BAB V
KESIMPULAN DAN SARAN

A. Kesimpulan

1. Hasil pada target makromolekul DPP4 yang terbaik adalah Acutosides D *(L. acutangula)* dengan *score* -10,8 pada glukokinase adalah α-Carotene *(C. moschata)* dengan *score* -11,25, pada PTP1B adalah Auroxanthin *(C. moschata)* dengan *score* -9,60, dan pada α glukosidase adalah Acutosides B *(L. acutangula)* dengan *score* -11,15.
2. Hasil model interaksi yang memiliki model interaksi terbaik pada target makromolekul DPP4 adalah Lutheoxanthine *(C. moschata)*, pada glukokinase adalah Zeaxanthine *(C. moschata)*, pada PTP1B adalah Luteolin-7-glucosides *(L. acutangula)*, dan pada α-glukosidase adalah Kuguacin B *(M. charantia.)*
3. Hasil prediksi profil farmakokinetika dari 12 senyawa yang dengan *docking score* terbaik menunjukkan bahwa Kuguacin B adalah senyawa yang memiliki profil farmakokinetik terbaik karena memenuhi persyaratan *Lipinsky rules of five* sehingga dapat digunakan oral, memiliki absorbsi yang tingg, tidak menembus BBB dan dapat dimetabolisme dengan baik.

B. Saran

1. Hasil ini merupakan prediksi aktivitas biologis karena didapat dari simulasi pemodelan *software*. Sehingga perlu dilakukan uji *in vitro* dan *in vivo* pada Kuguacin B untuk mengetahui aktivitas senyawa tersebut.
2. Dapat dilakukan penelitian lebih lanjut dengan menggunakan target makromolekul antidiabetes selain empat makromolekul yang telah diujikan pada penelitian ini
3. Dapat dilakukan penelitian lanjutan dengan menggunakan studi hubungan struktur-aktivitas (HKSA) lima puluh sembilan senyawa didockingkan pada empat makromolekul target diatas.

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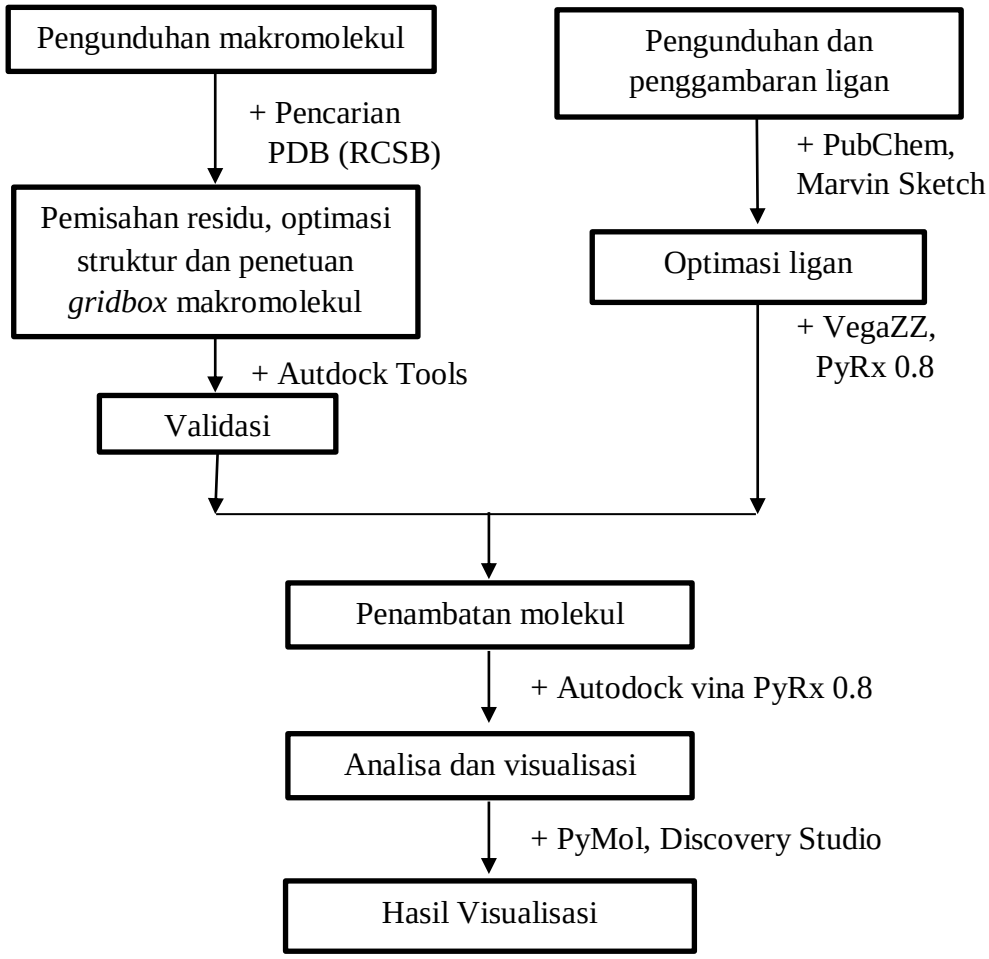
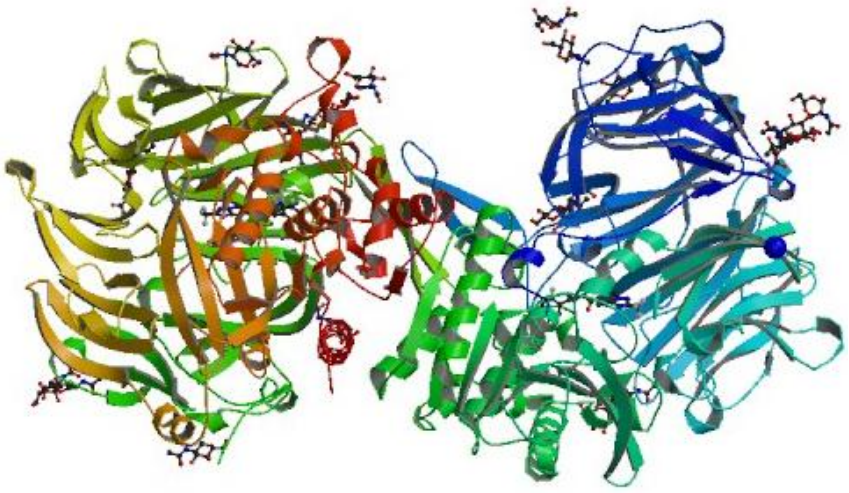
LAMPIRAN

