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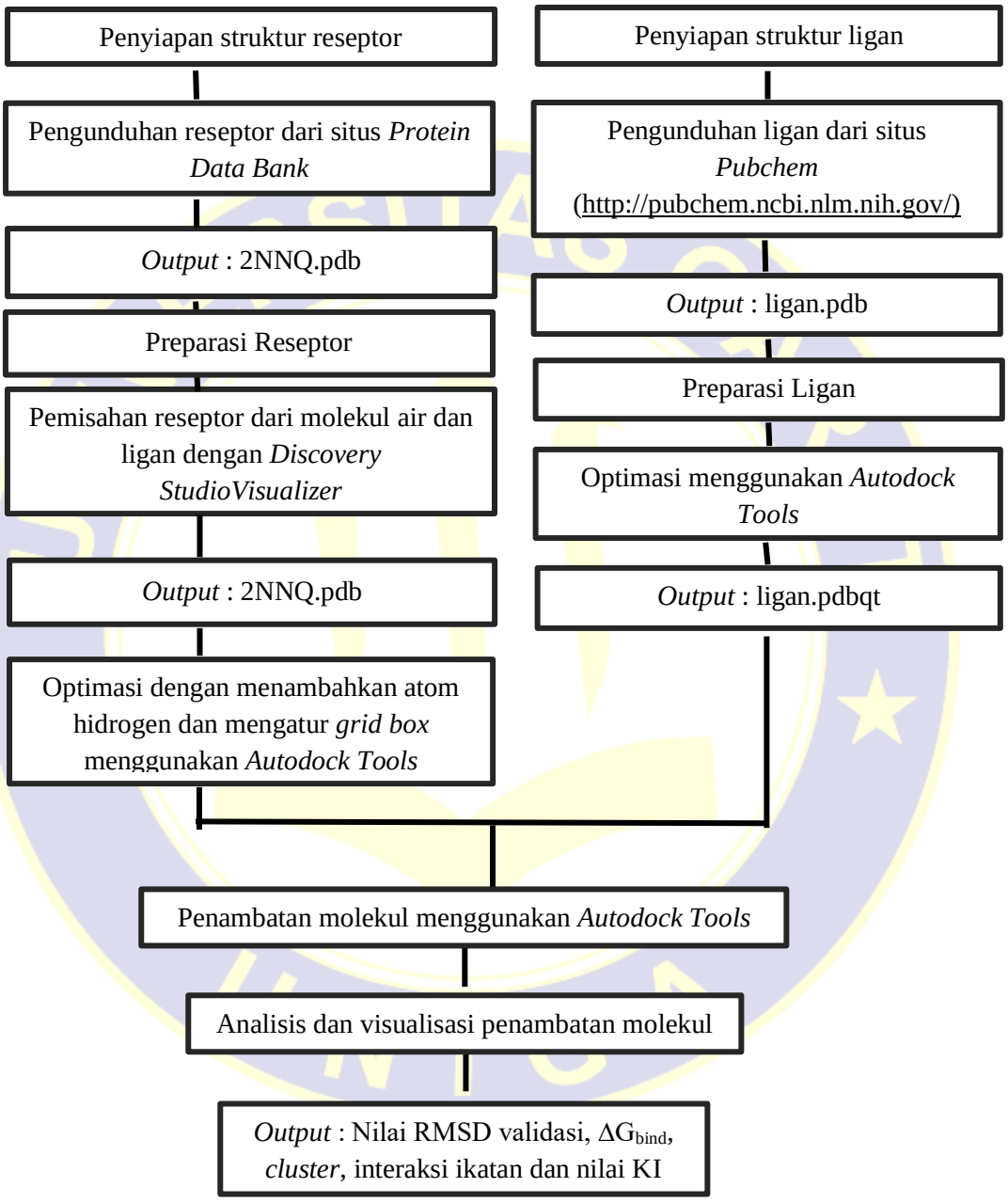
LAMPIRAN 1

