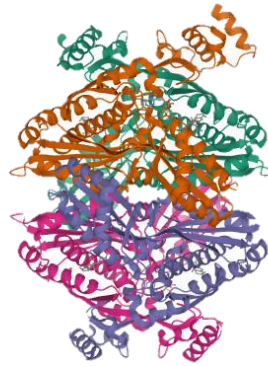


LAMPIRAN

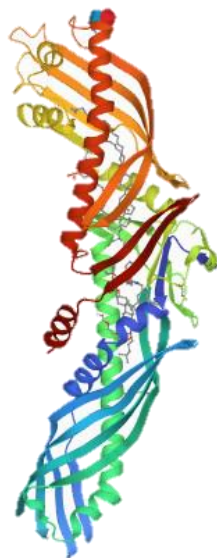
Lampiran 1. Struktur 3D Makromolekul

A. Struktur 3D Makromolekul HMGCR dengan Kode PDB 1HW9



(Sumber : www.rcsb.org)

B. Struktur 3D Makromolekul CETP dengan Kode PDB 4EWS



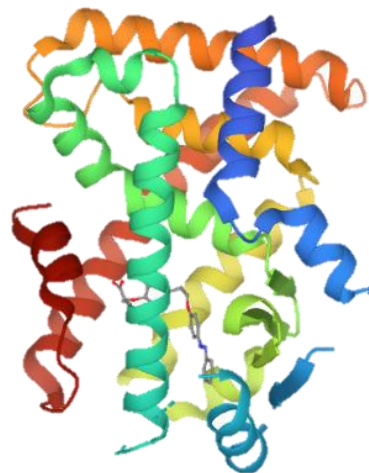
(Sumber : www.rcsb.org)

C. Struktur 3D Makromolekul *Pancreatic lipase* dengan Kode PDB 1LPB



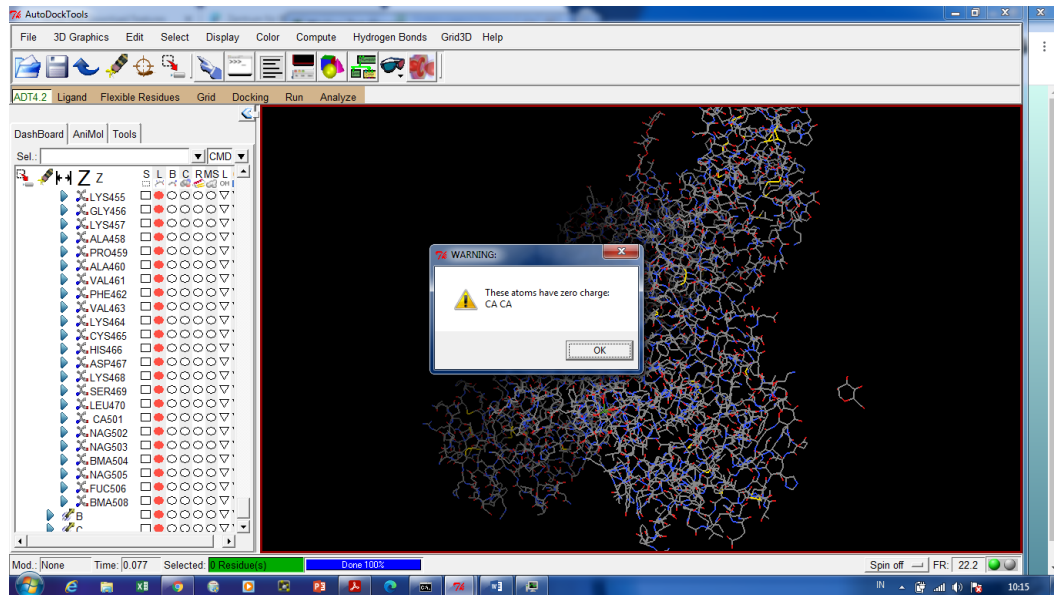
(Sumber : www.rcsb.org)

