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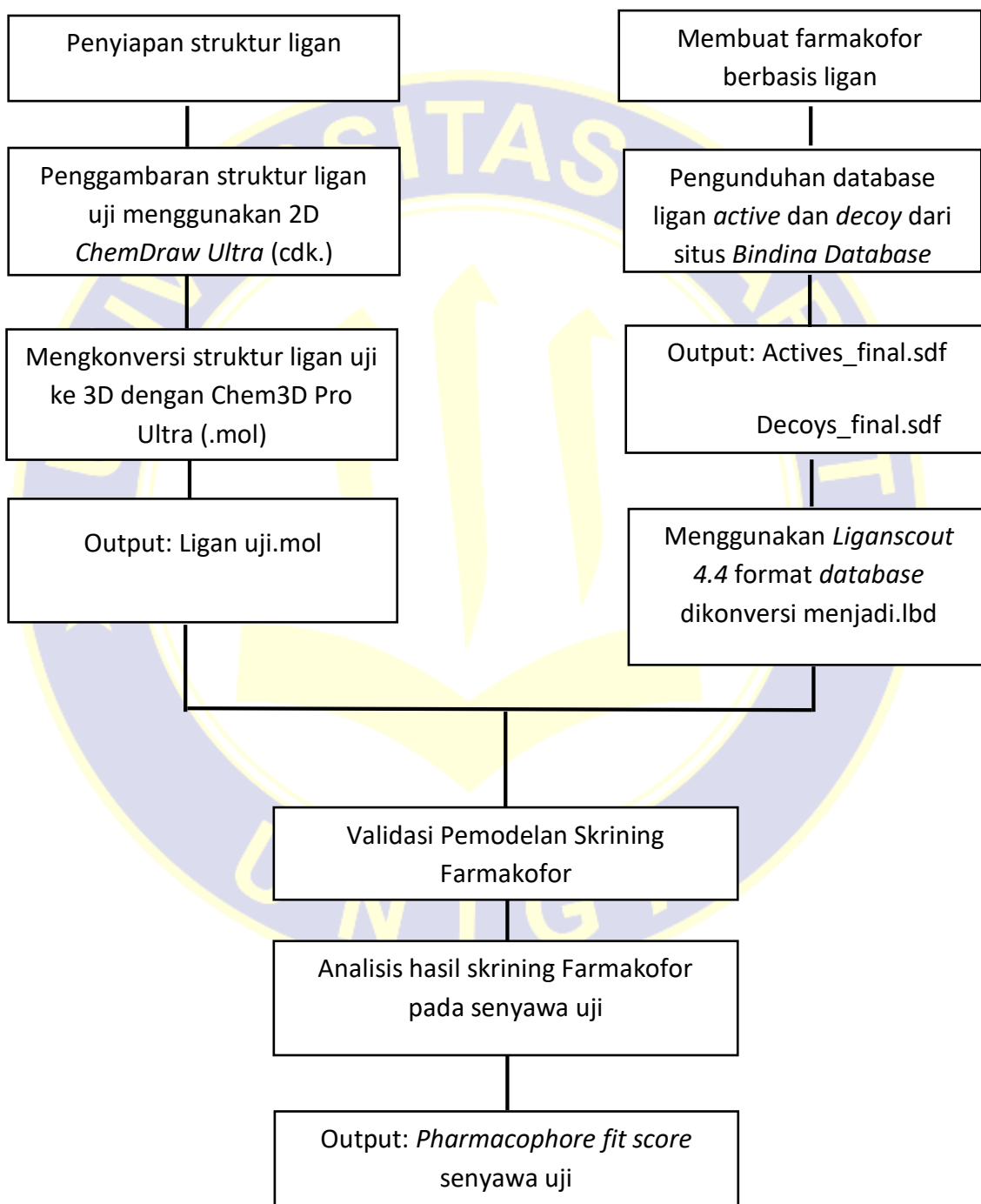
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LAMPIRAN 1

