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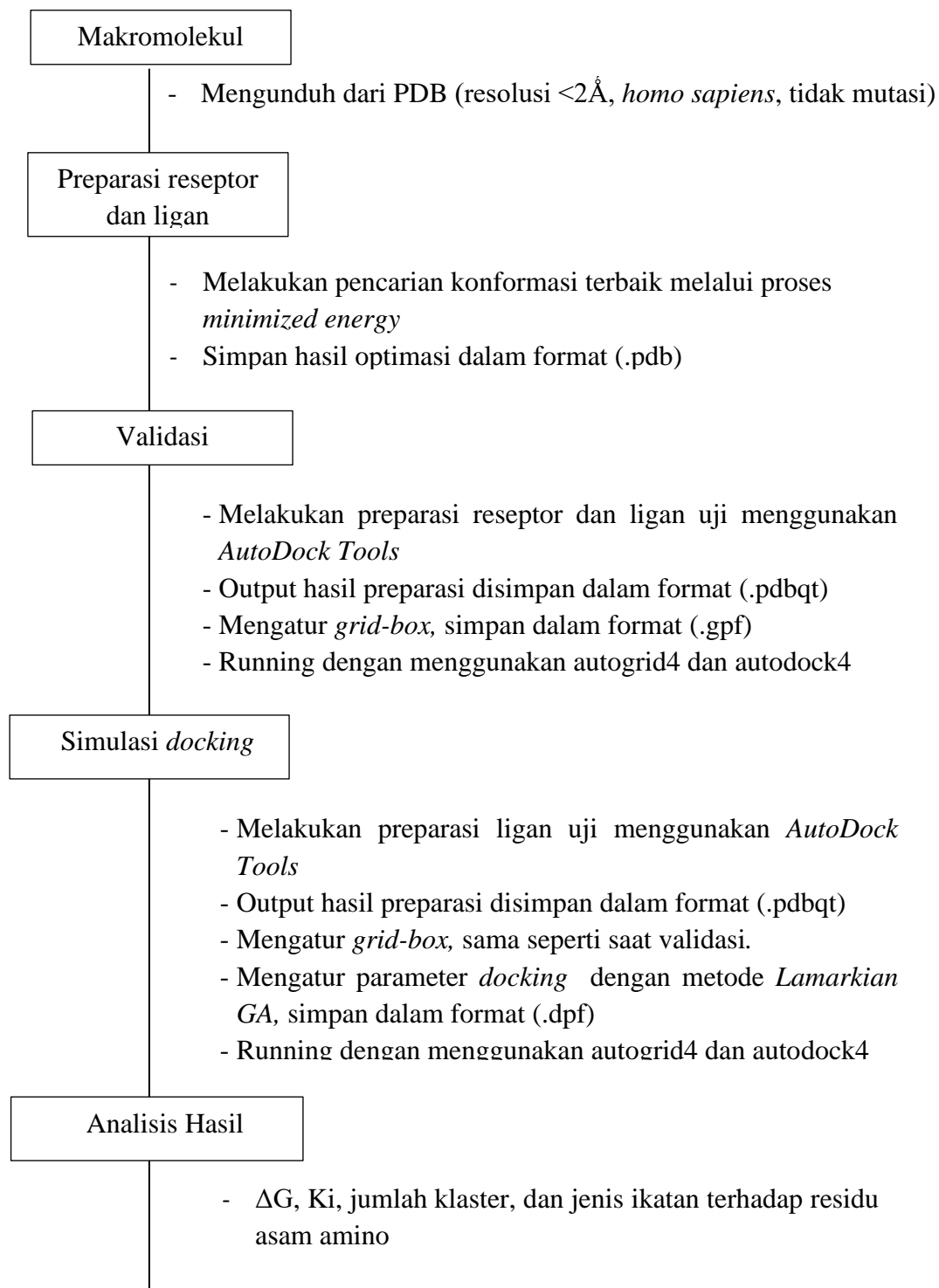
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LAMPIRAN 1

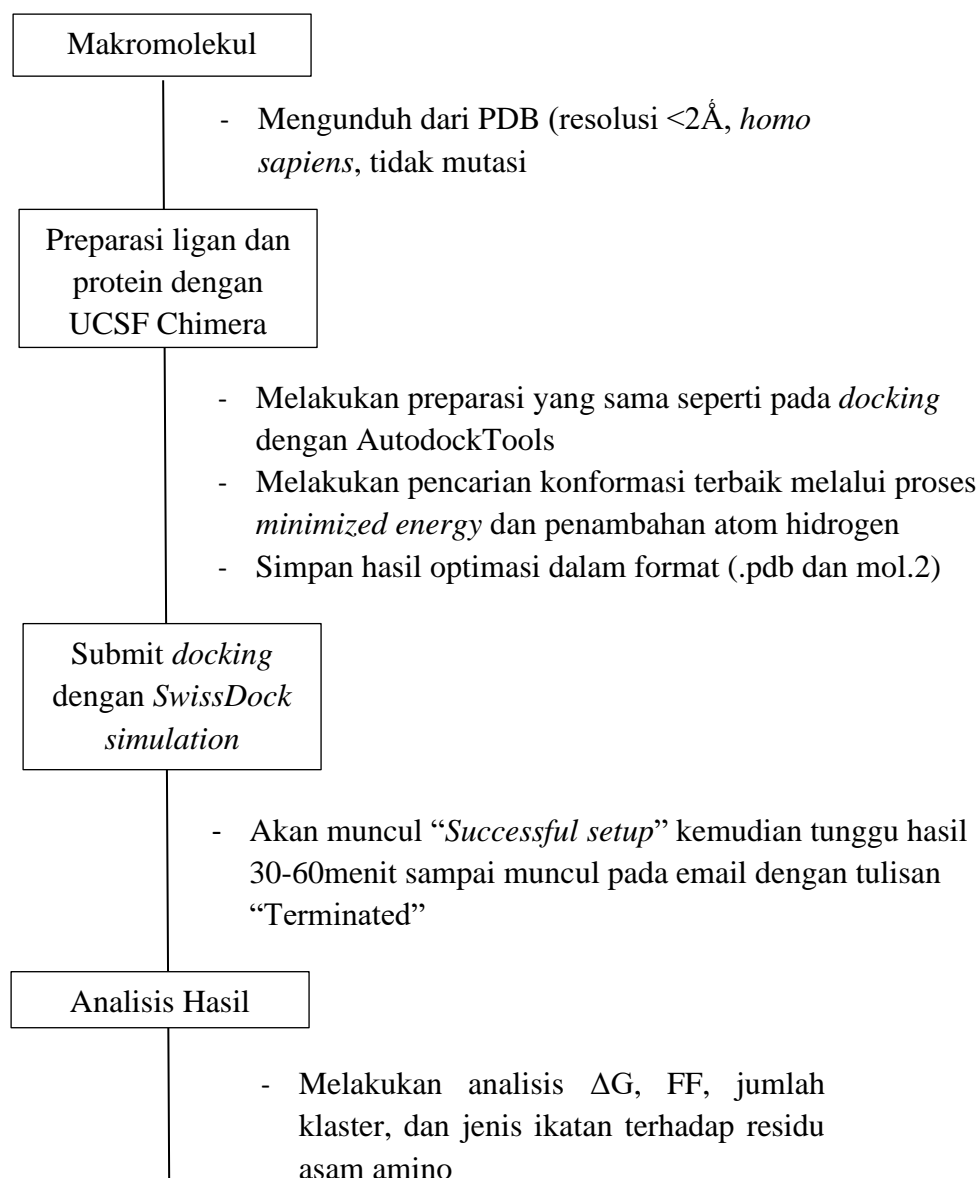
Skema kerja *Molecular Docking* dengan *AutodockTools* pada senyawa uji dengan protein *FAB-Antibody*



Gambar 1.1 Skema alur penelitian *Molecular Docking* Senyawa uji terhadap Protein *FAB-Antibody*