SKEMA ALUR PENELITIAN PENAMBATAN MOLEKUL

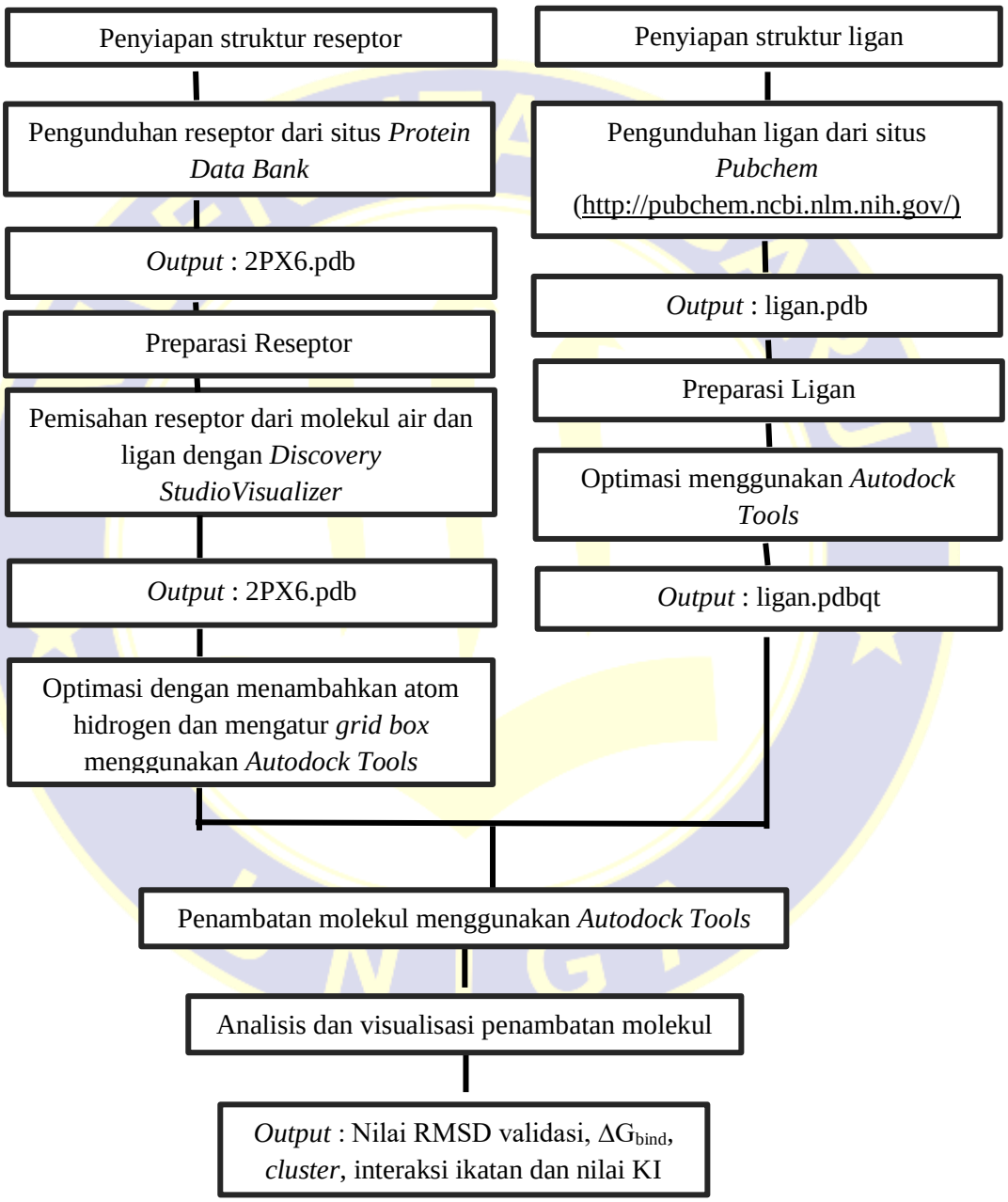


Gambar I.6 Skema alur penelitian penambatan molekul dari reseptor aFABP

LAMPIRAN 1

(LANJUTAN)

SKEMA ALUR PENELITIAN PENAMBATAN MOLEKUL

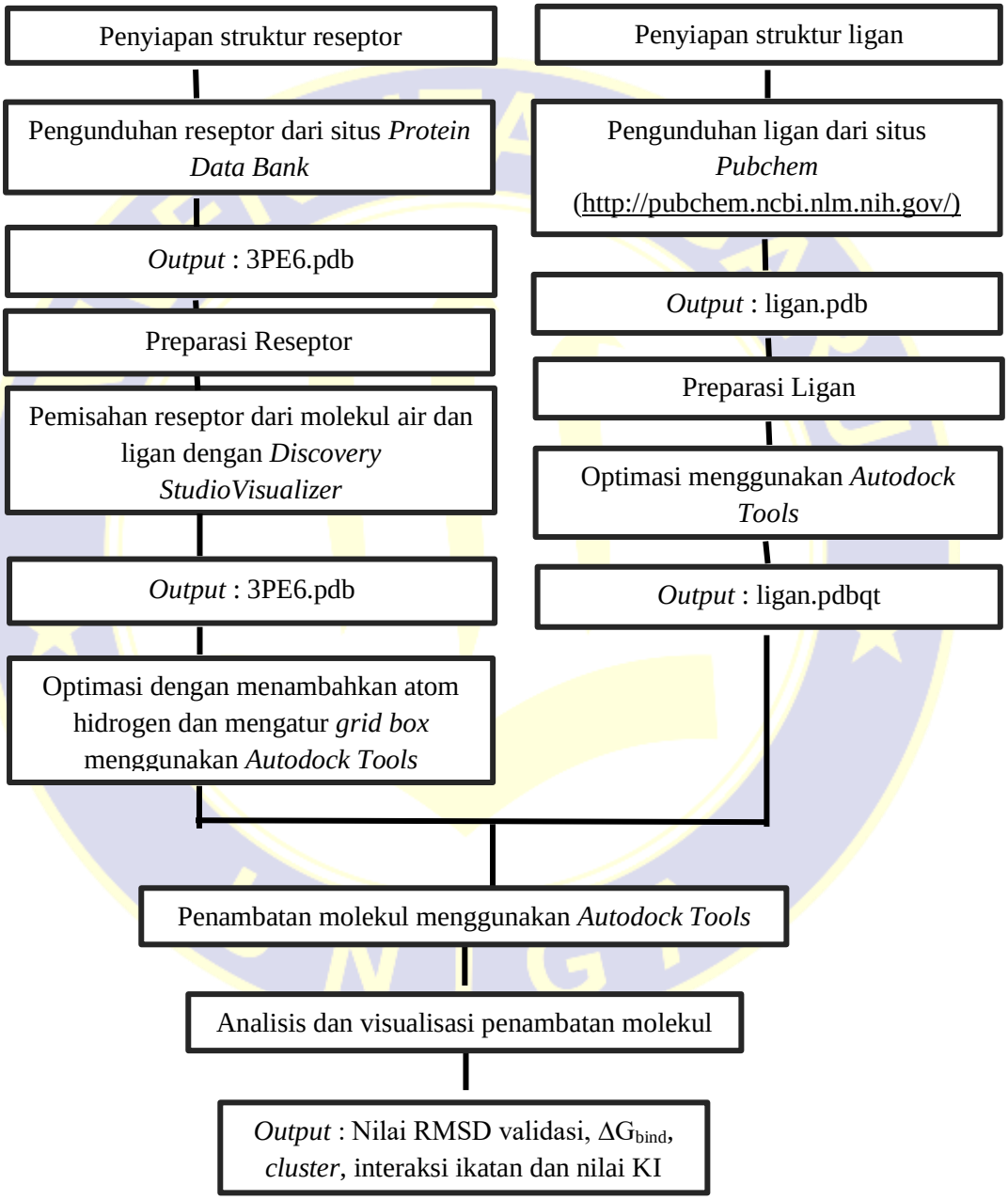


Gambar I.6 Lanjutan

LAMPIRAN 1

(LANJUTAN)