D. Struktur 3D Makromolekul PPAR α dengan kode PDB 4CI4

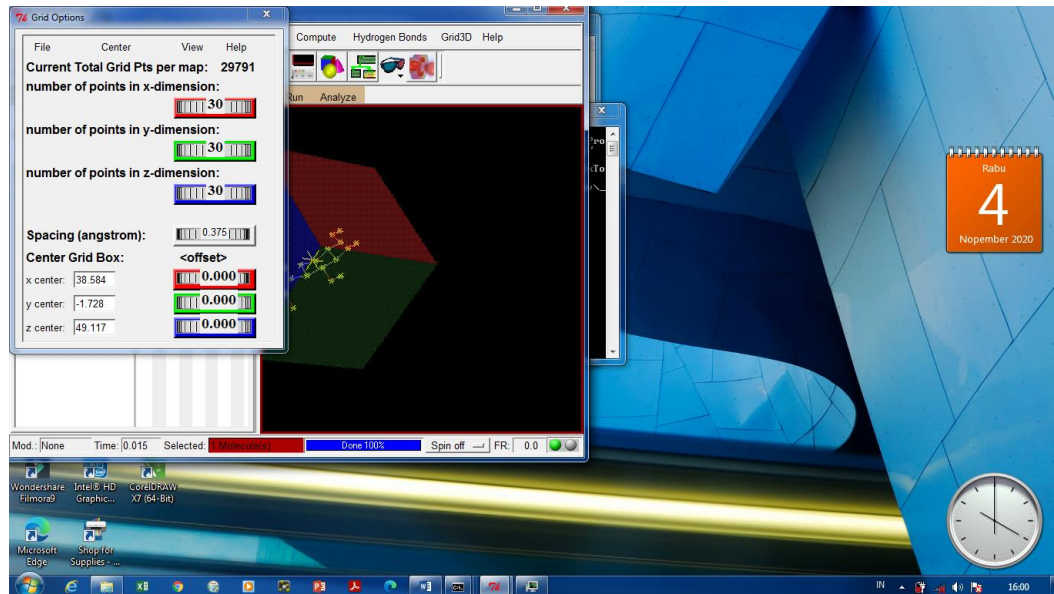


(Sumber : www.rcsb.org)