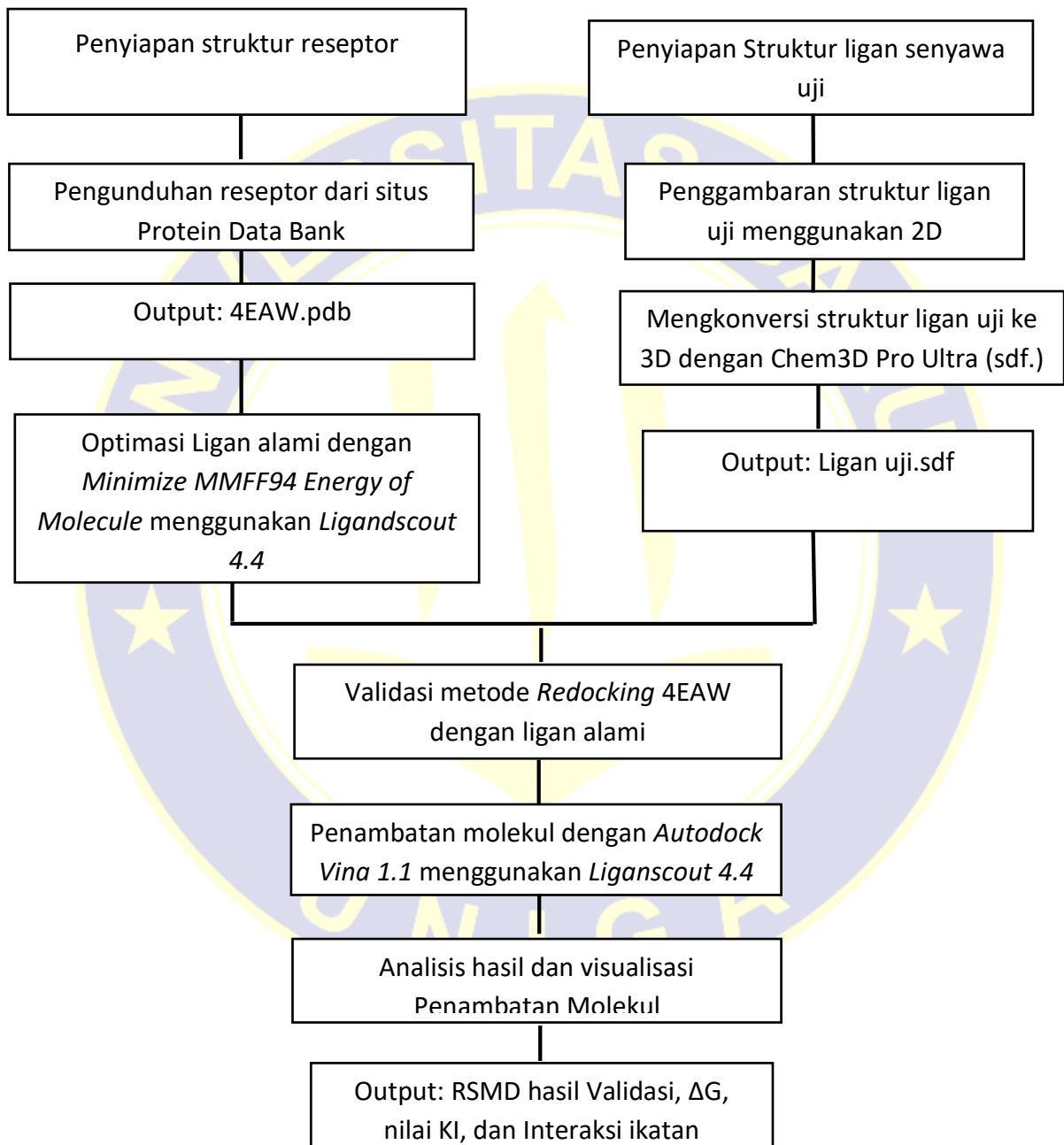
ALUR PENELITIAN



Gambar II Skema alur penelitian skrining farmakofor

LAMPIRAN 2

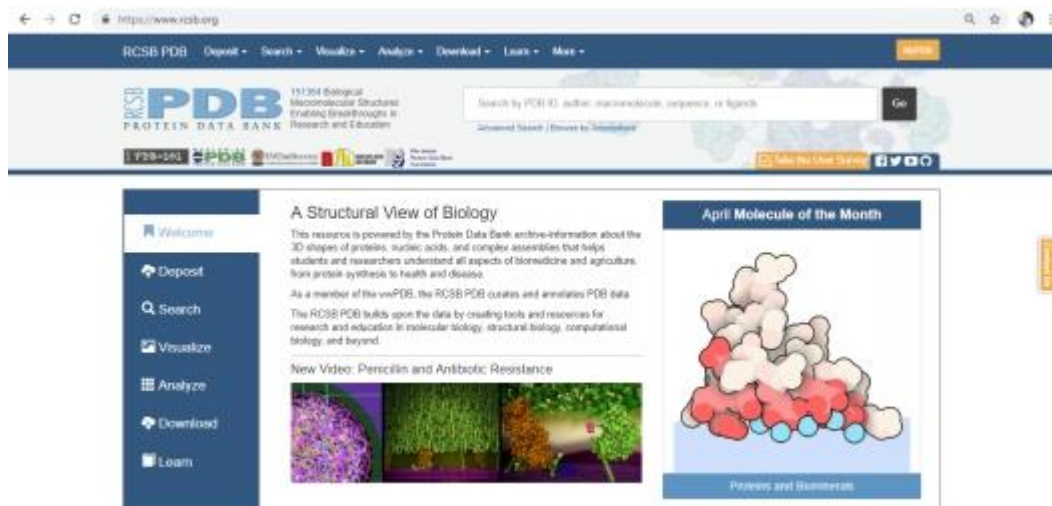
ALUR PENELITIAN PENAMBATAN MOLEKUL



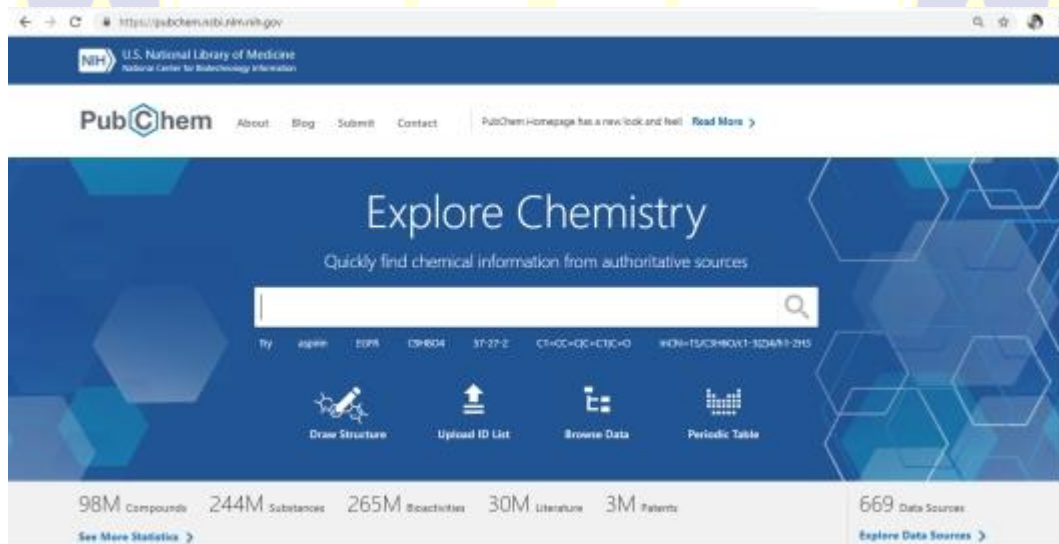
Gambar II.1 Skema alur penelitian penambatan molekul