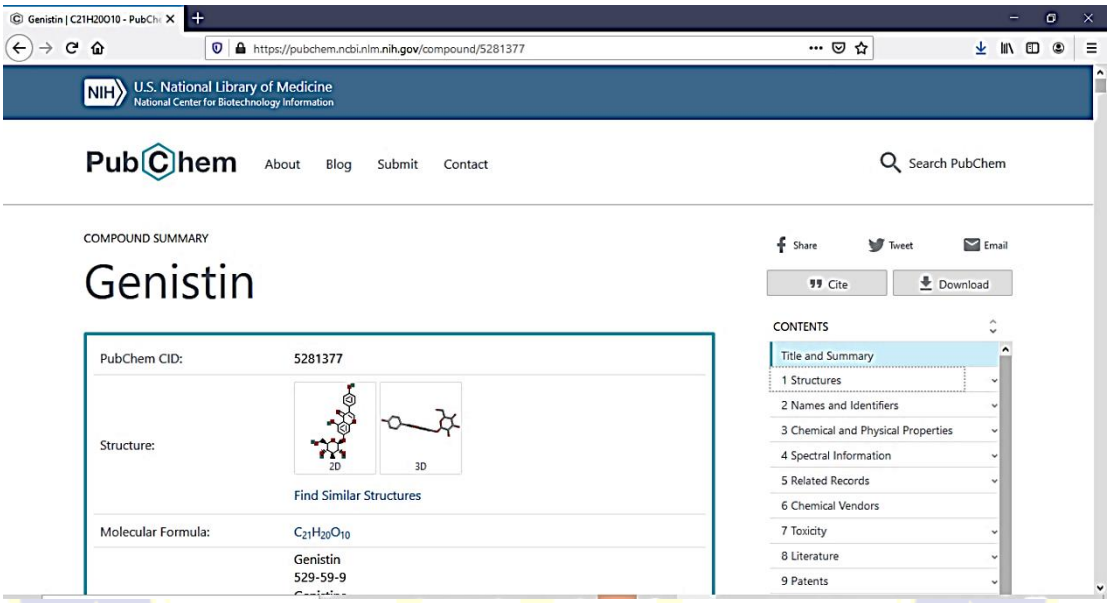
SKEMA ALUR PENELITIAN PENAMBATAN MOLEKUL



Gambar I.6 Lanjutan

LAMPIRAN 2

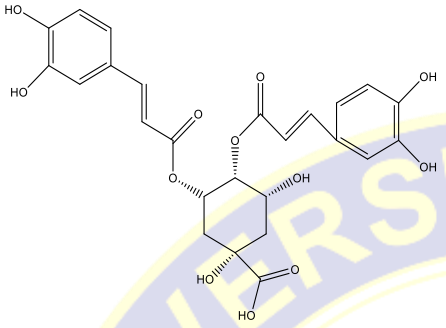
SITUS pubChem



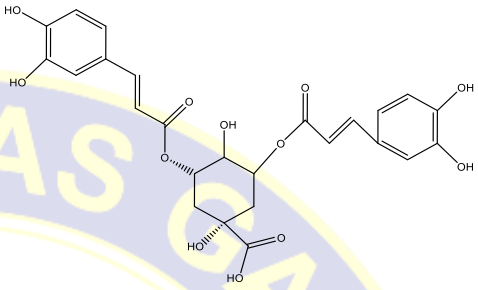
Gambar I.7 Situs pubchem

LAMPIRAN 3

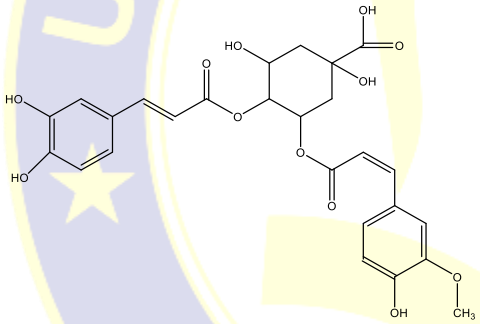
SENYAWA BIJI KOPI HIJAU ROBUSTA (*Coffea canephora*)



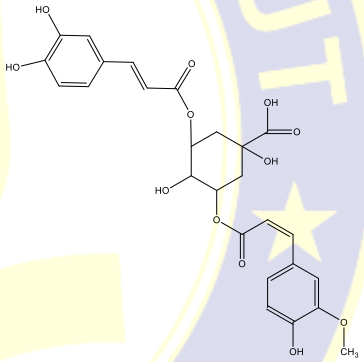
a. 3,4-O-Dicaffeoylquinic Acid Malonyl



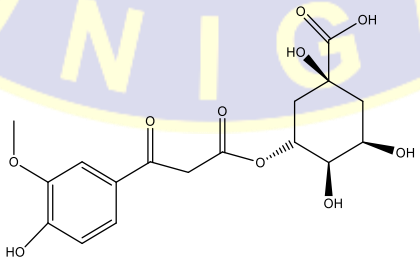
b. 3,5-O-Dicaffeoylquinic Acid Malonyl



c. 3-feruloyl-4-caffeoylquinic acid



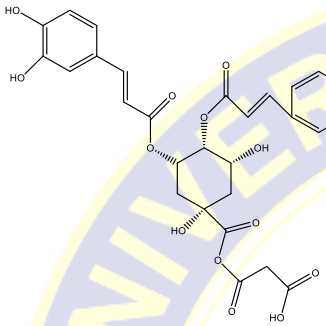
d. 3-feruloyl-5-caffeoylquinic



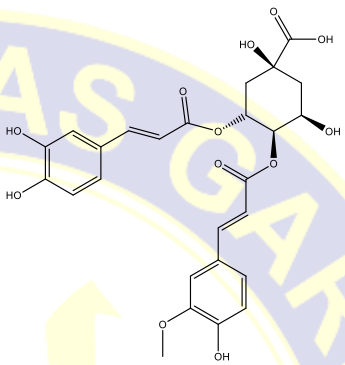
e. 3-O-feruloylquinic acid

LAMPIRAN 3

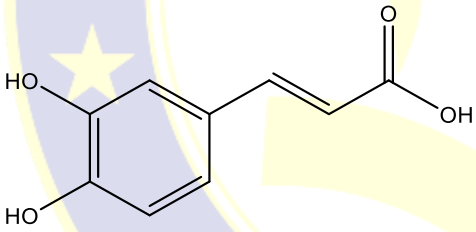
(LANJUTAN)