LAMPIRAN 2

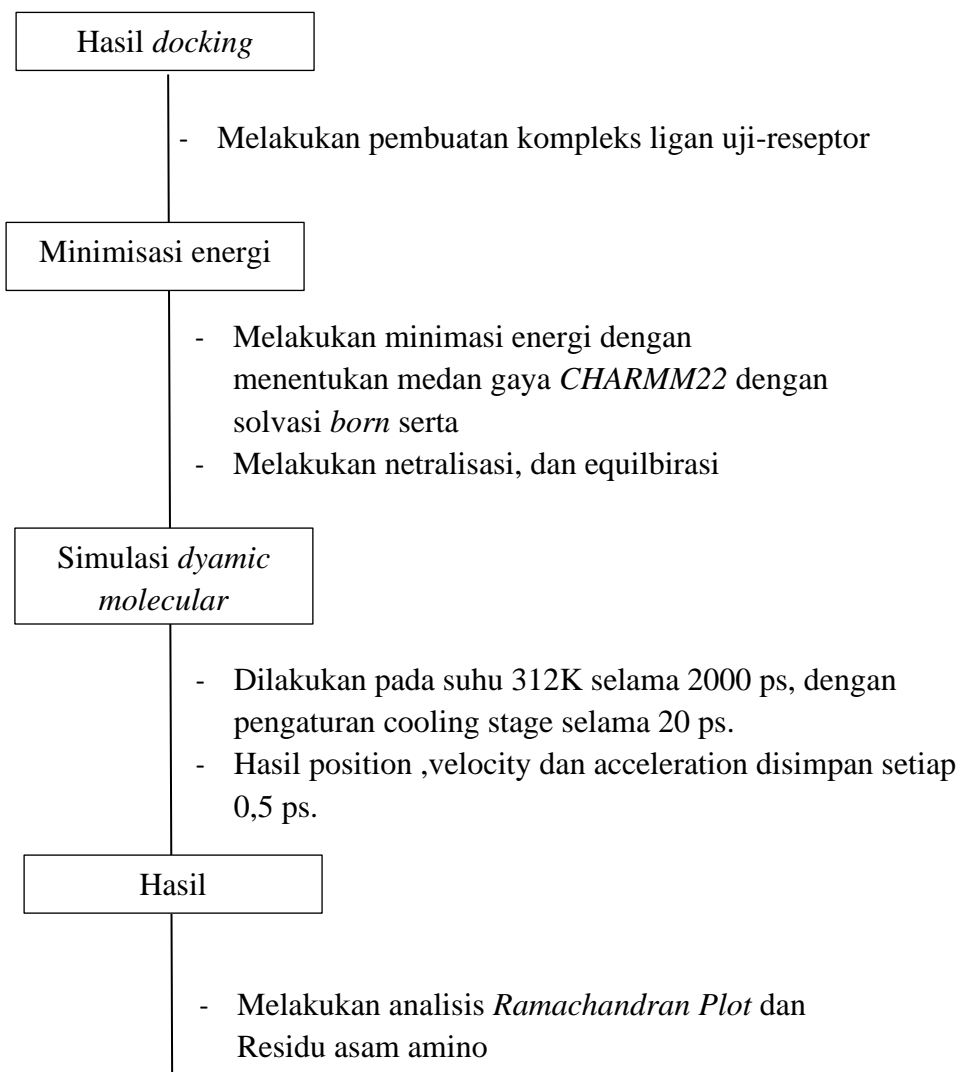
Skema kerja *Molecular Docking* dengan *SwissDock* pada Senyawa uji dengan reseptor protein *FAB- Antibody*



Gambar 2.1 Skema alur penelitian *Molecular Docking* dengan *SwissDock* pada senyawa uji dengan reseptor secara online

LAMPIRAN 3

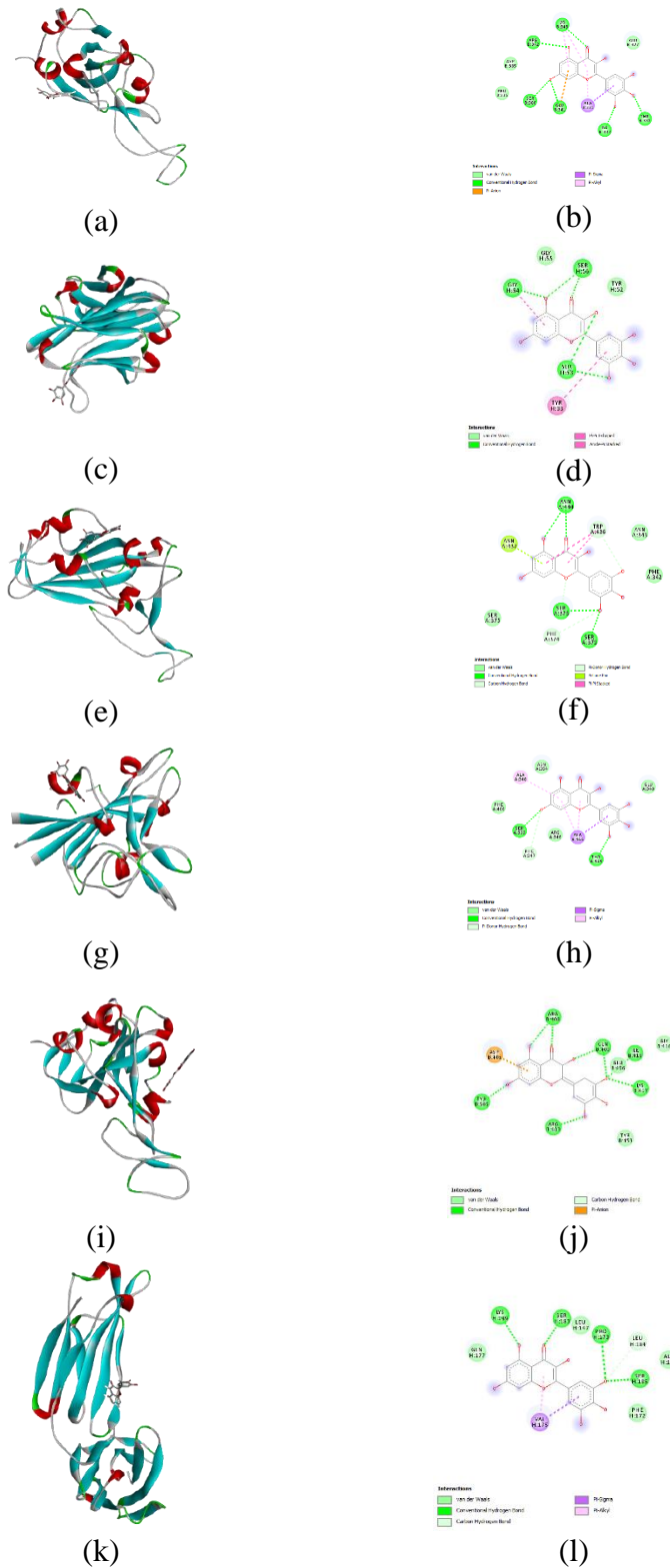
Skema alur penelitian *molecular dynamics* dari hasil *docking* sebelumnya menggunakan *molecular operating environment* (MOE)



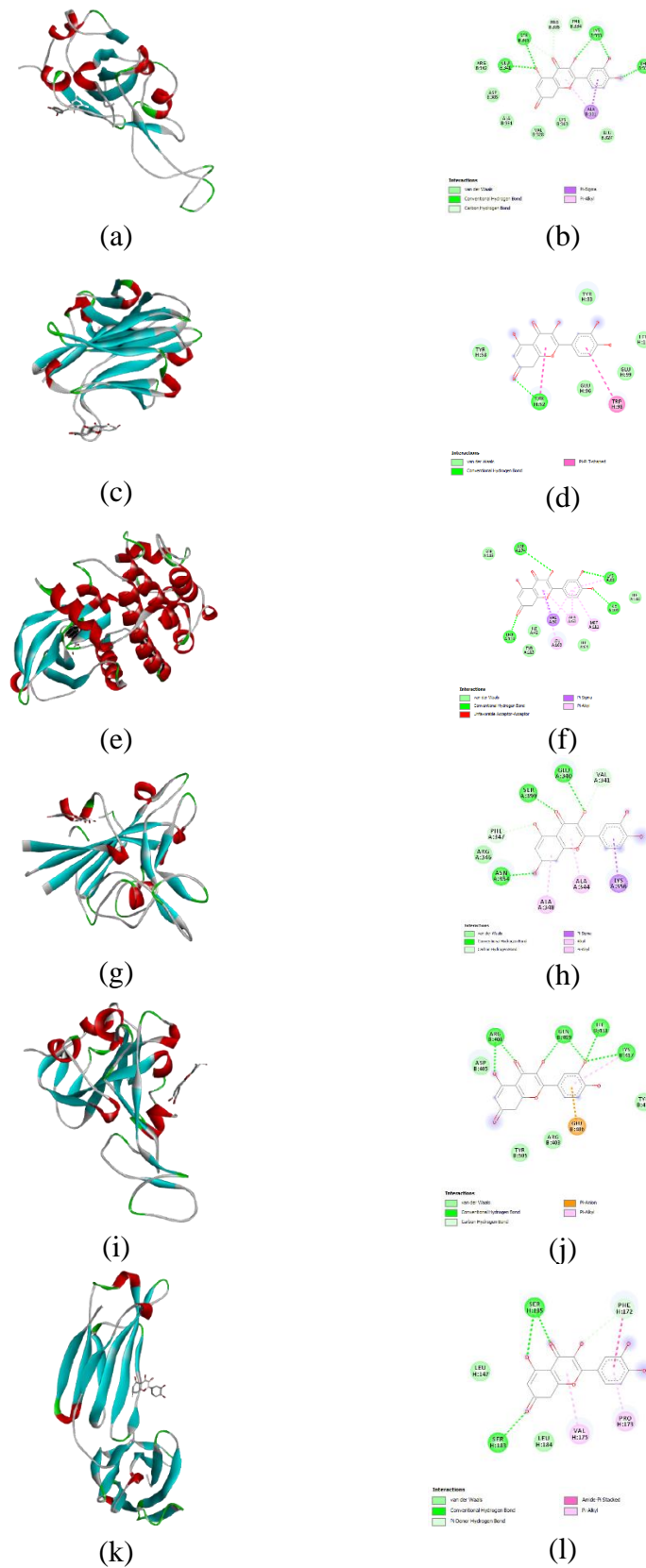
Gambar 3.1 Skema alur penelitian *molecular dynamics* dari hasil *docking* senyawa uji dengan protein *FAB- Antibody*