LAMPIRAN 3

SITUS DAN APLIKASI



Gambar III.1 Tampilan situs *Protein Data Bank*



Gambar III.2 Tampilan situs *Pubchem*

LAMPIRAN 3

(LANJUTAN)



Gambar III.3 Tampilan situs *Lipinski Rule of Five*



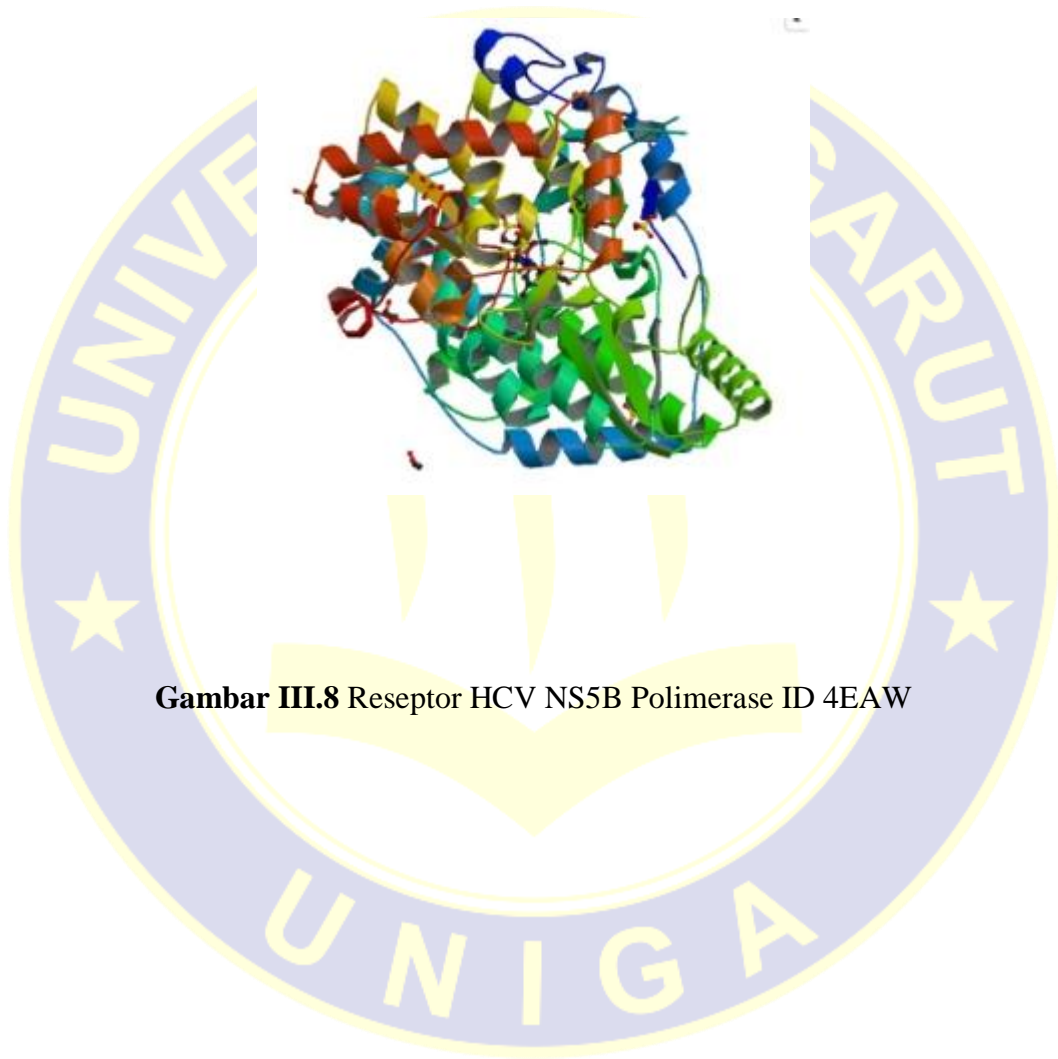
Gambar III.4 Tampilan situs *Binding Database*