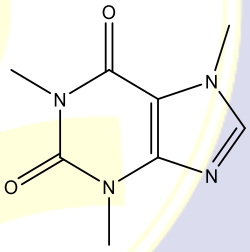
f. 4,5-O-dicaffeoylquinic acid



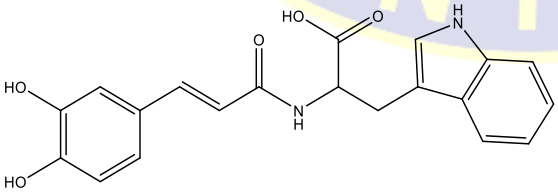
g. 4-O-feruloyl-5-caffeoylquinic acid



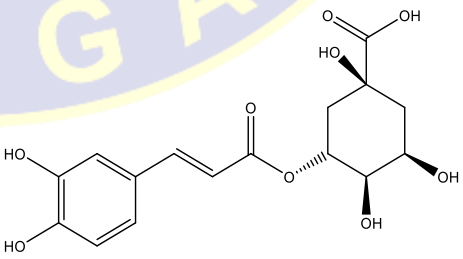
h. Caffeic Acid



i. Caffeine



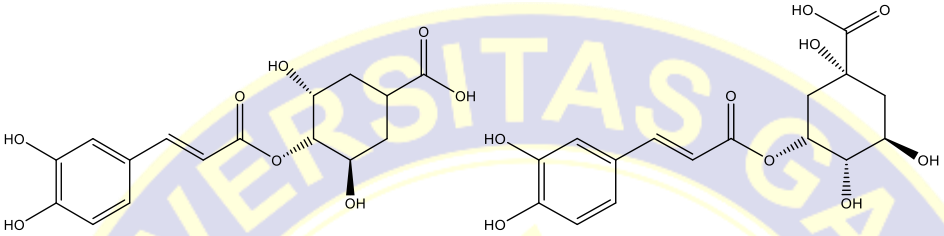
j. N-Caffeoyltryptophan



k. Chlorogenic Acid

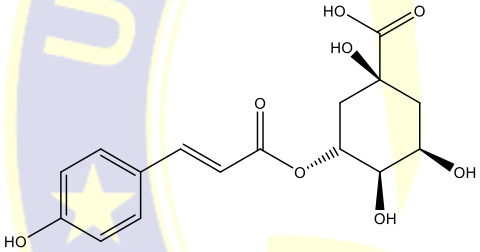
LAMPIRAN 3

(LANJUTAN)

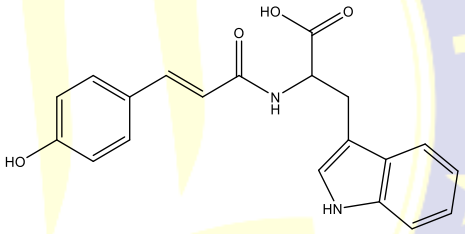


l. Cryptochlorogenic Acid

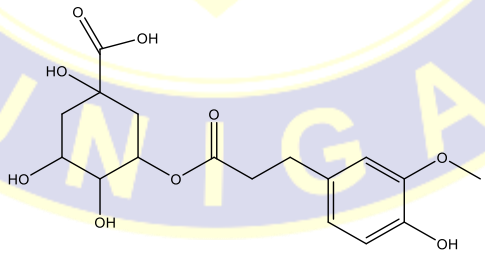
m. Neochlorogenic Acid



n. p-coumaroylquinic acid



o. p-coumaroylquinic-N-tryptophan

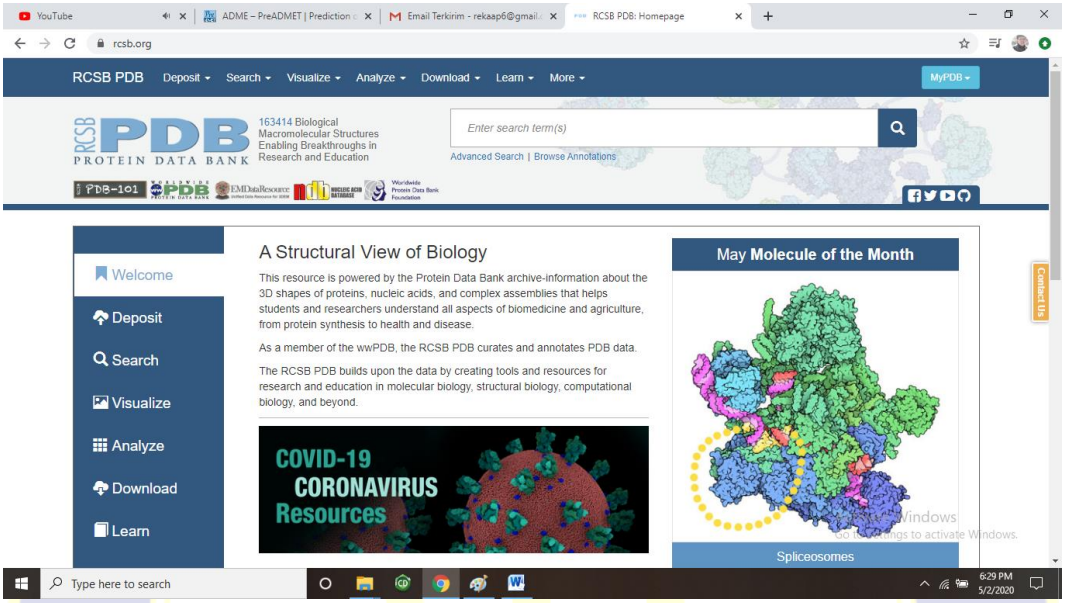


p. 5-O-feruloylquinic acid

Gambar I.8 Senyawa biji kopi hijau robusta (*Coffea canephora*)

LAMPIRAN 4

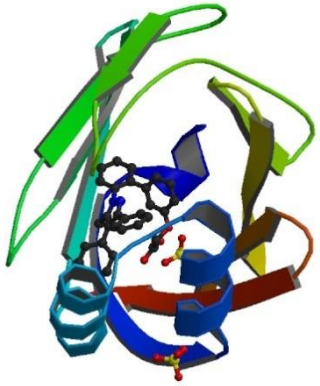
SITUS PDB (PROTEIN DATA BANK)



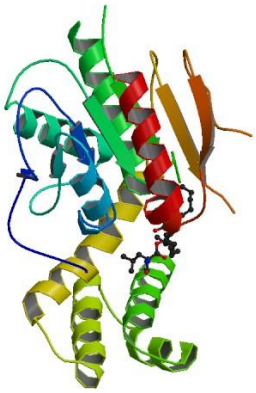
Gambar I.9 Situs PDB (Protein Data Bank)

LAMPIRAN 5

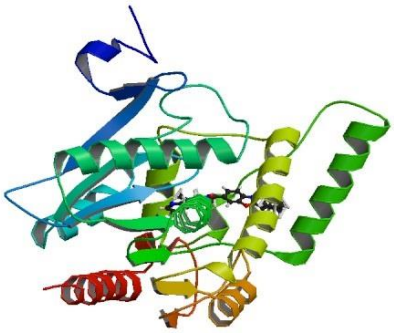
STRUKTUR 3D RESEPTOR



a. Reseptor*Adipocyte Fatty Acid Binding Protein*(aFABP)



b. Reseptor *Human Monoglyceride Lipase* (MGL)