LAMPIRAN 4

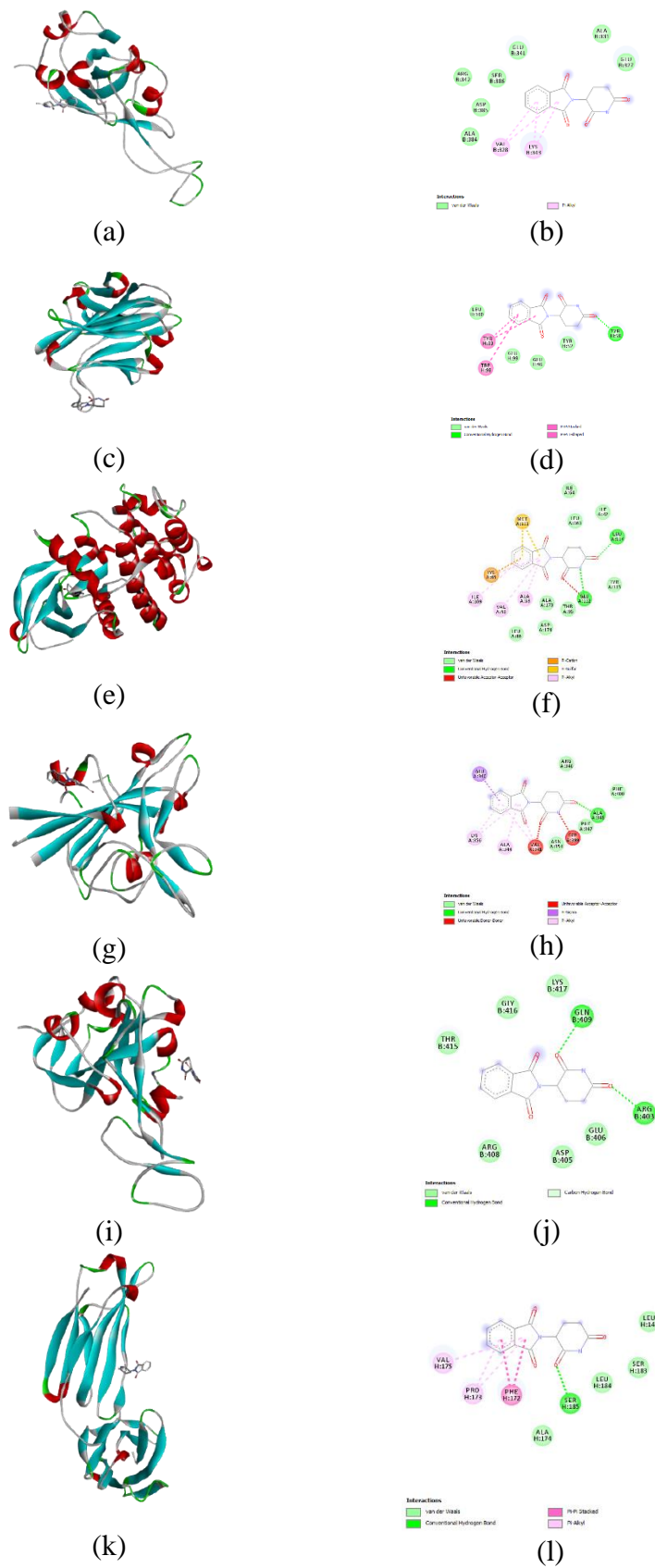
Hasil Visualisasi 3D & 2D *Molecular Docking* dengan *AutodockTools* pada senyawa uji mirisetin, mirisetin dan senyawa pembeding thalidomid



Gambar 4.1 Visualisasi 3D interaksi senyawa uji mirisetin dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 2D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA



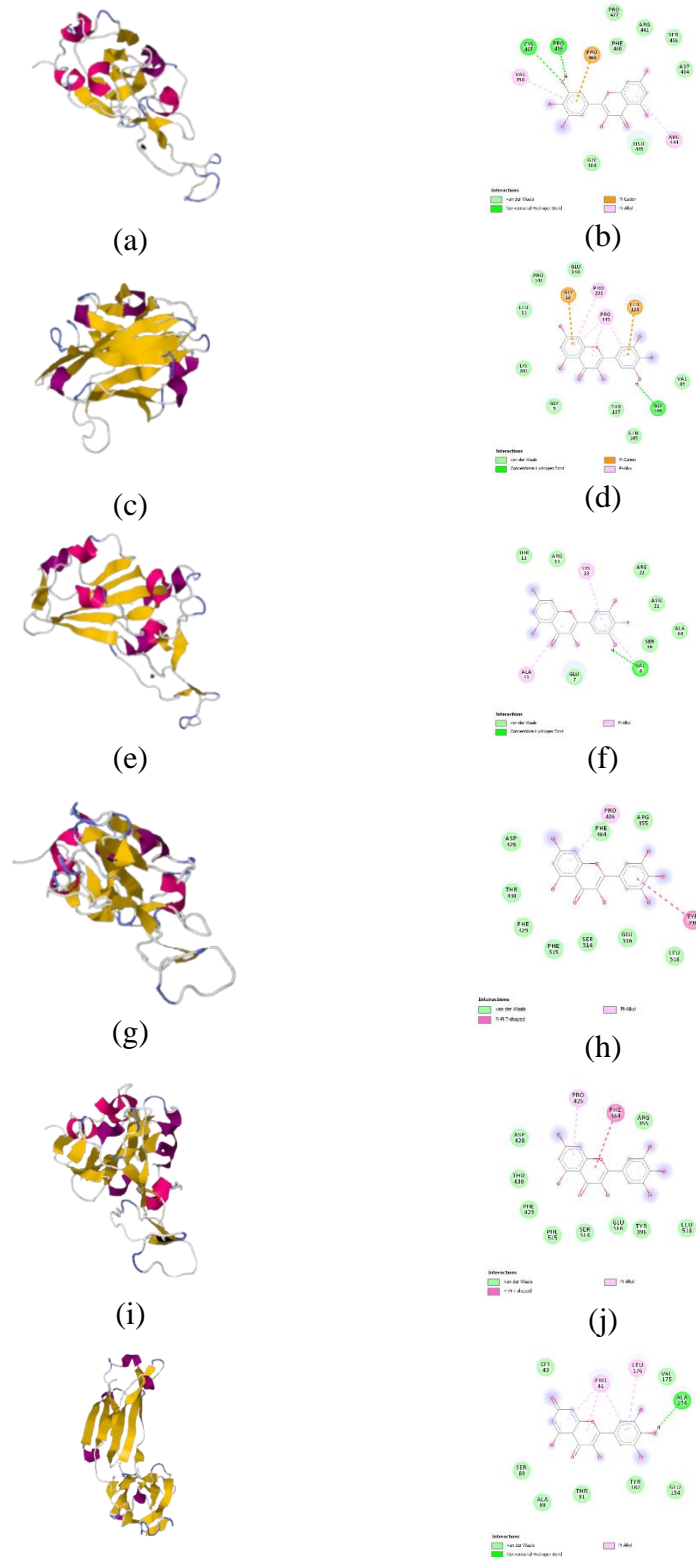
Gambar 4.2 Visualisasi 3D interaksi senyawa uji kuersetin dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 2D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA



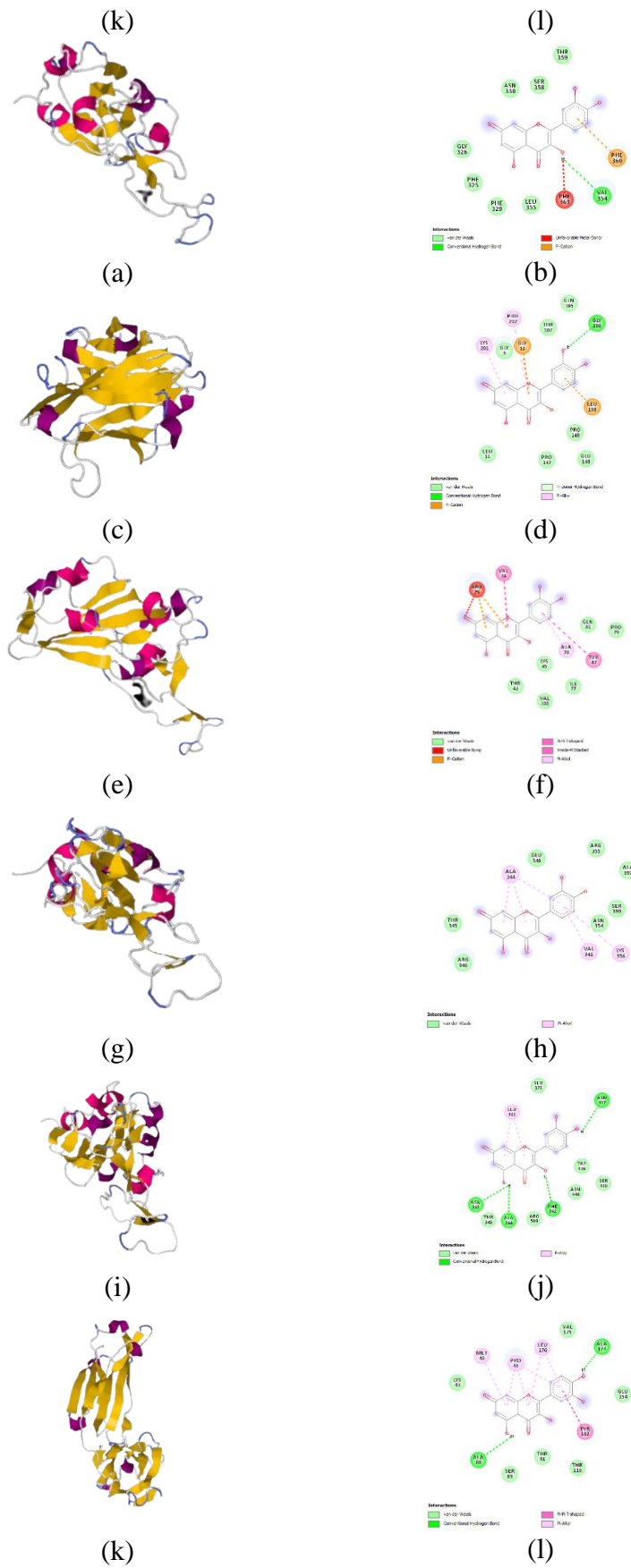
Gambar 4.3 Visualisasi 3D interaksi senyawa pembanding thalidomid dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 2D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA

LAMPIRAN 5

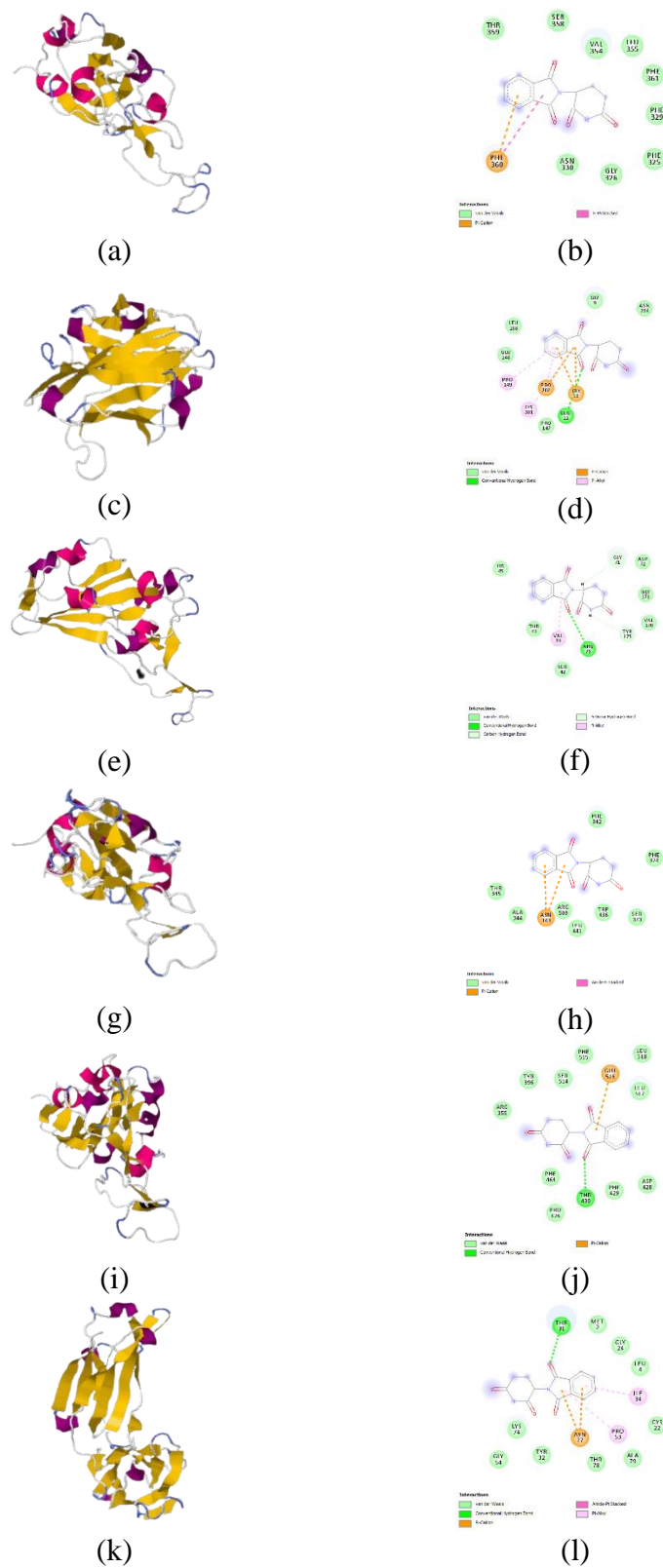
Hasil Visualisasi 3D & 2D *Molecular Docking* dengan *SwissDock* pada senyawa uji mirisetin, mirisetin dan senyawa pembanding thalidomid



Gambar 5.1 Visualisasi 3D interaksi senyawa uji mirisetin dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 2D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA



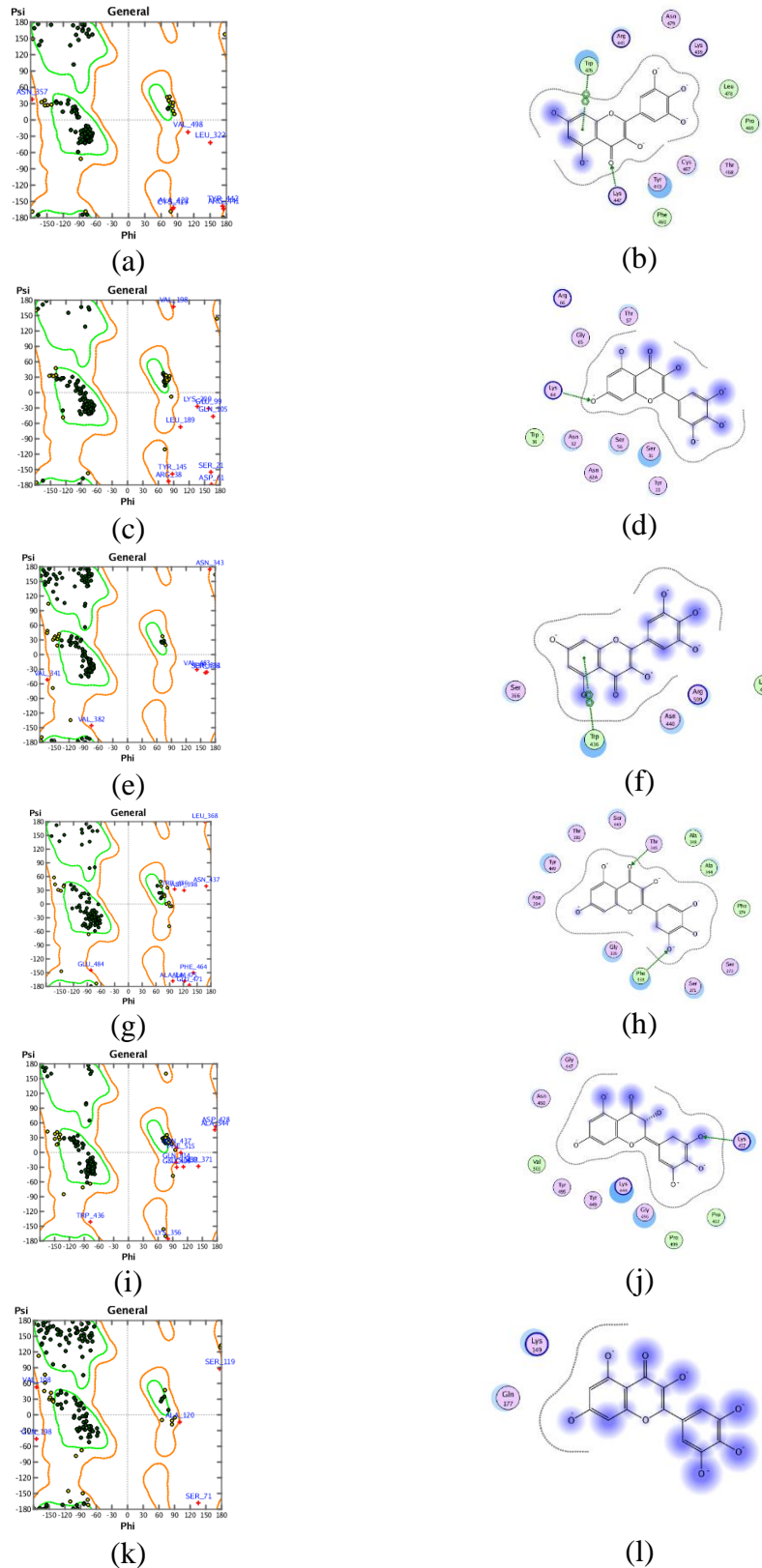
Gambar 5.2 Visualisasi 3D interaksi senyawa uji kuersetin dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 2D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA



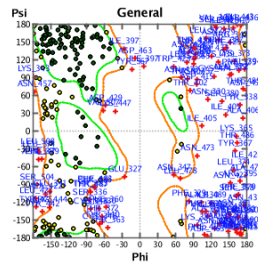
Gambar 5.3 Visualisasi 3D interaksi senyawa pembanding dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 2D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA

LAMPIRAN 6

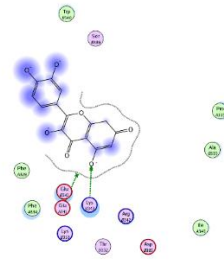
Hasil *Molecular Dynamic* dengan *Molecular Operating Environment* (MOE)



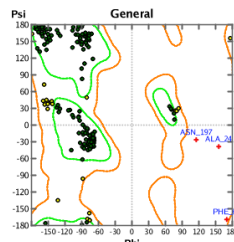
Gambar 6.1 Hasil Ramachandran Plot senyawa mirisetin dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 3D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA



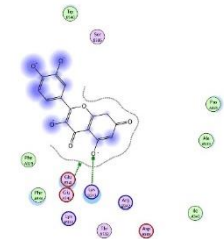
(a)



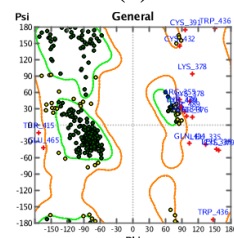
(b)



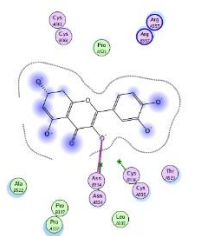
(c)



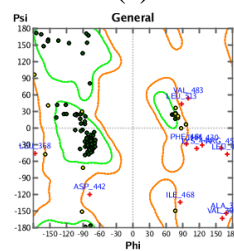
(d)



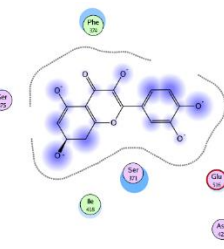
(e)



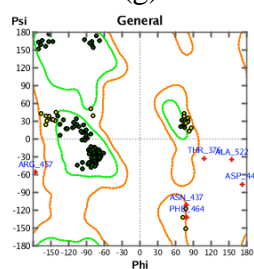
(f)



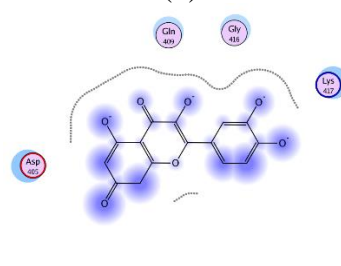
(g)



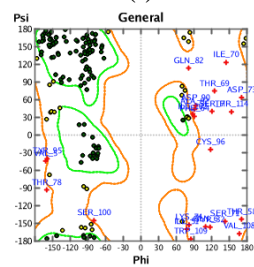
(h)



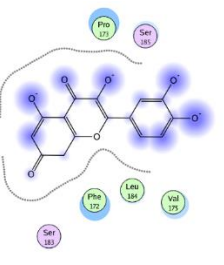
(i)



(j)

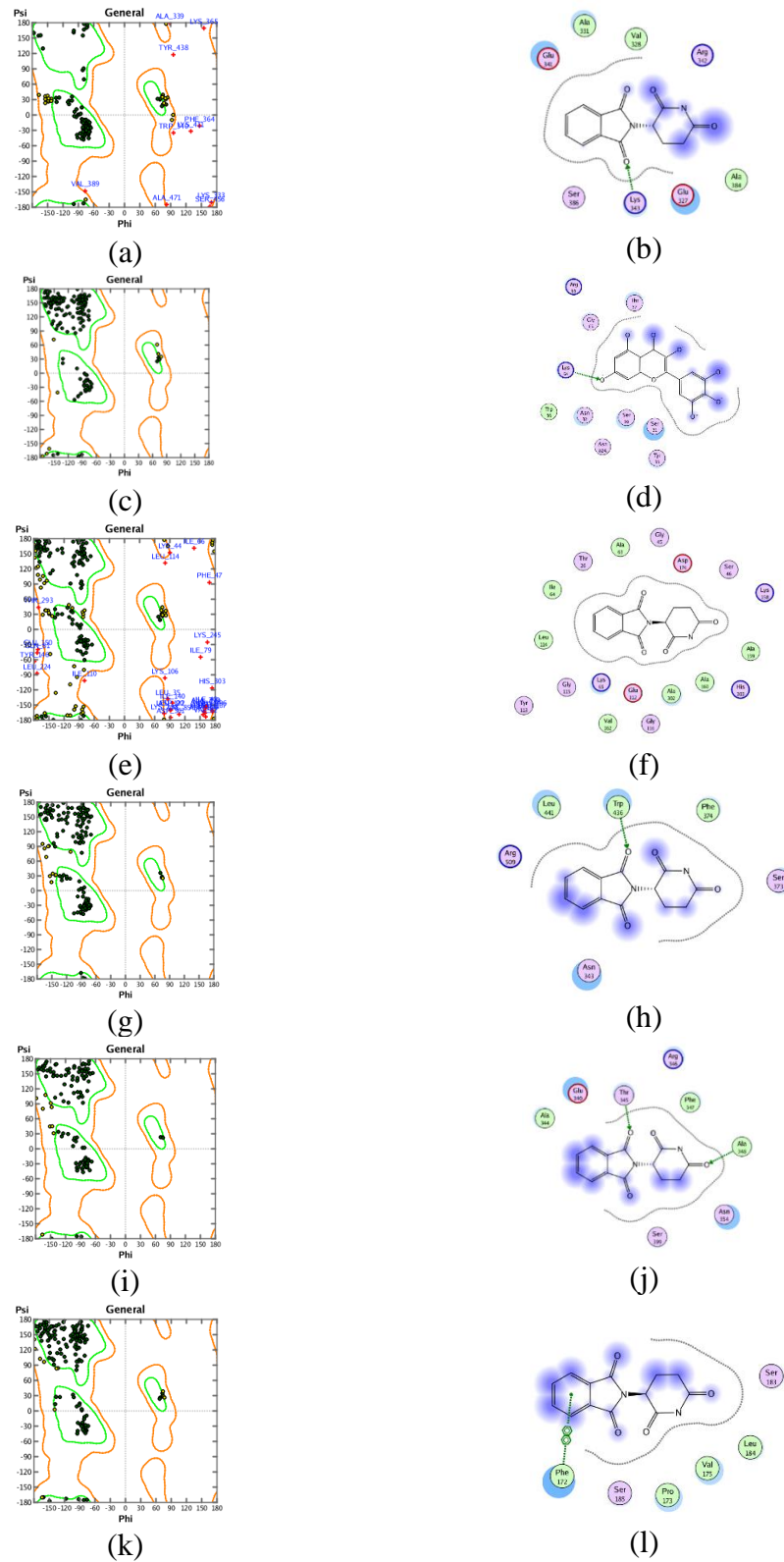


(k)