Gambar III.5 Tampilan situs DUD.E

LAMPIRAN 4

STRUKTUR 3D MAKROMOLEKUL PROTEIN



LAMPIRAN 5

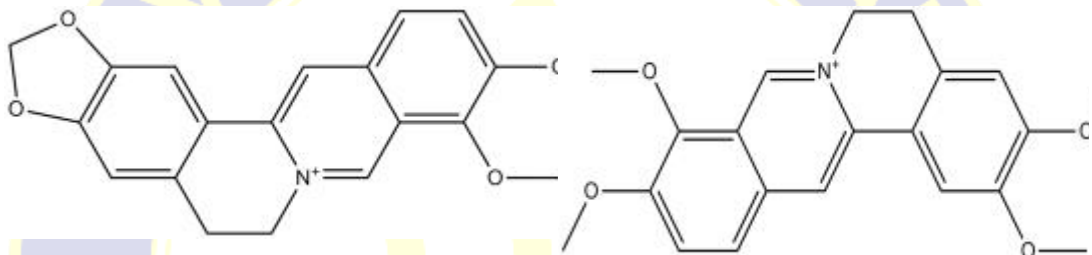
TUMBUHAN AKAR KUNING (*Arcangelisia Flava* (L) Merr)



Gambar I.I Tumbuhan akar Kuning (*Arcangelelisia Flava* (L) Merr)

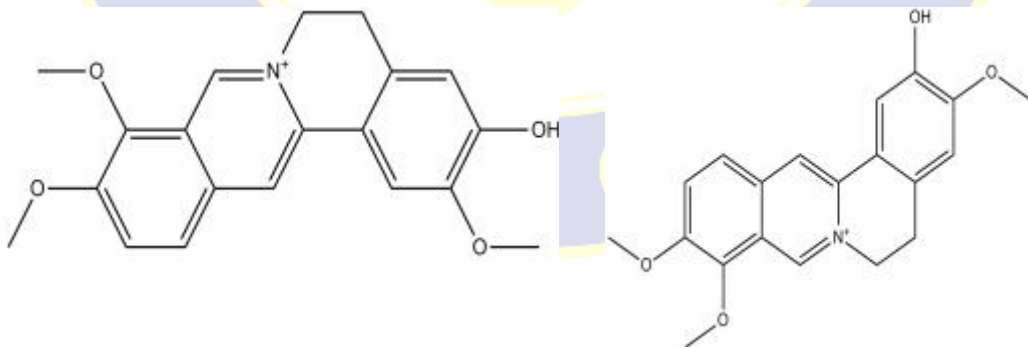
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STRUKTUR 2D SENYAWA UJI