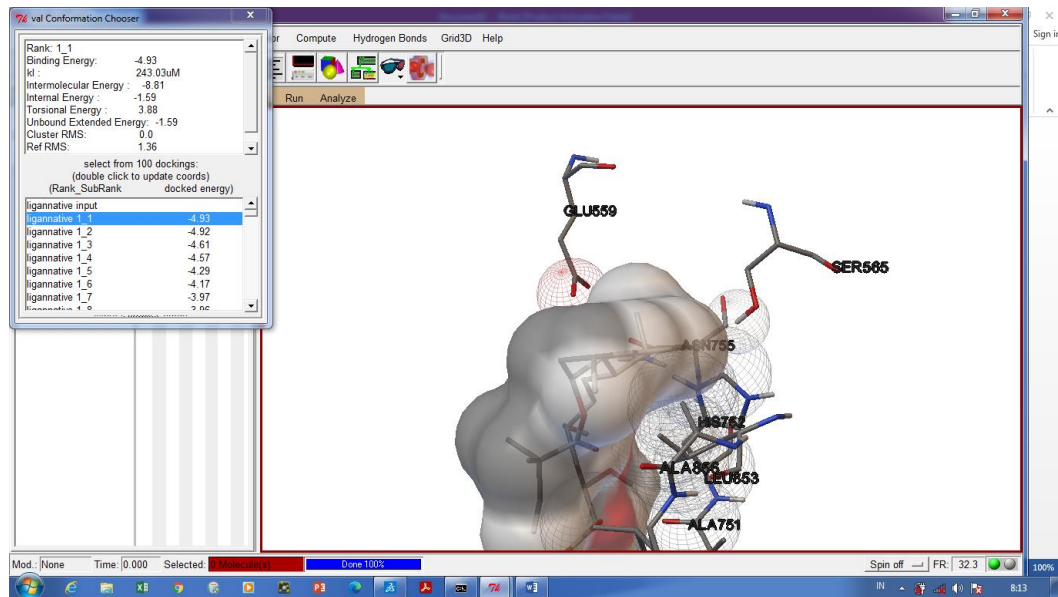
Lampiran 2. Preparasi protein target



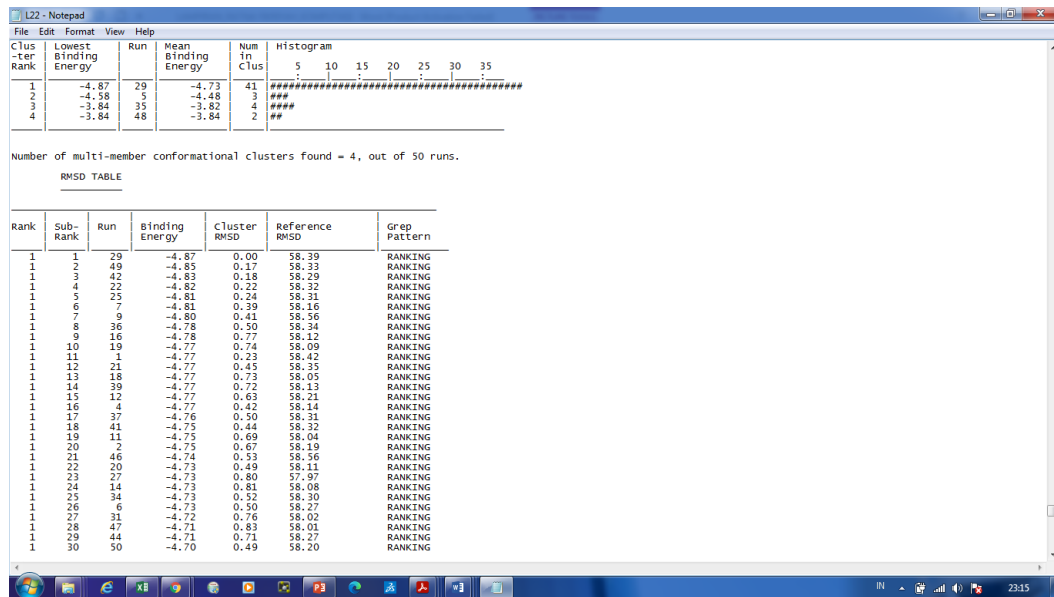
Lampiran 3. Penentuan grid box



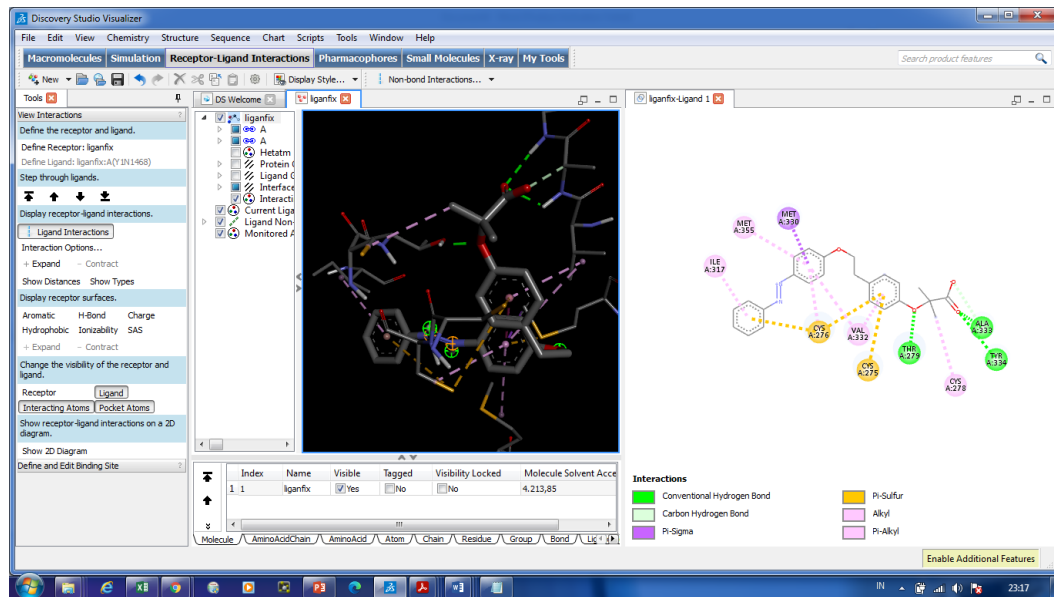
Lampiran 4. Analisa hasil *docking*



Lampiran 5. Penentuan *Lowest binding energy*



Lampiran 6. Visualisasi hasil *docking*



Lampiran 7. Nilai $\Delta G_{\text{binding}}$

No	Ligan Uji	$\Delta G_{\text{binding}}$ (kkal/mol)			
		HMGCR (1HW9)	CETP (4EWS)	<i>Pancreatic lipase</i> (1LPB)	PPAR α (4CI4)
	Ligan asli	-4,40 \pm 0,39	-10,30 \pm 0,15	-5,06 \pm 0,05	-10,19 \pm 0,51
<i>Basella alba</i> L.					
1.	<i>Acacetin</i>	-4,54\pm0,03	-6,86\pm0,13	-7,09 \pm0,04	-6,13 \pm0,03
2.	β sitosterol	-5,02\pm0,03	-10,36\pm0,06	-9,36\pm0,13	-8,75\pm0,04
3.	<i>Betalamic acid</i>	-3,59 \pm 0,17	-4,10 \pm 0,03	-4,17 \pm 0,09	-4,17 \pm 0,03
4.	<i>Ferulic acid</i>	-3,81\pm0,18	-4,56 \pm 0,09	-5,27 \pm 0,03	-5,24 \pm 0,07
6.	<i>Syringic acid</i>	-3,49 \pm 0,20	-4,14 \pm 0,07	-4,01 \pm 0,10	-4,91 \pm 0,09
7.	Vanilin	-3,03 \pm 0,13	-4,38 \pm 0,13	-3,21 \pm 0,09	-4,04 \pm 0,07
8.	Rutin	-0,98 \pm 0,03	-3,06 \pm 0,22	-1,86 \pm 0,07	-0,53 \pm 0,15
<i>Amaranthus viridis</i> L.					
1.	2-methoxy-4-vinylphenol	-3,41 \pm 0,08	-4,76 \pm 0,04	-4,83 \pm 0,07	-4,33 \pm 0,07
2.	9,12,15-octadecatrienoic acid	-3,41 \pm 0,07	-5,44 \pm 0,09	-5,24\pm0,01	-6,18\pm0,01
3.	<i>Linoleic acid</i>	-0,97 \pm 0,10	-5,05 \pm 0,06	-5,13 \pm 0,00	-5,36 \pm 0,06
