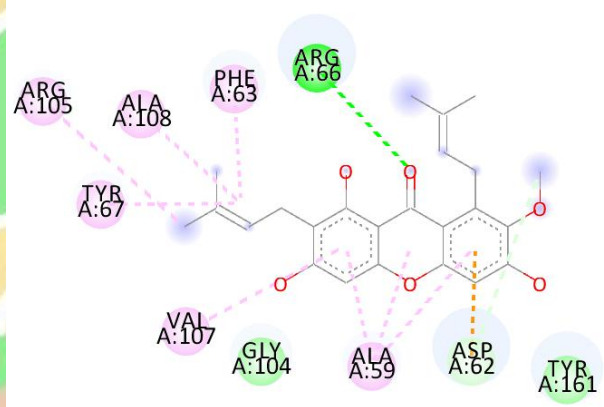
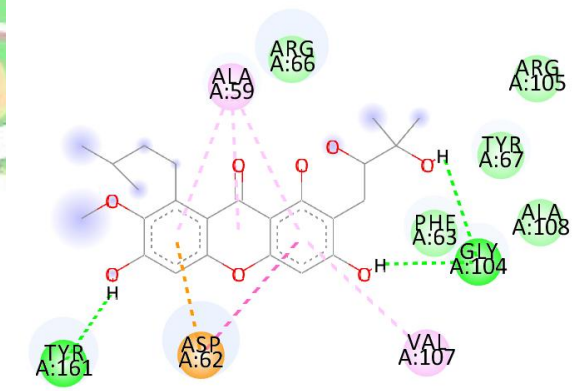
Metabolisme

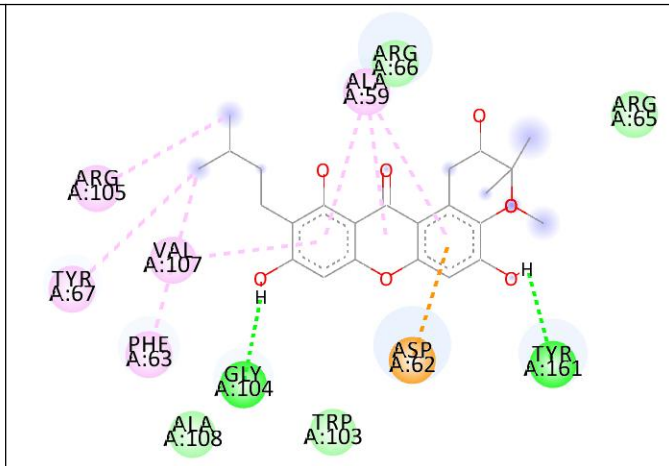
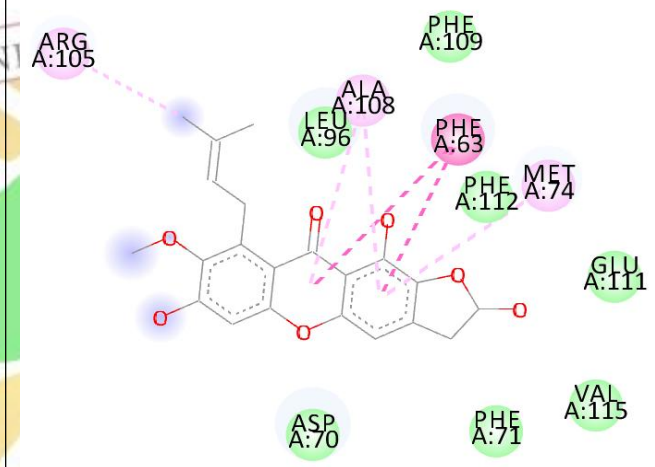
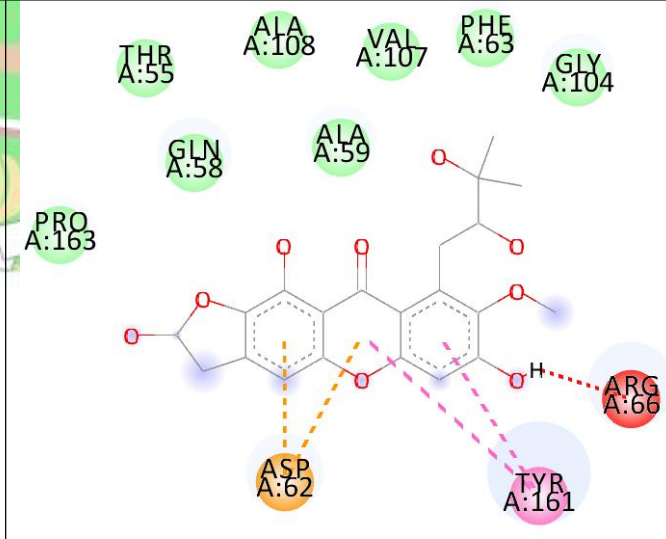
Senyawa	CYP3A4 Inhibition	CYPD6 Inhibition	CYP2C9 Inhibition	CYP2C19 Inhibition
Alfa Mangostin	Iya	Tidak	Iya	Iya
Derivate 1	Iya	Tidak	Iya	Iya
Derivate 2	Iya	Tidak	Iya	Iya
Derivate 3	Iya	Tidak	Iya	Iya
Derivate 4	Iya	Tidak	Iya	Iya
Derivate 5	Iya	Tidak	Iya	Iya
Derivate 6	Iya	Tidak	Iya	Iya