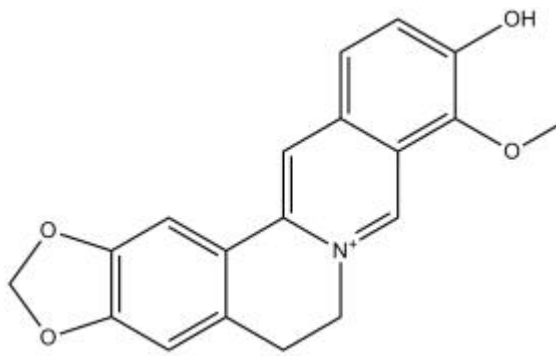
Gambar III.12 Berberine

Gambar III.13 Palmatine

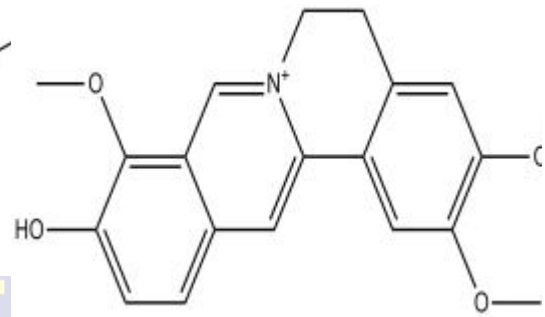


Gambar III.14 Jatrorrhizine

Gambar III.15 kolumbamine



Gambar III.16 Thalifendine

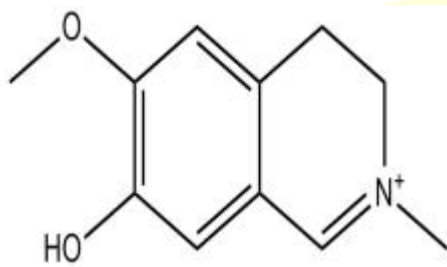


Gambar III.17 Dehydrocoridalmine

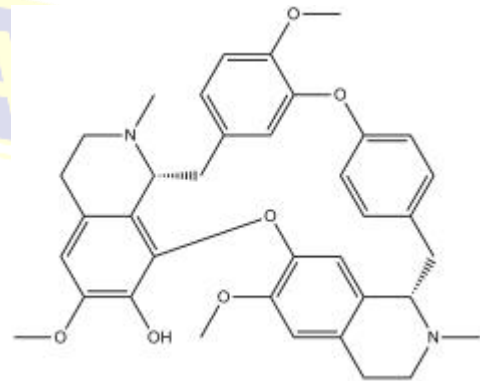


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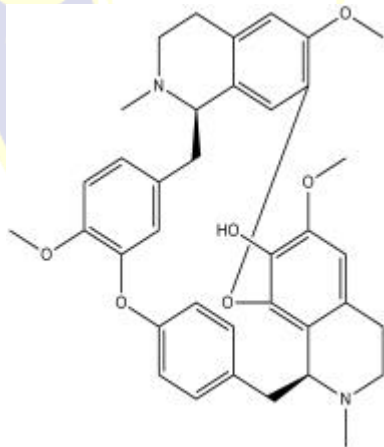
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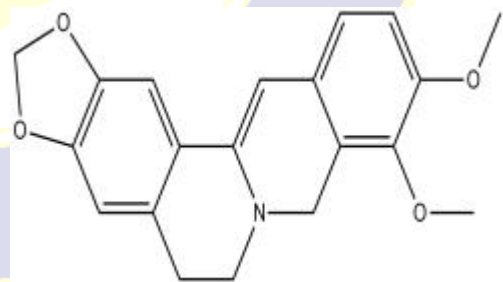
Gambar III.18 Pycnarhine



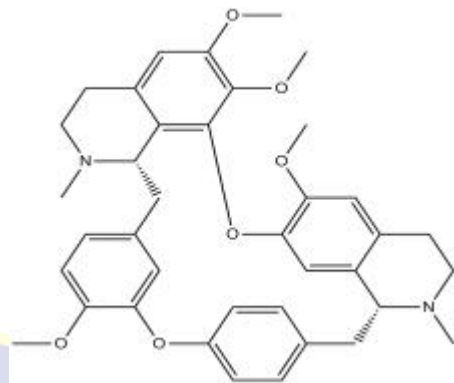
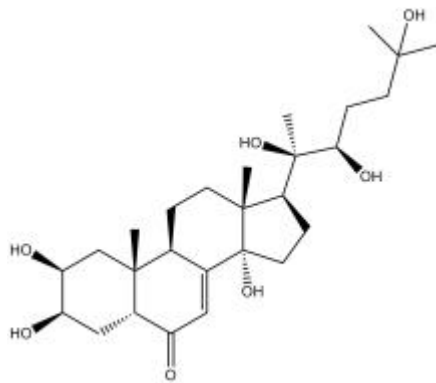
Gambar III.19 Limacine