Lampiran 1. Skema Jalannya Penelitian

Skema Jalannya Penelitian

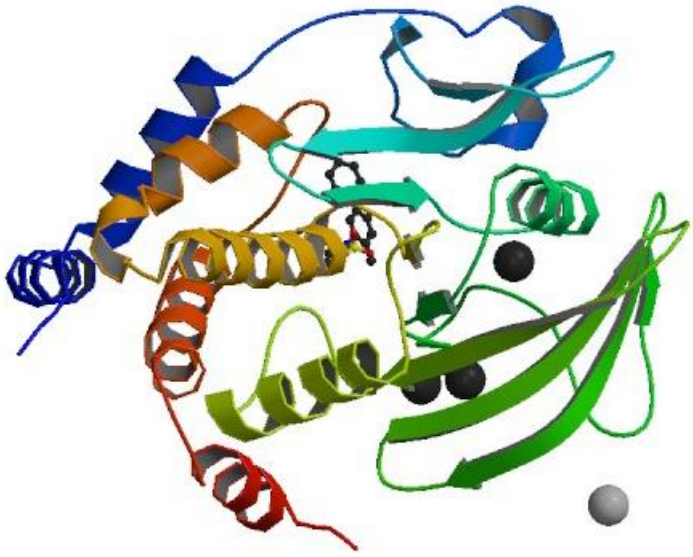


Lampiran 2. Struktur 3D Makromolekul DPP4 dengan Kode PDB 2QOE



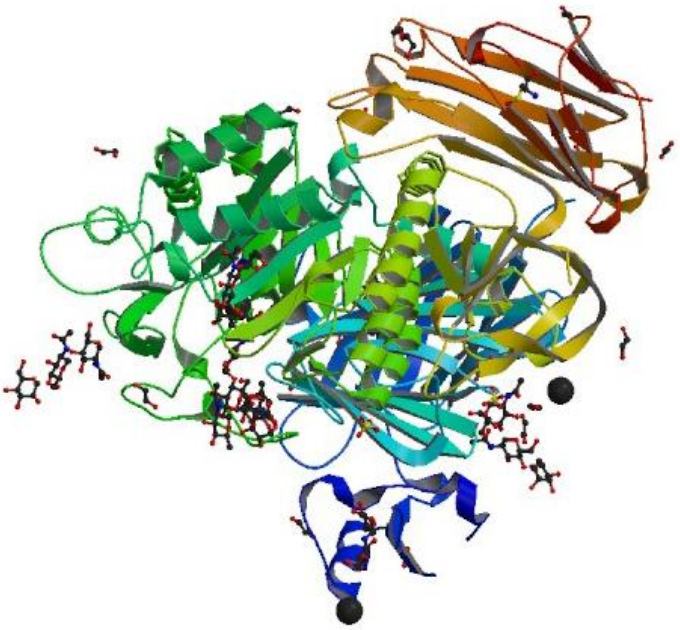
(Sumber : www.rscb.org)

Lampiran 3. Struktur 3D Makromolekul PTP1B dengan Kode PDB 5T19



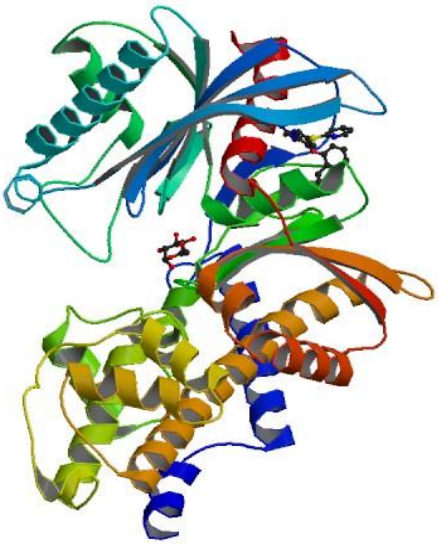
(Sumber : www.rscb.org)