(l)

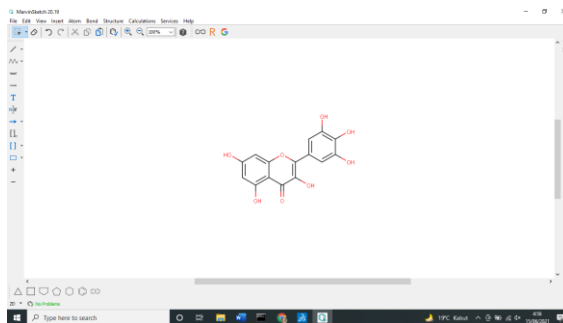
Gambar 6.2 Hasil Ramachandran Plot senyawa kuersetin dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 3D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA



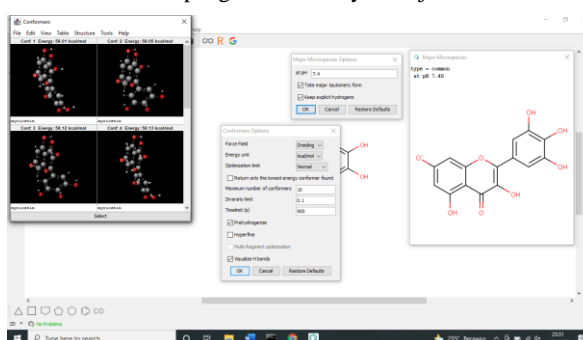
Gambar 6.3 Hasil Ramachandran Plot senyawa pembanding (thalidomid) dengan protein (a) 6WAQ (c) 6XCA (e) 7B30 (g) 7JMP (i) 7KN5 (k) 7KZA dan Visualisasi 3D interaksi senyawa dengan protein (b) 6WAQ (d) 6XCA (f) 7B30 (h) 7JMP (j) 7KN5 (l) 7KZA

LAMPIRAN 7

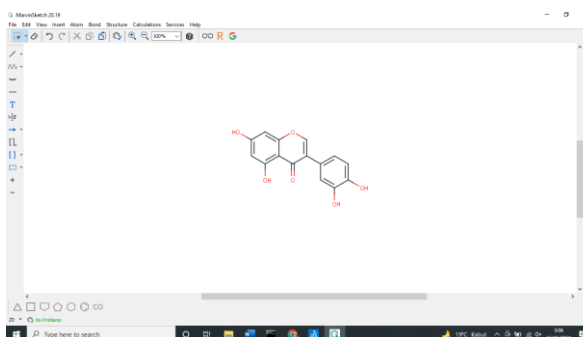
Proses Optimasi senyawa uji dengan *Marvinsketch* 20.19



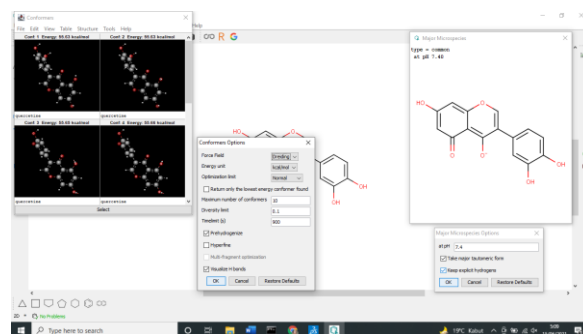
7.1 Proses penggambaran senyawa uji miresetin



7.2 Proses optimasi dengan menentukan nilai energi terkecil pada senyawa uji miresetin dengan *marvinsketch*



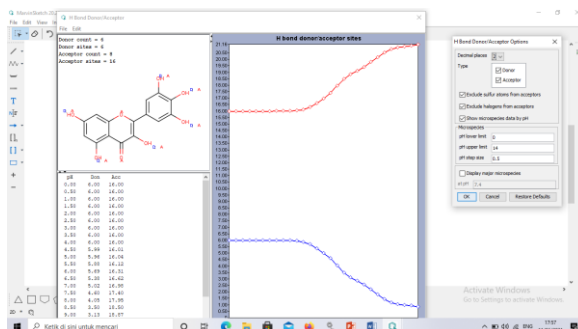
7.3 Proses penggambaran senyawa uji kuersetin



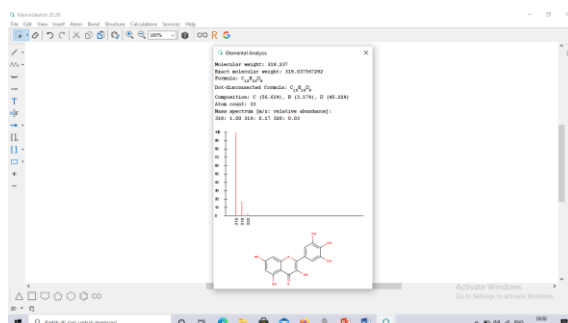
7.4 Proses optimasi dengan menentukan nilai energi terkecil pada senyawa uji kuersetin dengan *marvinsketch*

LAMPIRAN 8

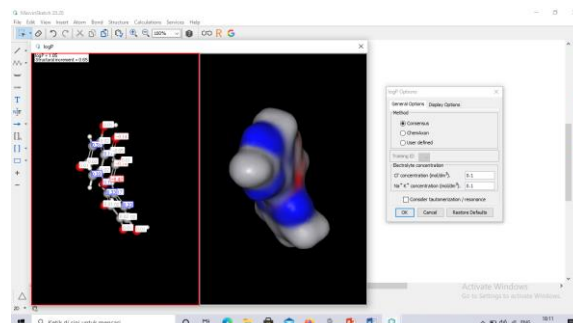
Pengujian *DrugScan*, PreADME dan Toksisitas pada senyawa uji kuersetin dan mirisetin



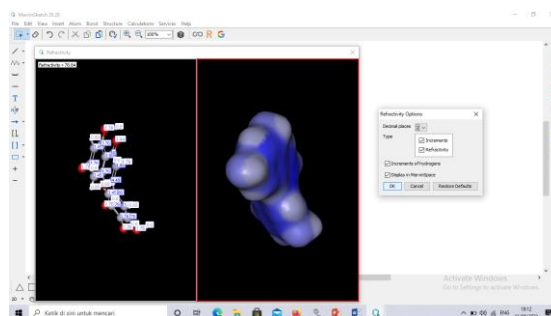
8.1 Proses *drugscan* pada *marvinsketch* untuk mengetahui absorpsi dilihat dari HBA dan HBD



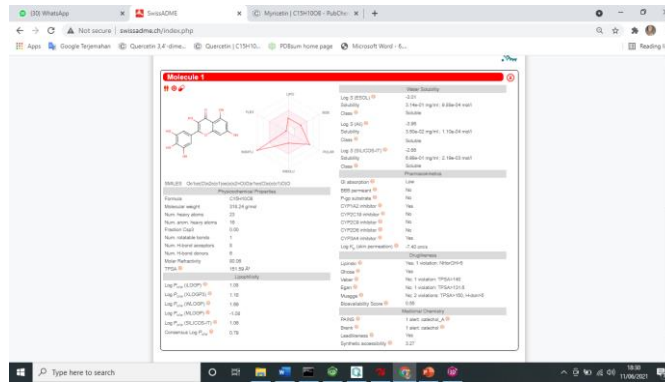
8.2 Proses *drugscan* pada *marvinsketch* untuk mengetahui nilai berat molekul pada senyawa uji



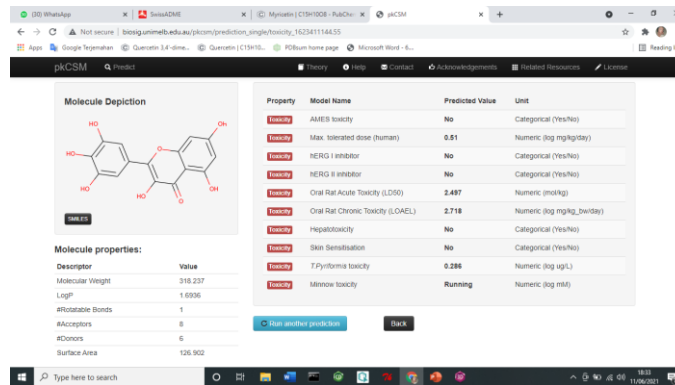
8.3 Proses *drugscan* pada *marvinsketch* untuk mengetahui lipofilitas dari suatu senyawa uji dilihat dari nilai Log P