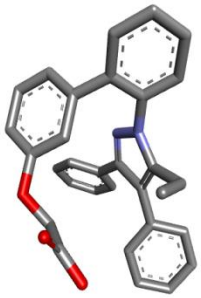


c. Reseptor *Human Fatty Acid Synthase* (FAS)

Gambar I.10 Struktur 3D reseptor

LAMPIRAN 6

LIGAN ALAMI



FABP Inhibitor

Ligan alami dari reseptor *Adipocyte*

Fatty Acid Binding Protein (aFABP)

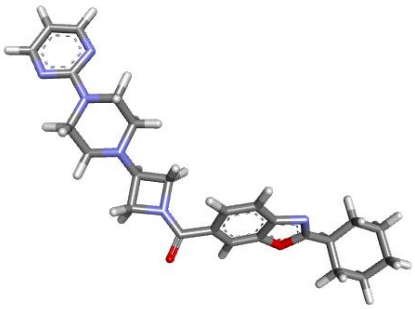
Orlistat

Ligan alami dari reseptor *Human Fatty*

Acid Synthase (FAS)

LAMPIRAN 6

(LANJUTAN)



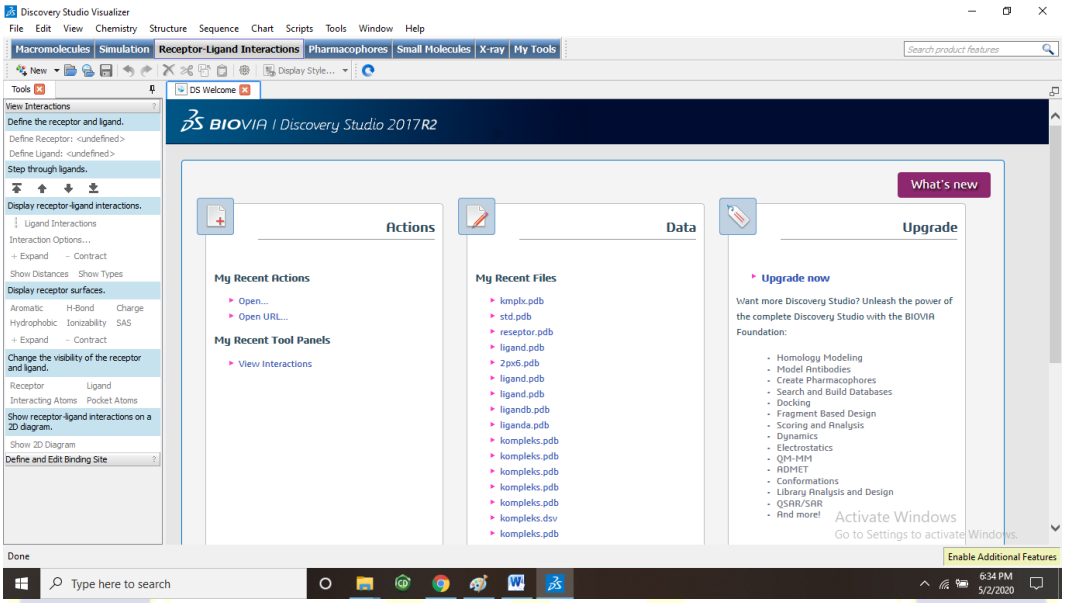
(2-cyclohexyl-1,3-benzoxazol-6-yl){3-[4-(pyrimidin-2-yl)piperazin-1-yl]azetidin-1-yl}methanone (MGL inhibitor)

Ligan alami dari reseptor *Human Monoglyceride Lipase* (MGL)

Gambar I.11 Ligan alami

LAMPIRAN 7

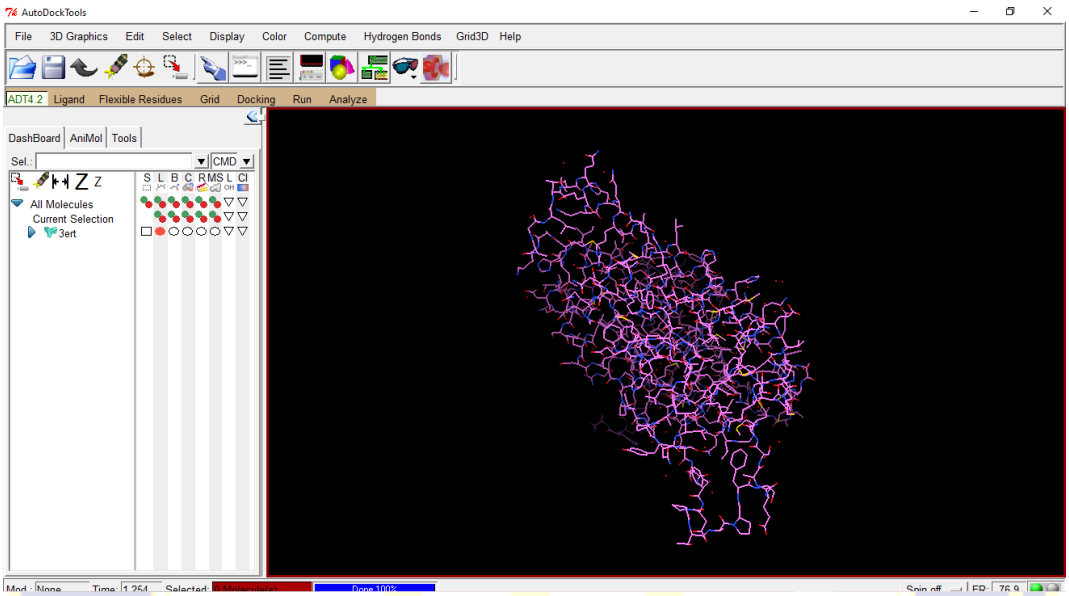
PERANGKAT LUNAK *DISCOVERY STUDIO VISUALIZER*