Lampiran 4. Struktur 3D Makromolekul α-glukosidase dengan Kode PDB 5NN8



(Sumber : www.rscb.org)

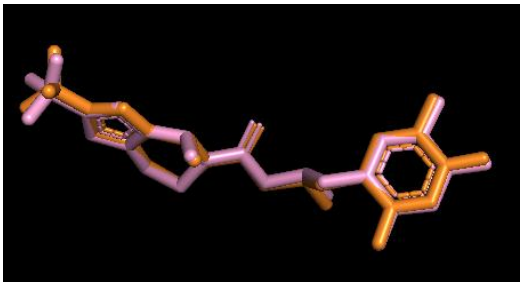
Lampiran 5. Struktur 3D Makromolekul Glukokinase dengan Kode PDB 4RCH



(Sumber : www.rscb.org)

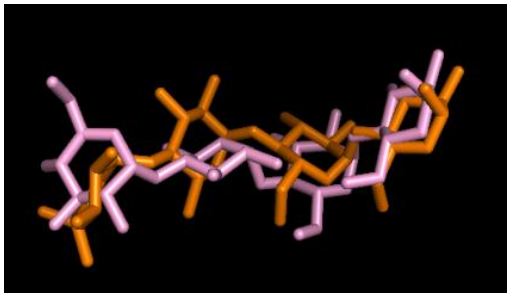
Lampiran 6. Overlay Ligan Uji dan Ligan Asli Menggunakan PyMOL

1. **2QOE**

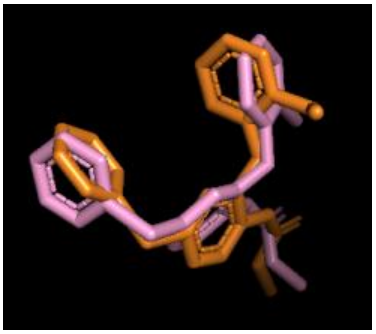


2. **5T19**

3. **5NN8**



4. **4RCH**



Lampiran 7. Hasil Docking Nilai Energi Ikatan pada target DPP4

No	Name	Average	SD
40			
38	Acutoside B	-10.525	0.414578099
23	Momordicosides D	-10.375	0.147901995
43	Acutoside G	-10.15	0.438748219
2	Auroxanthin	-9.85	0.16583124
39	Acutoside C	-9.65	0.05
37	Acutoside A	-8.975	0.04330127
13	Zeaxanthin	-8.9	0.751664819
9	Luteoxanthin	-8.9	0.244948974
12	Violaxanthin	-8.8	0.122474487
41	Acutoside E	-8.8	0.234520788
1	Alpha carotene	-8.725	0.356195171
7	Favoxanthin	-8.675	0.04330127
8	Lutein	-8.525	0.216506351
54	Luteolin-7-glucoside	-8.525	0.04330127
50	Carotene	-8.475	0.286138079
18	Kuguacin A	-8.375	0.04330127
46	Apigenin 7-glucoside	-8.375	0.04330127
6	Beta cryptoxanthin	-8.275	0.147901995
24	Omargliptine	-8.25	0.08660254
4	Beta carotene-5,6-epoxide	-8.1	0.663324958
17	Cucurbitacin	-8.1	0.3
21	Kuguacin G	-8.075	0.04330127
19	Kuguacin B	-8.075	0.04330127
31	1,8-dihydroxy-4-methylanthracene-9,10-dione	-8.075	0.04330127
28	Cholest-5-En-3-Ol	-8.05	0.206155281
42	Acutoside F	-7.925	0.791754381
20	Kuguacin D	-7.8	0
22	Kuguacin H	-7.7	0
3	Beta carotene	-7.65	0.287228132
15	Catechin	-7.65	0.08660254
16	Cholic Acid	-7.6	0
10	Neurosporene	-7.225	0.204633819
14	Zetacarotene	-7.125	0.779021823
11	Phytofluene	-6.7	0.604152299