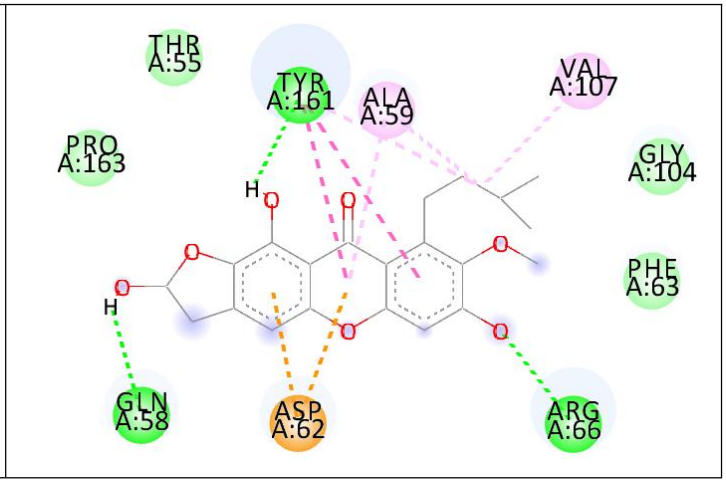
Ekskresi

Senyawa	Total Clearance (Log Ml/Min/Kg)	Renal OCT2 Substrate
Alfa Mangostin	0,557	Tidak
Derivate 1	0,017	Tidak
Derivate 2	0,091	Tidak
Derivate 3	0,044	Tidak
Derivate 4	0,461	Tidak
Derivate 5	-0,264	Tidak
Derivate 6	0,445	Tidak

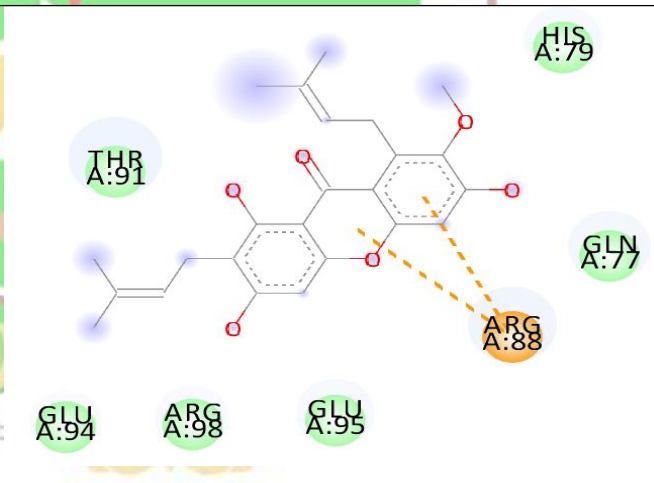
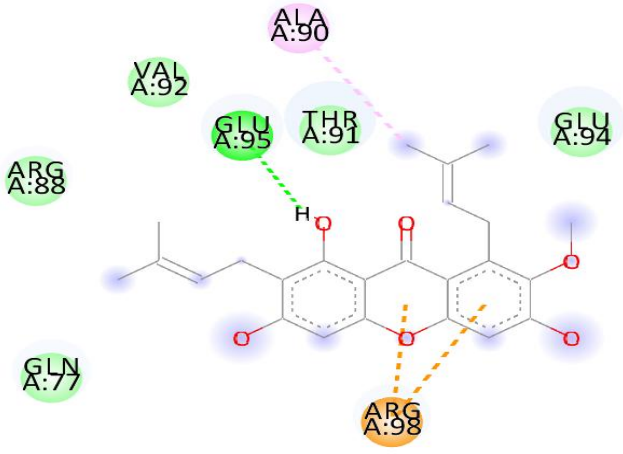
Lampiran 3. Visualisasi Hasil 2D Interaksi Senyawa Alfa Mangostin dan Derivate-Derivat Alfa Mangostin Terhadap Makromolekul 4IEH