Gambar I.12 Perangkat lunak *discovery studio visualizer*

LAMPIRAN 8

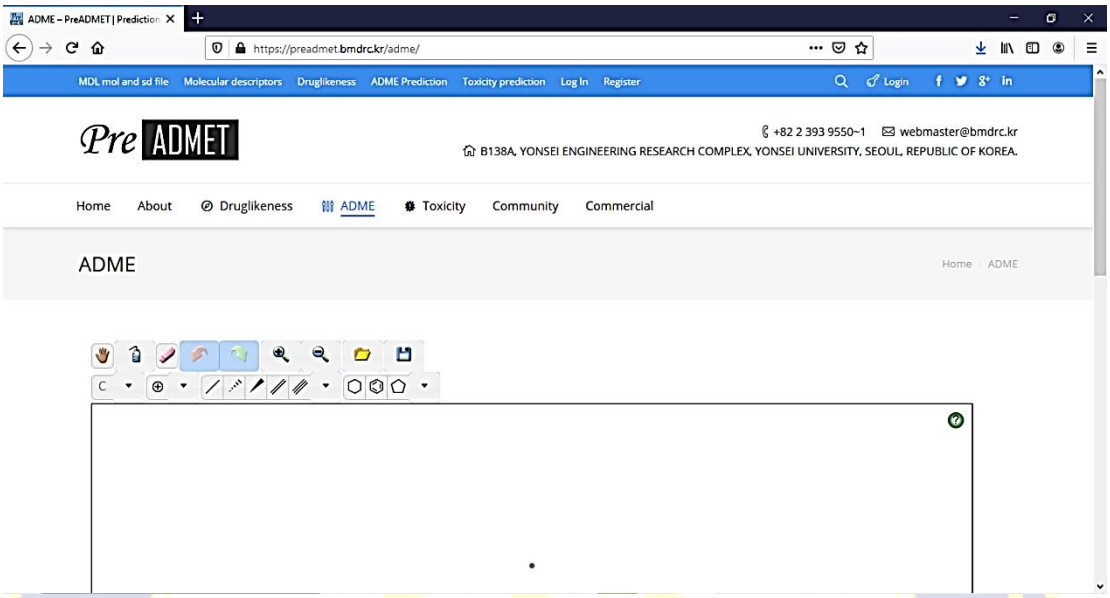
PERANGKAT LUNAK AUTODOCK TOOLS



Gambar I.13 Perangkat lunak autodock tools

LAMPIRAN 9

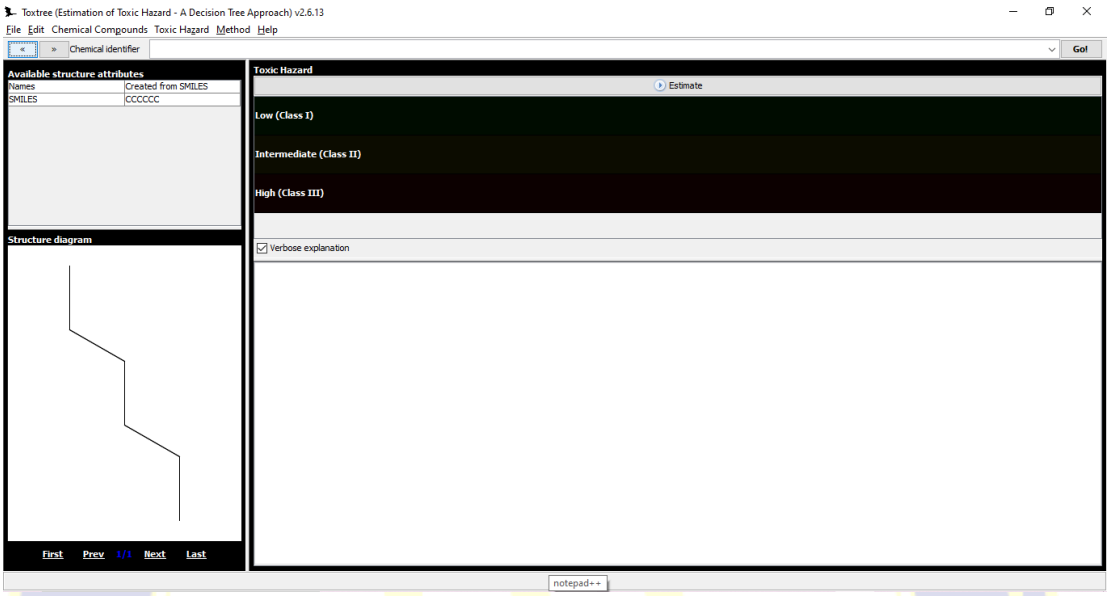
SITUS *PRE-ADMET*



Gambar I.14 Situs *pre-ADMET*

LAMPIRAN 10

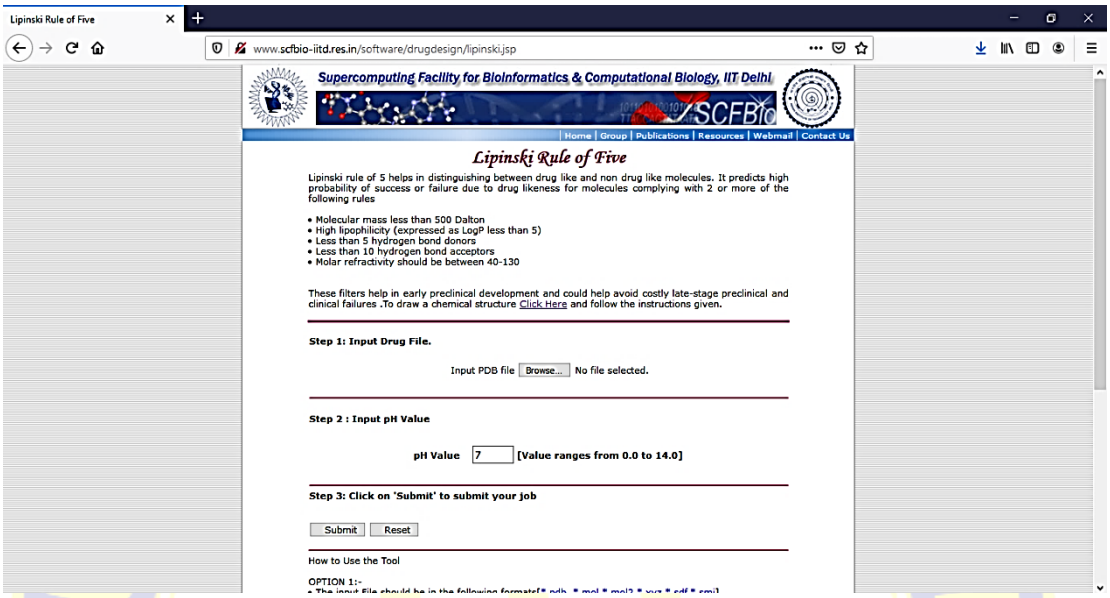
PERANGKAT LUNAK TOXTREE



Gambar I.15 Perangkat lunak toxtree

LAMPIRAN 11

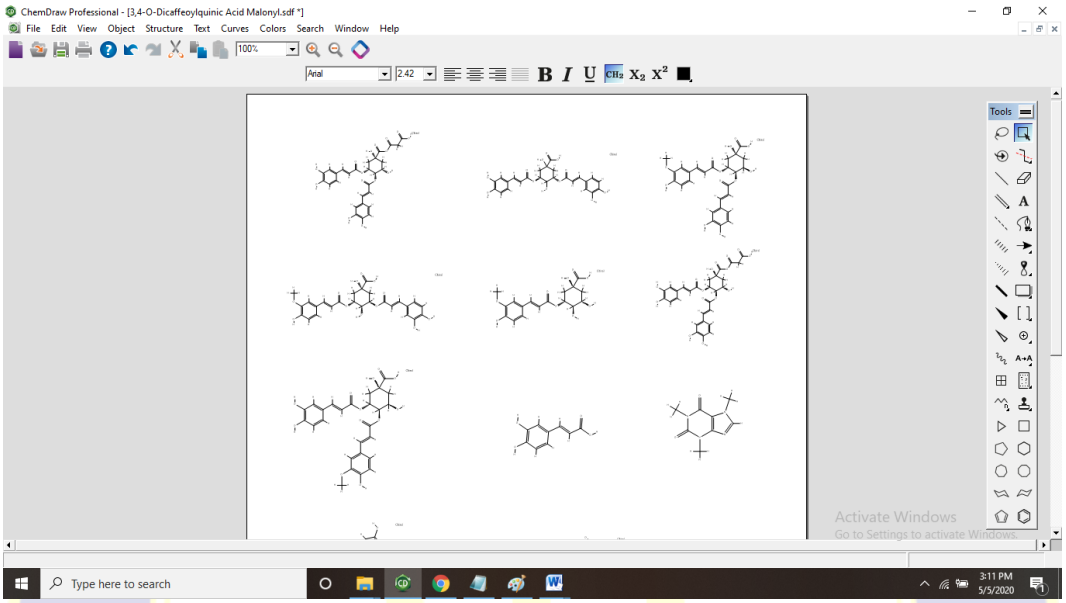
SITUS *LIPINSKI'S RULE OF FIVE*



Gambar I.16 Situs *lipinski's rule of five*

LAMPIRAN 12

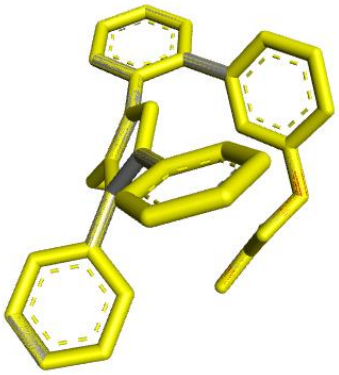
PERANGKAT LUNAK *CHEM DRAW*



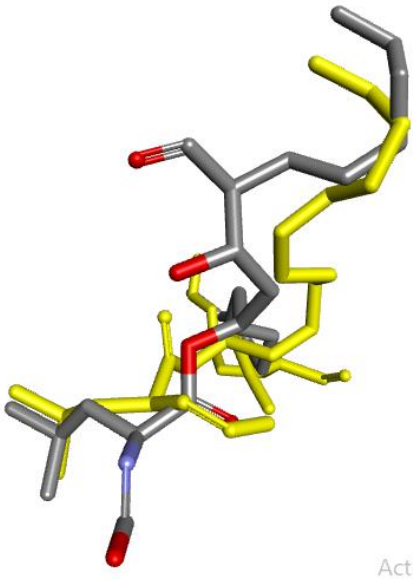
Gambar I.17 Perangkat lunak *chem draw*

LAMPIRAN 13

HASIL VALIDASI



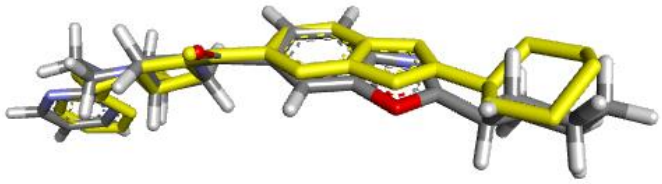
Visualisasi tumpang tindih ligan alami dengan ligan hasil *redocking* dari reseptor *Adipocyte Fatty Acid Binding Protein*(aFABP)