No	Name	Average	SD
55	Neryl Acetate	-6.375	0.04330127
47	Ascorbic Acid	-6.2	0
5	Citronellyl Tiglate	-5.9	0.070710678
32	1H-Indole	-5.9	0
36	9,12,15-octadecatrienoic acid_methyl_ester	-5.85	0.15
26	3,7,11,15-tetramethyl-2-hexadecen-1-ol	-5.825	0.356195171
52	Citronellyl Tiglate	-5.675	0.216506351
25	2,3-dihydro,3,5-dihydroxy-6-methyl-(4H)-pyran-4-one	-5.6	0
48	Alpha-Terpineol	-5.55	0.05
27	9,12,15-Octadecatrienoic_Acid,Methyl_Ester	-5.5	0.122474487
34	3,4-Dimethyl-2,4,6-octatriene	-5.475	0.04330127
29	(E)-beta-ocimene	-5.425	0.08291562
33	2-Methyl-6-Methylene-1,7-Octadien-3-One	-5.4	0.122474487
59	n-Hexadecanoic acid	-5.225	0.178535711
57	trans-Dihydrocarvone	-5.2	0
58	trans-Linaloloxide	-5.2	0.173205081
30	(Z)-beta-ocimene	-5.175	0.04330127
53	D,L-limonene	-5.15	0.08660254
45	Alpha –Thujone	-5	0
49	beta-Myrcene	-4.925	0.31124749
56	Sabiene	-4.8	0
44	Alpha- Thujene	-4.775	0.04330127
51	Sabinene Hydrate	-4.6	0.173205081
35	3-Methyl-1-butanol	-4.2	0
	sitagliptine	-8.875	0.326917421

Lampiran 8. Hasil Docking Nilai Energi Ikatan pada target Glukokinase

No	Name	Average	SD
1			
2	Auroxanthin	-10.7	0.187082869
13	Zeaxanthin	-10.55	0.610327781
3	Beta carotene	-10.4	0.821583836
14	Zetacarotene	-9.85	0.111803399
8	Lutein	-9.7	0.234520788
11	Phytofluene	-9.475	0.31124749
24	Omargliptine	-9.475	0.04330127
50	Carotene	-9.475	0.383242743
9	Luteoxanthin	-9.4	0
21	Kuguacin G	-9.4	0
4	Beta carotene-5,6-epoxide	-9.375	0.460298816
7	Favoxanthin	-9.25	0.15
19	Kuguacin B	-9.225	0.04330127
6	Beta cryptoxanthin	-9.175	0.376662979
18	Kuguacin A	-9.1	0
31	1,8-dihydroxy-4-methylanthracene-9,10-dione	-9.1	0
46	Apigenin 7-glucoside	-9.075	0.04330127
12	Violaxanthin	-9.025	0.408503366
23	Momordicosides D	-9	0.291547595
28	Cholest-5-En-3-Ol	-8.925	0.04330127
10	Neurosporene	-8.9	0.070710678
54	Luteolin-7-glucoside	-8.8	0
15	Catechin	-8.5	0
22	Kuguacin H	-8.3	0.367423461
43	Acutoside G	-8.225	0.794905655
20	Kuguacin D	-8.125	0.04330127
16	Cholic Acid	-7.875	0.389711432
17	Cucurbitacin	-7.725	0.389711432
37	Acutoside A	-7.425	0.369966215
40	Acutoside D	-6.975	0.697764287
26	3,7,11,15-tetramethyl-2-hexadecen-1-ol	-6.95	0.229128785
52	Citronellyl Tiglate	-6.75	0.08660254
27	9,12,15-Octadecatrienoic_Acid,Methyl_	-6.65	0.111803399

No	Name	Average	SD
	Ester		
36	9,12,15-octadecatrienoic acid_methyl_ester	-6.65	0.327871926
5	Citronellyl Tiglate	-6.6	0.141421356
39	Acutoside C	-6.6	0.552268051
41	Acutoside E	-6.475	1.008402202
55	Neryl Acetate	-6.275	0.04330127
48	Alpha-Terpineol	-6.2	0
53	D,L-limonene	-6.2	0
57	trans-Dihydrocarvone	-6.025	0.04330127
34	3,4-Dimethyl-2,4,6-octatriene	-6	0
58	trans-Linaloloxide	-5.85	0.05
56	Sabiene	-5.8	0
44	Alpha- Thujene	-5.775	0.04330127
59	n-Hexadecanoic acid	-5.775	0.08291562
29	(E)-beta-ocimene	-5.775	0.04330127
30	(Z)-beta-ocimene	-5.7	0
45	Alpha –Thujone	-5.7	0
33	2-Methyl-6-Methylene-1,7-Octadien-3-One	-5.625	0.04330127
42	Acutoside F	-5.625	0.825757228
49	beta-Myrcene	-5.575	0.04330127
32	1H-Indole	-5.3	0
47	Ascorbic Acid	-5.1	0
25	2,3-dihydro,3,5-dihydroxy-6-methyl-(4H)-pyran-4-one	-4.8	0
38	Acutoside B	-4.75	8.001406126
35	3-Methyl-1-butanol	-3.7	0
51	Sabinene Hydrate	-2.9	5.022947342
	(4Z,12Z)-Cyclopentadeca-4, 12-dienone	-8.1	0