Gambar III.20 Homoaromoline



Gambar III.21 dihydroberberine

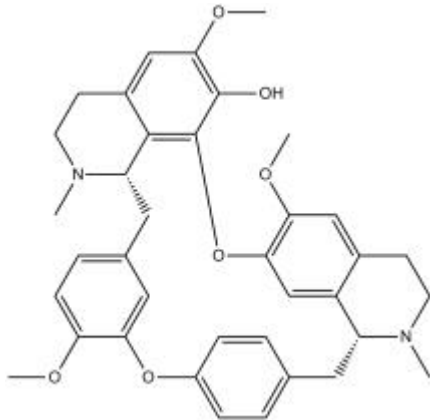


Gambar III.22 20-hydroxyecdysone **Gambar III.23** Tetradine

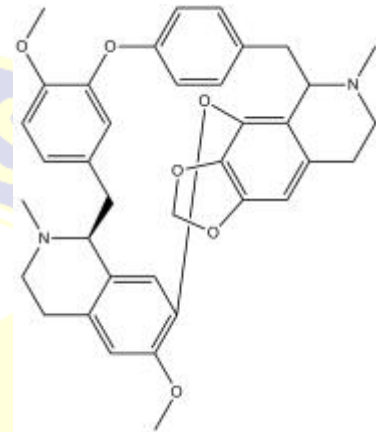


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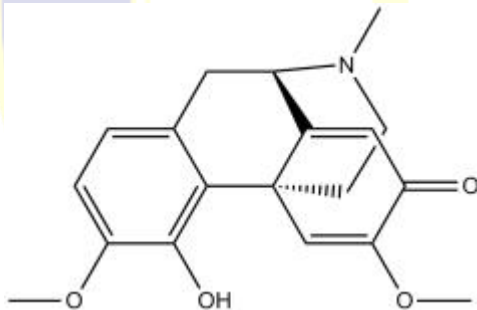
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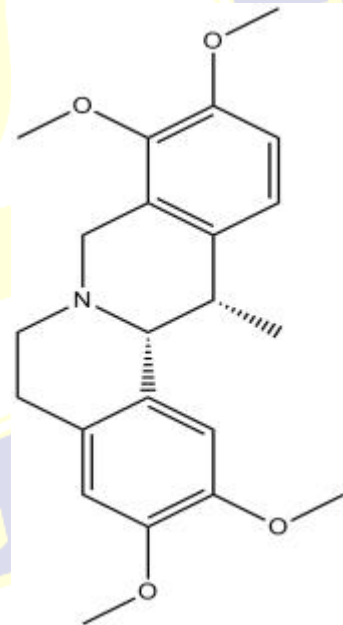
Gambar III.24 Fangchinoline



Gambar III.25 Cepharanthine



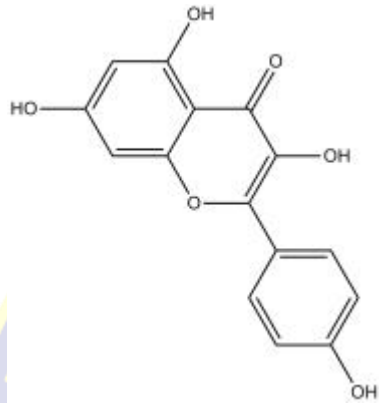
Gambar III.26 sinoacutine



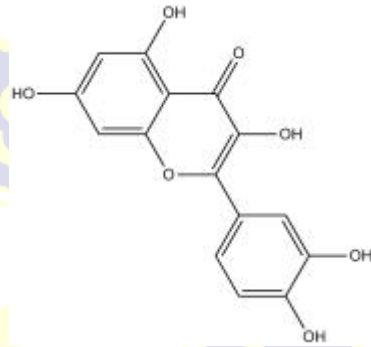
Gambar III.27 Coridaline

LAMPIRAN 9

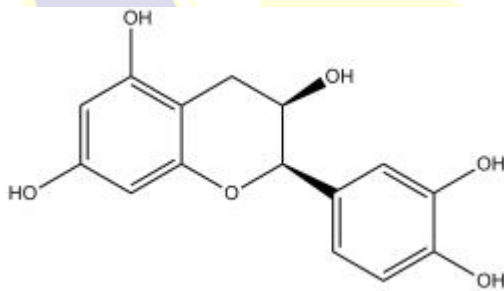
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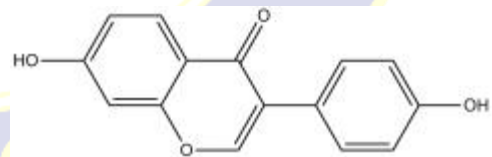
Gambar III.28 Kaempferol