Visualisasi tumpang tindih ligan alami dengan ligan hasil *redocking* dari reseptor *Human Fatty Acid Synthase*(FAS)

LAMPIRAN 13

(LANJUTAN)



Visualisasi tumpang tindih ligan alami dengan ligan hasil *redocking* dari reseptor *Human Monoglyceride Lipase*(MGL)

Gambar I.18 Hasil validasi

Tabel V.2. Grid Box, Nilai RMSD, Nilai ΔG (Energi Bebas)

Reseptor	Grid Box	RMSD	ΔG (Energi Bebas)
Adipocyte Fatty Acid Binding Protein(aFABP) Kode 2NNQ	x : 4.52 y : 7.609 z : 18.565	1,254 Å	-11,34
Human Fatty Acid Synthase(FAS) Kode 2PX6	x : 12.75 y : -4.297 z : 25.282	1.99 Å	-2.50
Human Monoglyceride Lipase(MGL) Kode 3PE6	x : -10.87 y : 20.03 z : -9.412	0,689 Å	-13.33

LAMPIRAN 14

HASIL PENAMBATAN MOLEKUL

Tabel V.3. Hasil Penambatan Senyawa Aktif Dari Tanaman Kopi Hijau Robusta (*Coffea canepghora* (L.)) Dan Identifikasi Interaksi Hidrogen Menggunakan *Discovery Studio Visualizer*® Terhadap Reseptor Target *Adipocyte Fatty Acid Binding Protein* (aFABP) Kode 2NNQ