Lampiran 9. Hasil Docking Nilai Energi Ikatan pada target PTP1B

No	Name	Average	SD
2			
43	Acutoside G	-9.125	0.248746859
54	Luteolin-7-glucoside	-9.1	0
46	Apigenin 7-glucoside	-8.875	0.04330127
38	Acutoside B	-8.625	0.216506351
9	Luteoxanthin	-8.475	0.108972474
23	Momordicosides D	-8.475	0.108972474
17	Cucurbitacin	-8.425	0.129903811
19	Kuguacin B	-8.225	0.653356717
28	Cholest-5-En-3-Ol	-8.15	0.08660254
31	1,8-dihydroxy-4-methylanthracene-9,10-dione	-8.1	0
50	Carotene	-8.1	0
18	Kuguacin A	-8.05	0.438748219
16	Cholic Acid	-8.025	0.04330127
22	Kuguacin H	-8.025	0.334477204
41	Acutoside E	-7.9	0.173205081
21	Kuguacin G	-7.825	0.389711432
40	Acutoside D	-7.725	0.04330127
7	Favoxanthin	-7.7	0
6	Beta cryptoxanthin	-7.7	0.3
4	Beta carotene-5,6-epoxide	-7.65	0.657647322
24	Omargliptine	-7.6	0.346410162
8	Lutein	-7.525	0.258602011
1	Alpha carotene	-7.475	0.660965203
39	Acutoside C	-7.45	0.08660254
12	Violaxanthin	-7.425	0.178535711
13	Zeaxanthin	-7.35	0.217944947
10	Neurosporene	-7.25	0.364005494
42	Acutoside F	-7.175	0.04330127
15	Catechin	-7.1	0
55	Neryl Acetate	-7.1	0
37	Acutoside A	-7.075	0.248746859
3	Beta carotene	-6.95	0.638357267
14	Zetacarotene	-6.9	0.234520788
20	Kuguacin D	-6.875	0.303108891

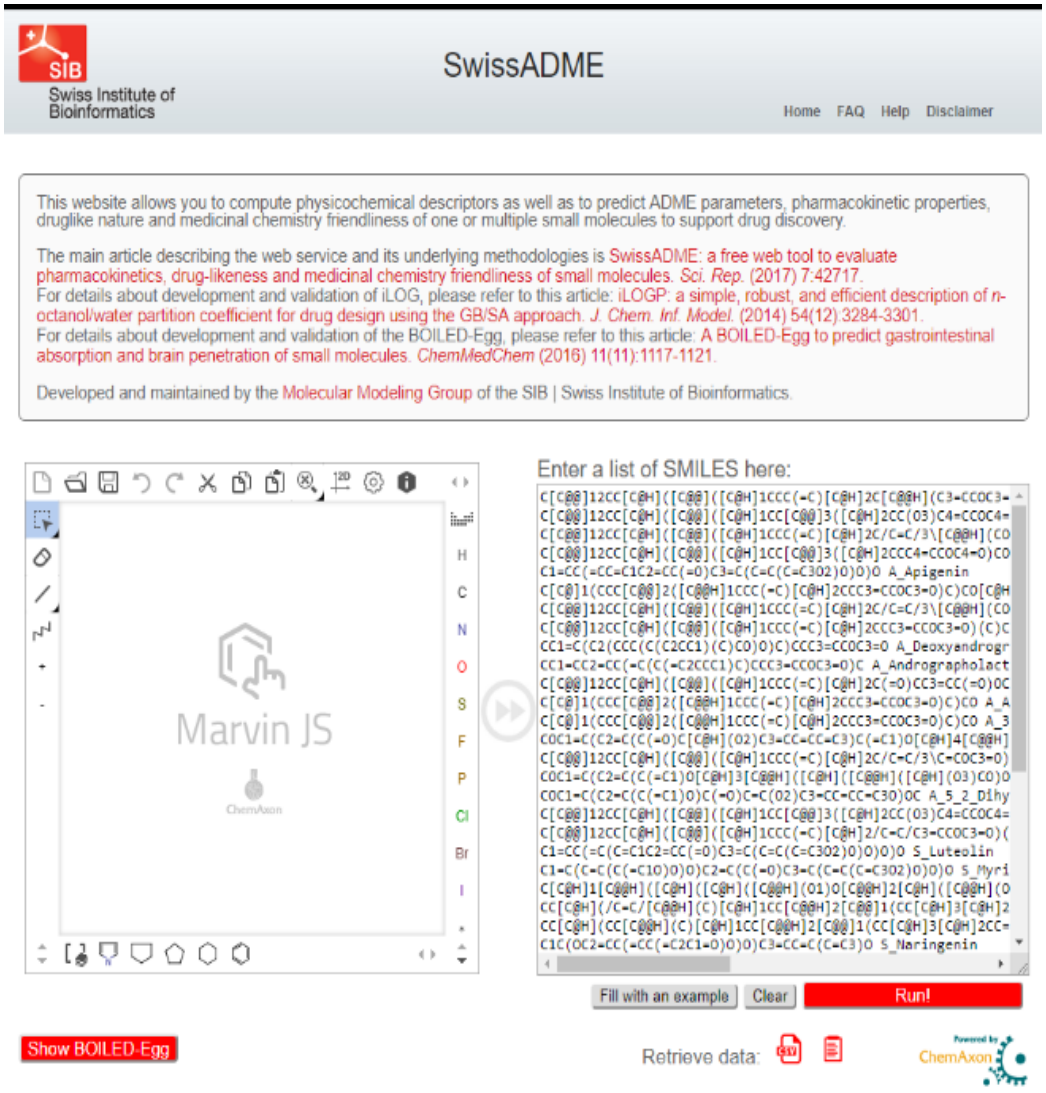
11	Phytofluene	-6.85	0.701783442
48	Alpha-Terpineol	-6.7	0
53	D,L-limonene	-6.7	0
52	Citronellyl Tiglate	-6.7	0.070710678
5	Citronellyl Tiglate	-6.525	0.08291562
45	Alpha –Thujone	-6.4	0
56	Sabiene	-6.3	0
57	trans-Dihydrocarvone	-6.3	0
34	3,4-Dimethyl-2,4,6-octatriene	-6.2	0
44	Alpha- Thujene	-6.2	0
36	9,12,15-octadecatrienoic acid_methyl_ester	-6.1	0.070710678
29	(E)-beta-ocimene	-6.05	0.08660254
47	Ascorbic Acid	-6.025	0.04330127
33	2-Methyl-6-Methylene-1,7-Octadien-3-One	-6	0
59	n-Hexadecanoic acid	-5.95	0.05
30	(Z)-beta-ocimene	-5.95	0.05
51	Sabinene Hydrate	-5.9	0
27	9,12,15-Octadecatrienoic_Acid,Methyl_Ester	-5.775	0.449305019
49	beta-Myrcene	-5.775	0.04330127
32	1H-Indole	-5.7	0
25	2,3-dihydro,3,5-dihydroxy-6-methyl-(4H)-pyran-4-one	-5.425	0.326917421
58	trans-Linaloloxide	-5.225	0.535607132
35	3-Methyl-1-butanol	-4.575	0.04330127
26	3,7,11,15-tetramethyl-2-hexadecen-1-ol	-3.075	5.41865989
	3-bromo-4[difloro(phosphono)methyl]-N-methyl-nalpha-(methylsulfonyl)-L-Phenylalaninamide	-8.65	0.05