Gambar III.29 quercetine



Gambar III.30 Epicatechine



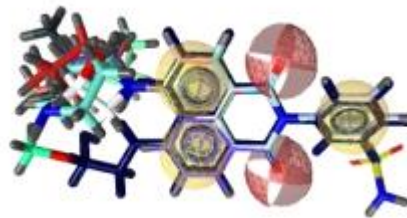
Gambar III.31 Daidzeine

LAMPIRAN 10

SKRINING FARMAKOFOR



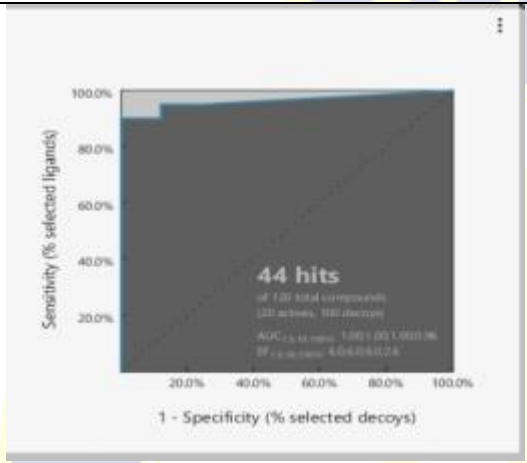
Gambar V.1 Hasil Skrining farmakofor reseptor HCV NS5B *Polymerase*



Gambar V.2 Model 1 farmakofor Ligan HCV NS5B *Polymerase*. Gambar divisualisasi menggunakan *Ligandscout*

LAMPIRAN 11

(LANJUTAN)

MODEL	AUC	HITS
	0,96	44

Tabel V.1 ROC Curve HCV NS5B polymerase

LAMPIRAN 12

(LANJUTAN)

NO	Nama senyawa	Matching Features	Fit Score
1.	Talipendine		51,29
2.	Palmatine		51,25
3.	Dehidrocoridalmine		51,24
4.	Berberine		51,15
5.	Columbamine		51,15
6.	Jatrorrhizine		51,15
7.	Quarcetine		43,12
8.	Kaempferol		35,63
9.	Ribavirin		61,53

Table V.2 Hasil Skrining Farmakofor HCV NS5B *Polymerase* Terhadap HCV NS5B *Polymerase*

Keterangan : Warna kuning = Interaksi hidrofobik

Warna merah = Akseptor ikatan hydrogen

Warna hijau = Donor ikatan hydrogen

Warna biru = Cincin aromatic

LAMPIRAN 13

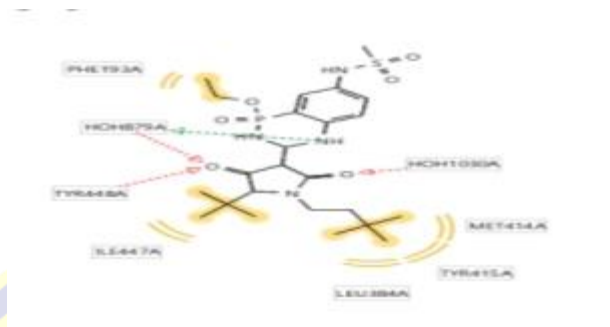
ATURAN *LIPINSKI'S RULE OF FIVE*

Senyawa Uji	Donor Ikatan Hidrogen	Akseptor Ikatan Hidrogen	Bobot Molekul	LogP	Memenuhi Syarat/Tidak
Thalifendine	0	0	322,340	3,371	Memenuhi
Tetrandrine	5	8	628,140	5,002	Tidak memenuhi
Palmatine	0	0	352,410	3,385	Memenuhi
Dehidrocoridalmine	0	0	338,383	3,082	Memenuhi
Berberine	0	3	337,375	2,215	Memenuhi
Columbamine	1	1	338,383	3,082	Memenuhi
Jatrorrhizine	1	4	338,383	3,082	Memenuhi
Quaracetine	1	4	302,238	1,988	Memenuhi
Kaempferol	3	4	286,239	2,282	Memenuhi
Cepharantine	3	7	540,620	5,826	Tidak memenuhi
Dihydroberberine	3	6	520,236	5,856	Tidak Memenuhi
Epicatechine	7	3	290,277	3,122	Memenuhi
Fangchinoline	4	5	610,343	7,062	Tidak memenuhi
Homoaromoline	2	9	540,620	5,856	Tidak memenuhi
Corydaline	5	8	612.335	5,215	Tidak memenuhi
Sinoacutine	5	9	365,221	6,032	Tidak Memenuhi
Daidzeine	1	8	254,244	1,033	Memenuhi
20-hydroxyecdysone	0	7	452,226	5,261	Tidak Memenuhi
Limacine	6	5	610,353	7,072	Tidak Memenuhi
Pycnarrhine	3	7	162.192	1,012	Memenuhi