4.	<i>Eicosyl ester</i>	0,61 \pm 0,03	-5,81 \pm 0,02	-2,67 \pm 0,07	-4,95 \pm 0,06
5.	Rutin	-1,06 \pm 0,08	-6,54\pm0,08	-2,54 \pm 0,33	-0,76 \pm 0,05

Lampiran 8. Prediksi ADME

1. Lipinski's Rules terhadap Ligan Uji

Ligan	Bobot Molekul	H-Bond acceptors	H-Bond donors	Log P	Druglikeness
<i>Basella alba</i> L.					
Acacetin	284,267	5	2	2,88	Diterima
β sitosterol	414,718	1	1	8,025	Diterima
Ferulic acid	194,186	3	2	1,499	Diterima
<i>Amaranthus viridis</i> L.					
Rutin	610,52	16	10	-1,51	Ditolak
2-methoxy-4-vinylphenol	150,177	2	1	2,044	Diterima
9,12,15-octadecatrienoic acid	278,436	1	1	5,661	Diterima

Lampiran 9. Nilai farmakokinetika

Parameter farmakokinetik		Ligan uji				
		<i>Basella alba</i> L		<i>Amaranthus viridis</i> L.		
		<i>Acacetin</i>	β sitosterol	<i>Ferulic acid</i>	Rutin	9,12,15-octadecatrienoic acid
Absorpsi	Papp (Caco-2)	-4.839	-4.726	-4.943	-6.606	-4.729
	Pgp-inhibior	0,644	0.91	0.134	0.365	0.307
	Pgp-substrate	0,006	0.077	0.026	0.168	0.044
	HIA (%)	54,4	92,4	63,5	21	80,5
Distribusi	PPB (%)	88,552	78	50,002	76,65	88.333
	VD (L/kg)	-0,182	0.156	-0,813	-1.052	-0.79
	BBB	0,47	0.886	0.565	0.018	0.891
Metabolisme	CYP1A2	0.979	0.034	0.234	0.197	0.47
	CYP3A4	0.89	0.069	0.012	0.518	0.006
	CYP2C9	0,318	0.048	0.059	0.199	0.034
	CYP2C19	0,371	0.063	0.061	0.072	0.021
	CYP2D6	0,78	0.358	0.184	0.29	0.142
Eliminasi	T1/2 (jam)	1.599	1.865	0.913	2.138	1.728
	Cl (mL/min/kg)	1,882	1.135	1.696	0.641	1.203