Lampiran 10. Hasil Docking Nilai Energi Ikatan pada target Alpha glukosida

No	Name	Average	SD
38			
43	Acutoside G	-9.225	0.739509973
19	Kuguacin B	-8.7	0
23	Momordicosides D	-8.675	0.535607132
40	Acutoside D	-8.6	0
21	Kuguacin G	-8.475	0.04330127
22	Kuguacin H	-8.475	0.216506351
54	Luteolin-7-glucoside	-8.425	0.277263413
18	Kuguacin A	-8.4	0
2	Auroxanthin	-8.325	0.04330127
24	Omargliptine	-8.2	0
28	Cholest-5-En-3-Ol	-8.2	0
41	Acutoside E	-8.125	0.108972474
17	Cucurbitacin	-8.1	0.3
16	Cholic Acid	-8.075	0.04330127
42	Acutoside F	-7.975	0.294745653
46	Apigenin 7-glucoside	-7.975	0.163935963
13	Zeaxanthin	-7.925	0.277263413
37	Acutoside A	-7.9	0
12	Violaxanthin	-7.725	0.147901995
3	Beta carotene	-7.725	0.04330127
9	Luteoxanthin	-7.6	0.339116499
8	Lutein	-7.6	0.070710678
50	Carotene	-7.6	0.254950976
7	Favoxanthin	-7.575	0.04330127
1	Alpha carotene	-7.45	0.16583124
10	Neurosporene	-7.425	0.576085931
39	Acutoside C	-7.4	0.122474487
4	Beta carotene-5,6-epoxide	-7.4	0.254950976
20	Kuguacin D	-7.375	0.04330127
15	Catechin	-7.125	0.04330127
6	Beta cryptoxanthin	-7.025	0.04330127
11	Phytofluene	-6.75	0.572276157
14	Zetacarotene	-6.55	0.16583124
31	1,8-dihydroxy-4-methylanthracene-9,10-dione	-6.525	0.04330127

No	Name	Average	SD
52	Citronellyl Tiglate	-6.175	0.08291562
5	Citronellyl Tiglate	-6.125	0.04330127
48	Alpha-Terpineol	-5.7	0
57	trans-Dihydrocarvone	-5.7	0
55	Neryl Acetate	-5.625	0.147901995
26	3,7,11,15-tetramethyl-2-hexadecen-1-ol	-5.575	0.2384848
32	1H-Indole	-5.5	0
47	Ascorbic Acid	-5.475	0.04330127
56	Sabiene	-5.45	0.08660254
53	D,L-limonene	-5.4	0
27	9,12,15-Octadecatrienoic_Acid,Methyl_Ester	-5.375	0.248746859
30	(Z)-beta-ocimene	-5.3	0
51	Sabinene Hydrate	-5.275	0.216506351
29	(E)-beta-ocimene	-5.2	0
33	2-Methyl-6-Methylene-1,7-Octadien-3-One	-5.2	0
34	3,4-Dimethyl-2,4,6-octatriene	-5.2	0
36	9,12,15-octadecatrienoic acid_methyl_ester	-5.175	0.192028644
49	beta-Myrcene	-5.1	0.1
25	2,3-dihydro,3,5-dihydroxy-6-methyl-(4H)-pyran-4-one	-5.05	0.08660254
44	Alpha- Thujene	-5.025	0.227760839
45	Alpha –Thujone	-4.925	0.426468053
59	n-Hexadecanoic acid	-4.9	0.122474487
58	trans-Linaloloxide	-4.875	0.147901995
35	3-Methyl-1-butanol	-4	0