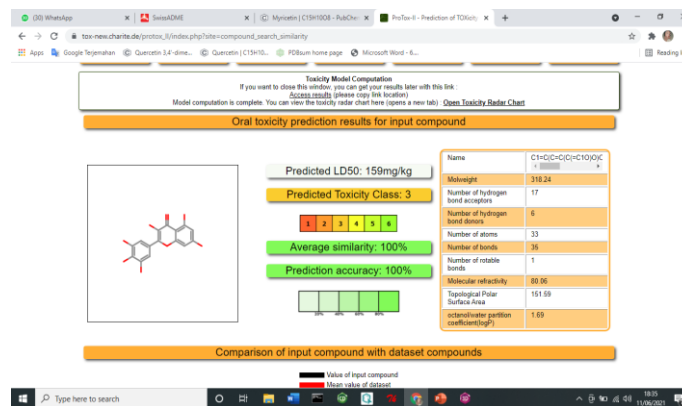
8.4 Proses *drugscan* pada *marvinsketch* untuk mengetahui kepolaran suatu senyawa uji dilihat dari nilai *Refractivity molar*



8.5 Pengujian ADME pada webservice SwissADME



8.6 Pengujian Toksitas pada webservice pkCSM tools



8.7 Pengujian toksitas pada webservice ProTox II online

ADME – PreADMET | Prediction of ADME/Tox

ID	Value
BBB	1.49973
Buffer_solubility_mg_L	5803.83
Caco2	22.2815
CYP_2C19_inhibition	Inhibitor
CYP_2C9_inhibition	Inhibitor
CYP_2D6_inhibition	Non
CYP_2D6_substrate	Non
CYP_3A4_inhibition	Inhibitor
CYP_3A4_substrate	Non
HIA	100.000000
MDCK	204.401
Pgp_inhibition	Non
Plasma_Protein_Binding	-1.#IND00
Pure_water_solubility_mg_L	3921.34
Skin_Permeability	-1.86648
SKlogD_value	0.965160
SKlogP_value	0.965160
SKlogS_buffer	-0.441560
SKlogS_pure	-0.611840

8.8 Pengujian ADME pada webservice PreADMET

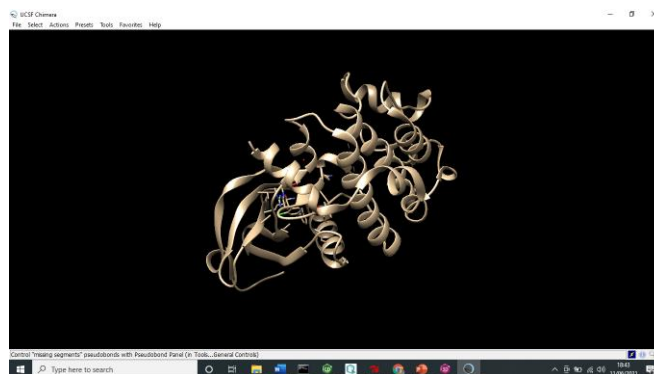
LAMPIRAN 9

Proses Preparasi Protein FAB – Antibody dengan software Chimera 1.15 dan PyRx 8.0

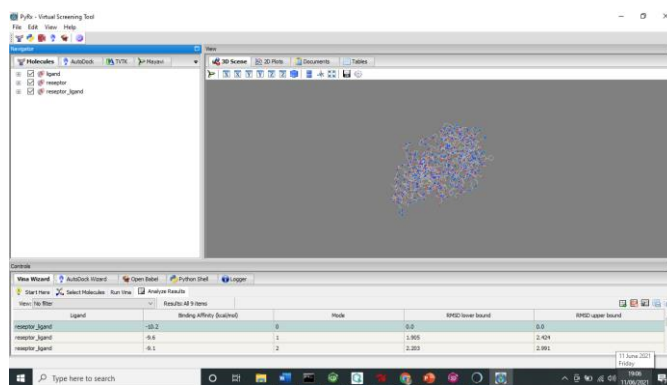


9.1 Pengunduhan protein Fab – Antibody pada website PDB (protein data bank)

<http://www.rcsb.org/pdb/home/home.do>.



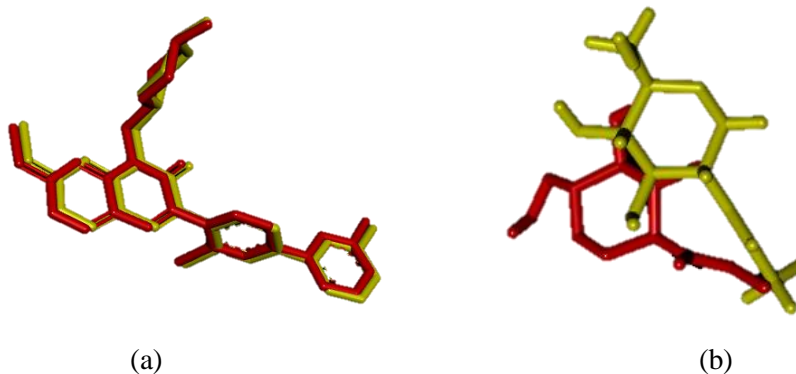
9.2 Pemisahan native ligan pada software Chimera 1.15



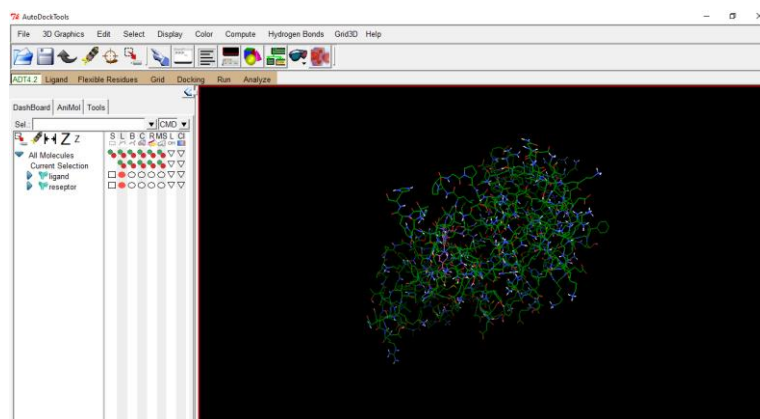
9.3 Protein dan ligan disiapkan dengan menggunakan konversi Autodock dan open babel didalam PyRx 8.0

LAMPIRAN 10

Proses Validasi *Molecular Docking*



Gambar 10.1 Hasil Visualisasi Tumpang Tindih Konformasi Struktur 7B30 (merah) dan Hasil simulasi *molecular docking* (kuning)



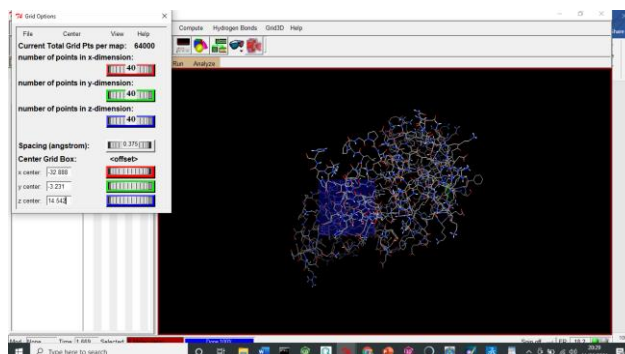
Gambar 10.2 Melakukan validasi *docking* pada *AutodockTools*

Rank	Sub-Rank	Run	Binding Energy	Cluster	Reference RMSD
1	1	18	-14.39	0.00	0.57
RANKING	2	91	-14.39	0.10	0.57
RANKING	3	14	-14.38	0.09	0.55
RANKING	4	16	-14.38	0.10	0.55
RANKING	5	83	-14.38	0.11	0.55
RANKING	6	22	-14.37	0.13	0.57
RANKING	7	32	-14.37	0.14	0.55
RANKING	8	7	-14.36	0.09	0.53
RANKING	9	68	-14.36	0.14	0.58
RANKING	10	84	-14.36	0.16	0.60
RANKING	11	64	-14.35	0.16	0.58
RANKING	12	20	-14.35	0.14	0.58
RANKING	13	66	-14.35	0.16	0.60