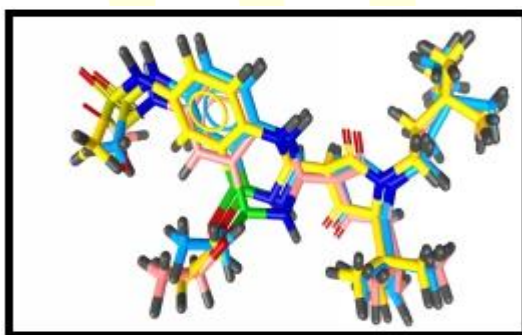
Tabel V.3 Sifat fisikokimia tumbuhan akar kayu kuning (*Arcangelisia Flava* (L) Merr) berdasarkan aturan *Lipinski's rule of five*

LAMPIRAN 14

RE-DOCKING



Gambar V.3. Interaksi *methanesulfonamide* dengan residu-residu asam amino pada sisi aktif enzim HCV NS5B *Polymerase*



Gambar V.4 *Overlay* reseptor HCV NS5B *Polymerase*



Gambar V.5 Interaksi HCV NS5B *Polymerase* dengan *Metaneusulfonamide* (Kode: 4EAW) dan model farmakofornya. Gambar divisualisasi menggunakan *Ligandscout*

LAMPIRAN 15

VALIDASI METODE

Senyawa	ΔG (kcal/mol)	RESIDU ASAM AMINO	RMSD (Å)	Ki(nM)
Ligan Alami Methanesulfonamide	-21,60	Tyr448A Phe193A Ile447A Met414A Leu384A Tyr415A	1,81	0,144
Ligan Pembanding Ribavirin	-18,34	Ser368A Tyr415A Tyr316A Tyr448A	1,83	0,035

Tabel V.4 Hasil Validasi *Re-docking* Ligan Alami, RSMD, Nilai ikatan Energi residu asam amino dan ribavirin

LAMPIRAN 16

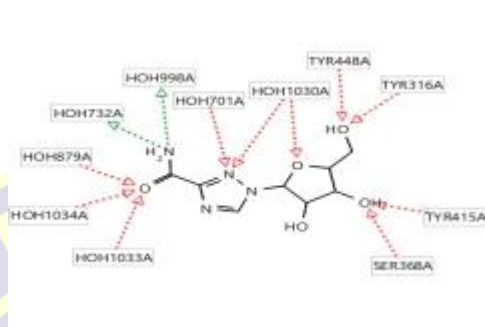
SIMULASI DOCKING

NO	SENYAWA	ΔG (kcal/mol)	RESIDU ASAM AMINO	Ki (nM)
1.	Thalipendine	-18,80	Phe193A	0,0163
2.	Palmatine	-19,40	Tyr415A,Ser368A Tyr316A, Phe193A	0,0059
3.	Dehidrocorydalmine	-19,90	Asn411A,Gly410A, Ser556A, Ile447A	0,0040
4.	Berberine	-15,90	Met414A, Tyr415A	2,18
5.	Columbamine	-17,00	Asp318A,Tyr448A, Met414A	0,340
6.	Jatrorrhizine	-16,50	Ser556A,Tyr448A,Met414A	0,792
7.	Quarcetine	-19,40	Asp319A,Tyr316A, Phe193A	0,0059
8.	Kaempferol	-18,70	Tyr316A, Tyr448A, Met414A	0,0193

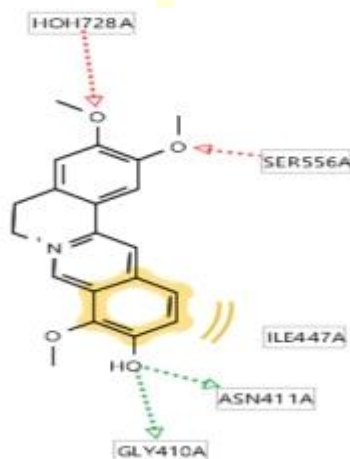
Table V.5 Hasil Simulasi *Docking*

LAMPIRAN 17

PENAMBATAN MOLEKUL



Gambar V.6 Interaksi obat standar Ribavirin dengan HCV NS5B *Polymerase* (kode :4EAW). Gambar divisualisasi menggunakan *Ligandscout*



Gambar V.7 Interaksi senyawa *dehydrocorydalmine* dengan reseptor HCV NS5B *Polymerase* (kode: 4EAW) Gambar divisualisasi menggunakan *Ligandscout*