Lampiran 11. Proses Prediksi ADME menggunakan Swiss ADME



Lampiran 12. Hasil *Lipinski's rule of five*

Molecule	*MW*	*#H-bond acceptors*	*#H-bond donors*	*Log P*	*Solubility*
(E) Beta-Ocimene	136.23	0	0	3.4	*Soluble*
(Z)-Beta-Ocimene	136.23	0	0	3.4	*Soluble*
1 _8-dihydroxy-4-methylanthracene-9 _10-dione	266.33	4	2	0.96	*Very soluble*
1H-Indole	117.15	0	1	1.98	*Soluble*
2 _3-Dihydro-3 _5-Dihydroxy-6-Methyl-4h-Pyran-4-One	144.13	4	2	-0.22	*Very soluble*
2-Methyl-6-Methylene-1 _7-Octadien-3-One	150.22	1	0	2.66	*Soluble*
3 _4-Dimethyl-2 _4 _6-octatriene	136.23	0	0	3.36	*Soluble*
3 _7 _11 _15-Tetramethyl-2-Hexadecen-1-OL	296.53	1	1	6.21	*Moderately soluble*
3-Methyl-1-butanol	88.15	1	1	1.16	*Very soluble*
9 _12 _15-octadecatrienoic acid_methyl_ester	278.43	2	1	5.18	*Moderately soluble*
9 _12 _15-Octadecatrienoic_Acid Methyl_Ester	292.46	2	0	5.55	*Moderately soluble*
Acutoside A	780.98	13	8	2.77	*Poorly soluble*
Acutoside B	1191.35	25	14	-1.03	*Poorly soluble*
Acutoside C	1207.35	26	15	-1.78	*Moderately soluble*
Acutoside D	1323.47	29	16	-2.21	*Poorly soluble*
Acutoside E	1323.47	29	16	-2.04	*Poorly soluble*
Acutoside F	1323.47	29	16	-2.22	*Poorly soluble*
Acutoside G	1455.58	33	18	-3.47	*Moderately soluble*
Alpha Carotene	536.87	0	0	11.06	*Insoluble*
Alpha- Thujene	136.23	0	0	3.15	*Soluble*
Alpha –Thujone	152.23	1	0	2.35	*Soluble*
Alpha-Terpineol	154.25	1	1	2.58	*Soluble*
Apigenin 7-glucoside	432.38	10	6	0.52	*Soluble*
Ascorbic Acid	176.12	6	4	-1.42	*Highly soluble*
Auroxanthin	600.87	4	2	7.84	*Poorly soluble*
Beta Carotene	536.87	0	0	11.13	*Insoluble*

Beta Carotene 5 _6-Epoxide	552.87	1	0	10.55	*Insoluble*
Beta-Cryptoxanthin	552.87	1	1	10.22	*Insoluble*
beta-Myrcene	136.23	0	0	3.43	*Soluble*
Carotene	536.87	0	0	11.06	*Insoluble*
	290.27	6	5	0.83	*Soluble*
Cholest-5-En-3-Ol	386.65	1	1	6.76	*Poorly soluble*
Cholic Acid	408.57	5	4	2.77	*Soluble*
Citronellyl Tiglate	238.37	2	0	4.21	*Soluble*
Citronellyl Tiglate	238.37	2	0	4.21	*Soluble*
Cucurbitacin B	558.7	8	3	3.24	*Moderately soluble*
D _L-limonene	136.23	0	0	3.37	*Soluble*
Flavoxanthine	584.87	3	2	8.52	*Poorly soluble*
Kuguacin A	470.68	4	2	4.82	*Moderately soluble*
Kuguacin B	456.7	3	2	5.69	*Poorly soluble*
Kuguacin D	428.6	4	1	4.14	*Moderately soluble*
Kuguacin G	500.67	6	1	3.93	*Moderately soluble*
Kuguacin H	484.67	5	1	4.25	*Moderately soluble*
Lutein	568.87	2	2	9.23	*Poorly soluble*
Luteolin-7-glucoside	448.38	11	7	0.15	*Soluble*
Luteoxanthin	600.87	4	2	8.16	*Poorly soluble*
Momordicoside D	783	13	9	2.01	*Poorly soluble*
Neryl Acetate	196.29	2	0	3.21	*Soluble*
Neurosporene	538.89	0	0	12.04	*Insoluble*
n-Hexadecanoic acid	256.42	2	1	5.2	*Moderately soluble*
Omarigliptin	398.43	8	1	1.51	*Soluble*
Phytofluene	542.92	0	0	12.21	*Insoluble*
Sabiene	136.23	0	0	3.25	*Soluble*
Sabinene Hydrate	154.25	1	1	2.34	*Soluble*
trans-Dihydrocarvone	154.25	1	0	2.54	*Soluble*
trans-Linaloloxide	170.25	2	1	2.03	*Very soluble*
Violaxanthin	600.87	4	2	8.4	*Poorly soluble*
Zeaxanthin	568.87	2	2	9.32	*Poorly soluble*
Zeta-Carotene	540.9	0	0	12.13	*Insoluble*