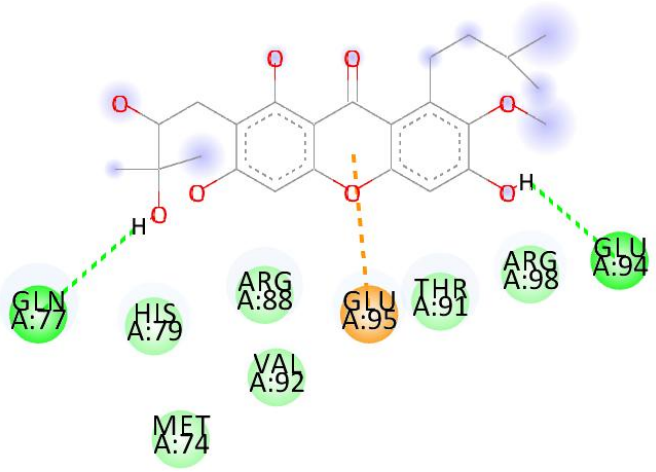
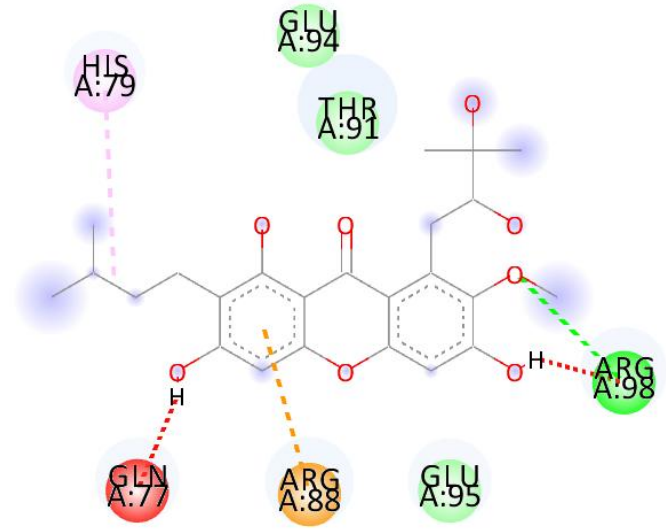
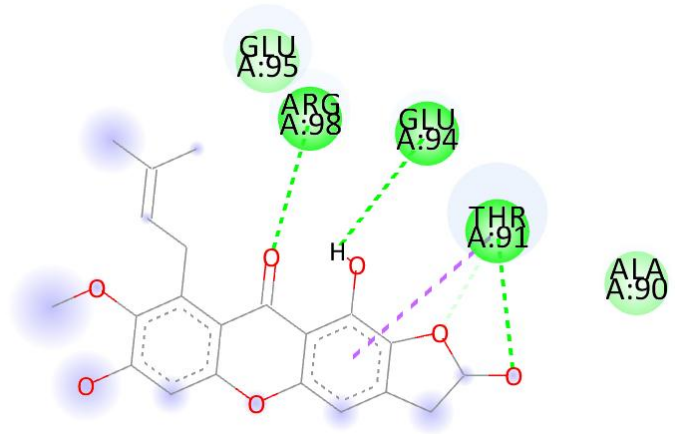
Nama senyawa	Visualisasi 2D
Alfa mangostin	
Derivate 1 alfa mangostin	
Derivate 2 alfa mangostin	

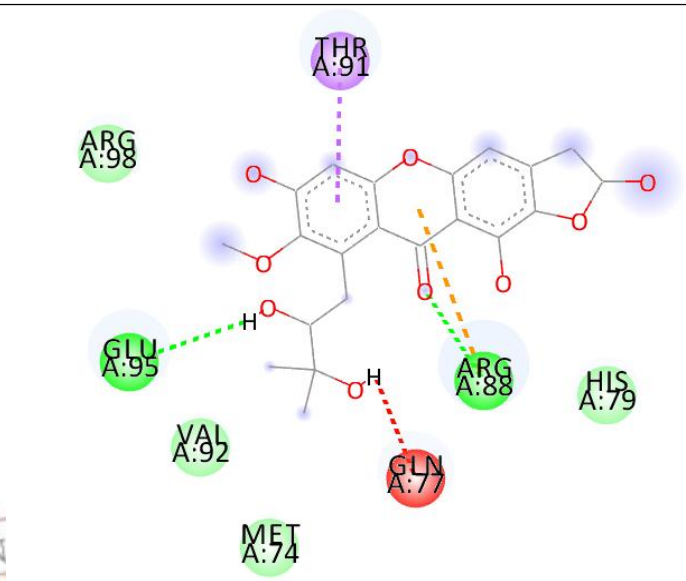
Derivate 3 alfa mangostin	
Derivate 4 alfa mangostin	
Derivate 5 alfa mangostin	

Derivate 6 alfa mangsotin	

Lampiran 4. Visualisasi Hasil 2D Interaksi Senyawa Alfa Mangostin dan Derivate-Derivat Alfa Mangostin Terhadap Makromolekul 4AQ3

Nama senyawa	Visualisasi 2D
Alfa mangostin	
Derivate 1 alfa mangostin	

Derivate 2 alfa mangostin	
Derivate 3 alfa mangostin	
Derivate 4 alfa mangostin	

Derivate 5 alfa mangostin	
Derivate 6 alfa mangsotin