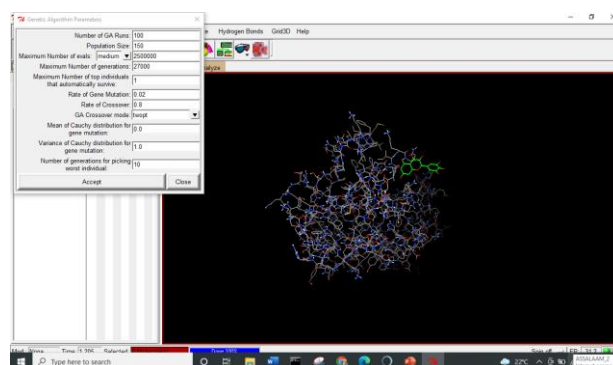
Gambar 10.3 Hasil validasi *molecular docking* pada software *AutodockTools* dengan hasil RMSD ≤ 2

LAMPIRAN 11

Proses *Molecular Docking* dengan software *AutodockTools* dan *SwissADME*



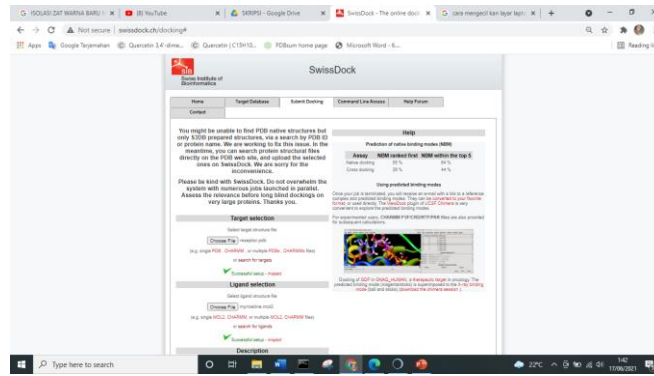
Gambar 11.1 Proses Pengaturan GridBox pada tahap proses simulasi *docking* pada *AutodockTools*



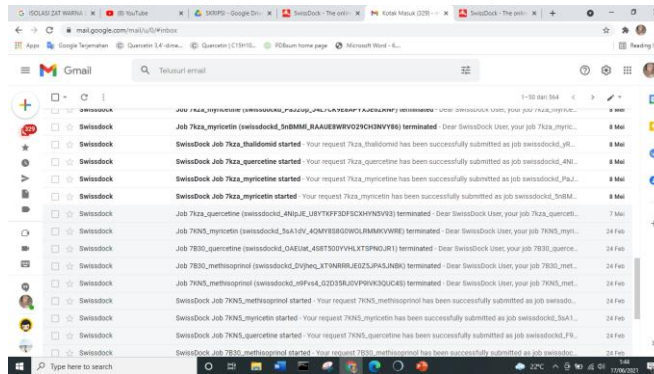
Gambar 11.2 Proses Pengaturan Running sebanyak 100x pada tahap proses simulasi *docking* pada *AutodockTools*

Rank	Sub-Group	Run	Binding Energy	Cluster	Reference
1		1	-7.55	0.00	29.04
1	RANKING	2	-7.55	0.00	29.03
1		3	-7.55	0.01	29.04
1	RANKING	4	-7.55	0.00	29.04
1		5	-7.55	0.02	29.04
1	RANKING	6	-7.55	0.00	29.04
1		7	-7.55	0.01	29.04
1	RANKING	8	-7.55	0.03	29.04
1		9	-7.55	0.01	29.04
1	RANKING	10	-7.55	0.01	29.03
1		11	-7.55	0.02	29.03
1	RANKING	12	-7.55	0.02	29.03

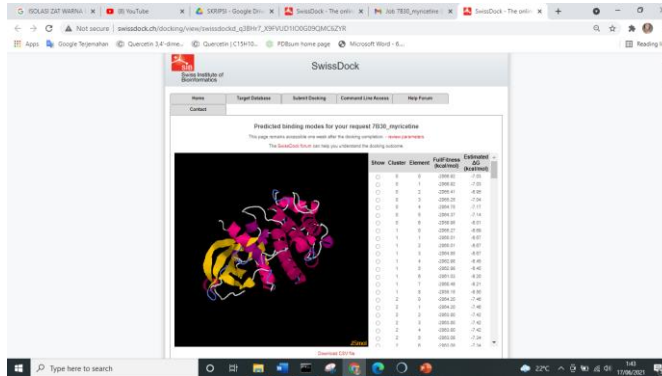
Gambar 11.3 Hasil Simulasi Docking dengan *AutodockTools* untuk melihat binding energy dan run terstabil



Gambar 11.4 menganalisis semua file input sebelum simulasi docking pada webservice *swissdock*



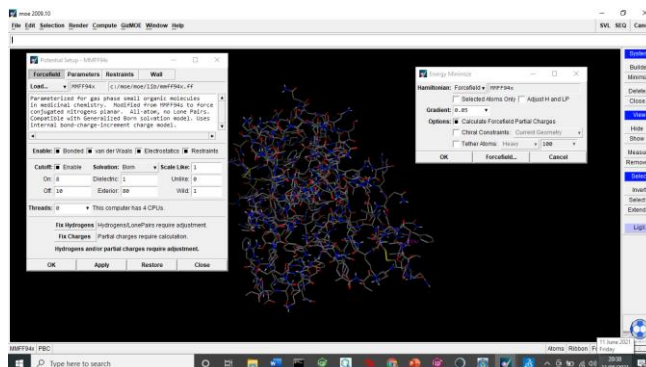
Gambar 11.5 Server *SwissDock* mengirimkan email dengan tautan untuk mengunduh hasil



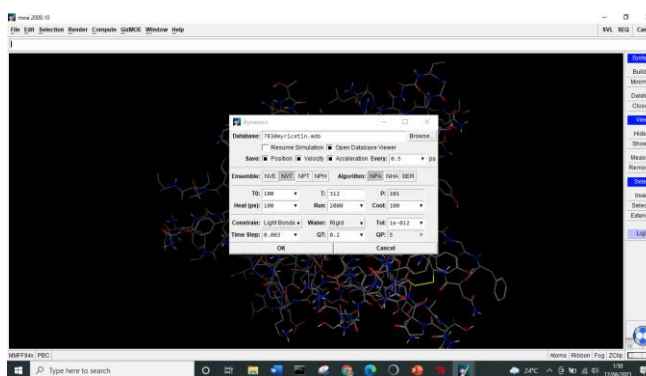
Gambar 11.6 Menunjukkan tabel interaktif dengan afinitas pengikatan yang dihitung untuk setiap pose

LAMPIRAN 12

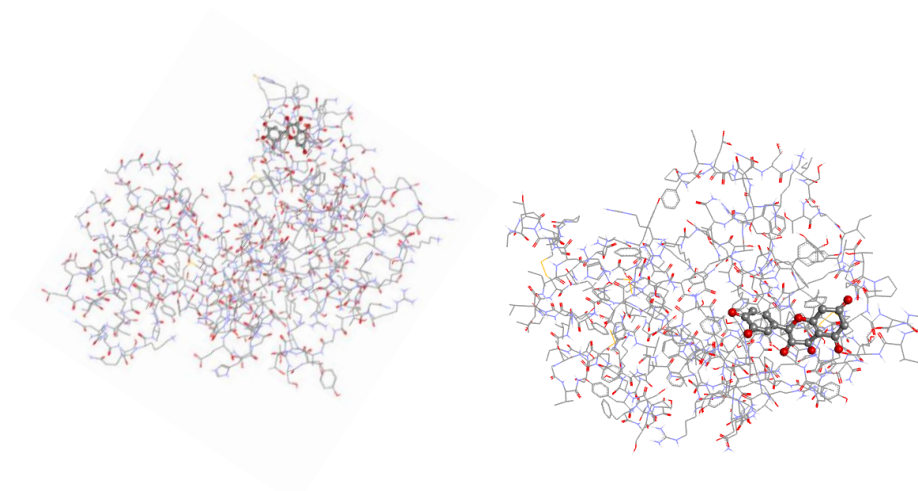
Proses *Molecular Dynamic* pada software *Molecular Operating Environment* (MOE)



Gambar 12.1 Penambahan solvasi *born* pada proses minimisasi energi



Gambar 12.2 Pengaturan simulasi molecular dinamik pada MOE 2009.10



(a)

(b)

Gambar 12.3 Visualisasi komponen protein sebelum (a) dan sesudah (b) *molecular dynamic* pada senyawa uji Kuersetin