Lampiran 13. Hasil Prediksi ADME

Molecule	*GI Abs*	*BBB Permeant*	*P-gp Substrate*	*CYP1A2 Inhibitor*	*CYP2C19 Inhibitor*	*CYP2C9 Inhibitor*	*CYP2D6 Inhibitor*	*CYP3A4 Inhibitor*
(E)-beta-ocimene	*Low*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
(Z)-beta-ocimene	*Low*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
1,8-dihydroxy-4-methylanthracene-9,10-dione	*High*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
1H-Indole	*High*	*Yes*	*No*	*Yes*	*No*	*No*	*No*	*No*
2,3-dihydro,3,5-dihydroxy-6-methyl-(4H)-pyran-4-one	*High*	*No*	*No*	*No*	*No*	*No*	*No*	*No*
2-Methyl-6-Methylene-1,7-Octadien-3-One	*High*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
3,4-Dimethyl-2,4,6-octatriene	*Low*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
3,7,11,15-tetramethyl-2-hexadecen-1-ol	*Low*	*No*	*Yes*	*No*	*No*	*Yes*	*No*	*No*
3-Methyl-1-butanol	*High*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
9,12,15-octadecatrienoic acid_methyl_ester	*High*	*Yes*	*No*	*Yes*	*No*	*Yes*	*No*	*No*
9,12,15-Octadecatrienoic_Acid,Methyl_Ester	*High*	*Yes*	*No*	*Yes*	*No*	*Yes*	*No*	*No*
9,12,15-Octadecatrienoic_Acid,Methyl_Ester	*High*	*Yes*	*No*	*Yes*	*No*	*Yes*	*No*	*No*
Acutoside A	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Acutoside B	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Acutoside C	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Acutoside D	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*

Molecule	*GI Abs*	*BBB Permeant*	*P-gp Substrate*	*CYP1A2 Inhibitor*	*CYP2C19 Inhibitor*	*CYP2C9 Inhibitor*	*CYP2D6 Inhibitor*	*CYP3A4 Inhibitor*
Acutoside E	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Acutoside F	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Acutoside G	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Alpha carotene	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Alpha- Thujene	*Low*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
Alpha –Thujone	*High*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
Alpha-Terpineol	*High*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
Apigenin 7-glucoside	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Ascorbic Acid	*Low*	*No*	*No*	*No*	*No*	*No*	*No*	*No*
Auroxanthin	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*Yes*
Beta carotene	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Beta carotene-5,6-epoxide	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Beta cryptoxanthin	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
beta-Myrcene	*Low*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
Carotene	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Catechin	*High*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Cholest-5-En-3-Ol	*Low*	*No*	*No*	*No*	*No*	*Yes*	*No*	*No*
Cholic Acid	*High*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Citronellyl Tiglate	*High*	*Yes*	*No*	*No*	*Yes*	*Yes*	*No*	*No*
Citronellyl Tiglate	*High*	*Yes*	*No*	*No*	*Yes*	*Yes*	*No*	*No*
Cucurbitacin	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*Yes*
D,L-limonene	*Low*	*Yes*	*No*	*No*	*No*	*Yes*	*No*	*No*

Molecule	*GI Abs*	*BBB Permeant*	*P-gp Substrate*	*CYP1A2 Inhibitor*	*CYP2C19 Inhibitor*	*CYP2C9 Inhibitor*	*CYP2D6 Inhibitor*	*CYP3A4 Inhibitor*
Favoxanthin	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*Yes*
Kuguacin A	*High*	*No*	*Yes*	*No*	*No*	*No*	*No*	*Yes*
Kuguacin B	*High*	*No*	*No*	*No*	*No*	*No*	*No*	*No*
Kuguacin D	*High*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Kuguacin G	*High*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Kuguacin H	*High*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Lutein	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Luteolin-7-glucoside	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Luteoxanthin	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Momordicosides D	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Neryl Acetate	*Low*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
Neurosporene	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
n-Hexadecanoic acid	*High*	*Yes*	*No*	*Yes*	*No*	*Yes*	*No*	*No*
Omargliptine	*High*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Phytofluene	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Sabiene	*Low*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
Sabinene Hydrate	*High*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
trans-Dihydrocarvone	*High*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
trans-Linaloloxide	*High*	*Yes*	*No*	*No*	*No*	*No*	*No*	*No*
Violaxanthin	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Zeaxanthin	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*
Zetacarotene	*Low*	*No*	*Yes*	*No*	*No*	*No*	*No*	*No*