No	Senyawa / Ligan	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1	Ligand Alami (FABP4 inhibitor)	-11.48	4	ARG106, CYS117, TYR128, ARG126,	4.8
2	3,4-O-Dicaffeoylquinic Acid Malonyl	-7.14	6	SER55, ALA75, ASP76, SER53, TYR128, THR60	5850
3	3,5-O-Dicaffeoylquinic Acid Malonyl	- 9.72	3	GLN95, ARG126, TYR128	74.96
4	3-feruloyl-4-caffeoylquinic acid	-7.15	5	SER55, HIS93, ARG106, ILE51, THR60	5700
5	3-feruloyl-5-caffeoylquinic acid	-7.86	4	SER55, ARG126, TYR128, TYR19.	1740
6	3-O-feruloylquinic acid	-5.85	5	ARG78, TYR19, ARG126, SER53, TYR128	51930
7	4,5-O-dicaffeoylquinic acid	-8.37	4	ARG106, ALA33, ARG126, MET20	738.30

8	4-O-feruloyl-5-caffeoylquinic acid	- 8.30	5	THR60, ARG126, ARG106, ILE51, LYS58	830.83
9	Caffeic Acid	- 5.88	4	ARG126, TYR19, TYR128, ARG78	48960
10	Caffeine	- 4.59	2	ARG106, ARG126,	434230
11	N-Caffeoyltryptophan	- 7.34	3	ILE51, SER55, ASP76,	4140
12	Chlorogenic Acid	- 7.19	3	SER55, ILE51, ARG126	5380
13	Cryptochlorogenic Acid	- 6.10	5	SER53, GLN95, ARG126, TYR128, ARG106.	34060
14	feruloylquinic acid	- 6.47	2	ARG126, ARG106	17950
15	Neochlorogenic Acid	- 6.53	2	ILE51, SER55	16360
16	p-coumaroylquinic acid	- 7.83	5	SER53, ARG78, TYR19, TYR128, ARG126	13720
17	p-coumaroylquinic-N-tryptophan	- 7.98	3	ARG106, ARG126, MET20	1420

LAMPIRAN 14

(LANJUTAN)

Tabel V.3. Hasil Penambatan Senyawa Aktif Dari Tanaman Kopi Hijau Robusta (*Coffea canepghora* (L.)) Dan Identifikasi Interaksi Hidrogen Menggunakan *Discovery Studio Visualizer*® Terhadap Reseptor Target *Human Fatty Acid Synthase* (FAS) Kode 2PX6

No	Senyawa / Ligan	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1	Ligand Alami (Orlistat)	-2.50	1	PHE2370	14660000
2	3,4-O-Dicaffeoylquinic Acid Malonyl	-5.44	2	GLU2366, TYR2343	102930
3	3,5-O-Dicaffeoylquinic Acid Malonyl	- 5.37	1	LEU2427	116120
4	3-feruloyl-4-caffeoylquinic acid	-3.71	3	LEU2427, ALA2363, GLU2366,	1900000
5	3-feruloyl-5-caffeoylquinic acid	-5.26	3	LEU2222, ILE2250, TYR2343	139780
6	3-O-feruloylquinic acid	-5.03	2	LEU2222, TYR2343	206140
7	4,5-O-dicaffeoylquinic acid	-3.97	2	ALA2363, LEU2427	1290000
8	4-O-feruloyl-5-caffeoylquinic acid	- 4.75	2	TYR2434, LEU2427,	528180
9	Caffeic Acid	- 5.15	2	ILE2250, GLU2251	167720

10	Caffeine	- 4.68	3	LEU2222, ILE2250, GLU2251	369440
11	N-Caffeoyltryptophan	-5.99	3	LEU2222, TYR2423, PHE2570	40600
12	Chlorogenic Acid	- 4.22	2	TYR2343, LEU2222	802350
13	Cryptochlorogenic Acid	- 4.71	1	LEU2222	355250
14	feruloylquinic acid	- 4.94	1	LEU2222	238490
15	Neochlorogenic Acid	- 4.37	2	TYR2343, LEU2222	627240
16	p-coumaroylquinic acid	- 6.97	4	LEU2222, GLU2251, HIS2481, TYR2309	42180
17	p-coumaroylquinic-N-tryptophan	- 6.21	2	SER2308, TYR2343	28100

LAMPIRAN 14

(LANJUTAN)

Table V.3. Hasil Penambatan Senyawa Aktif Dari Tanaman Kopi Hijau Robusta (*Coffea canepghora* (L.)) Dan Identifikasi Interaksi Hidrogen Menggunakan *Discovery Studio Visualizer*® Terhadap Reseptor Target *Human Monoglyceride Lipase* (MGL) Kode 3PE6

No	Senyawa / Ligan	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1	Ligand Alami (MGL inhibitor)	-13.33	4	SER181, MET123,ALA51, GLU190.	0.17034
2	3,4-O-Dicaffeoylquinic Acid Malonyl	-7.93	4	GLY219, SER155, ALA51, SER122	1530
3	3,5-O-Dicaffeoylquinic Acid Malonyl	- 7.96	4	SER155, ALA51, SER122, CYS242	1460
4	3-feruloyl-4-caffeoylquinic acid	-9.16	6	GLY210, ASP180, MET123, ALA51, SER175, GLY177	191.57
5	3-feruloyl-5-caffeoylquinic acid	-7.12	3	SER155, SER122, TYR19	6030
6	3-O-feruloylquinic acid	-7.66	3	HIS121, SER176, GLY177	2450
7	4,5-O-dicaffeoylquinic acid	-7.76	4	ASP180, ALA51, ARG240, CYS242	2040
8	4-O-feruloyl-5-	- 8.59	3	ASP180, PRO178,	508.42

	caffeoylquinic acid			ALA51	
9	Caffeic Acid	- 5.55	2	ALA51, PRO178	85230
10	Caffeine	- 5.61	1	ALA51	76910
11	N-Caffeoyltryptophan	- 8.98	4	GLY177, ALA51, MET123, GLY210,	261.79
12	Chlorogenic Acid	- 8.01	4	GLY177, LEU213, ALA51, MET123	1340
13	Cryptochlorogenic Acid	- 7.86	5	ARG240, ALA51, SER122, ILE179, PRO178	1730
14	feruloylquinic acid	- 7.00	5	ASP180, ALA51, MET123, SER122, GLY177	7330
15	Neochlorogenic Acid	- 7.29	4	MET123, PRO178, GLY177, ALA51	4500
16	p-coumaroylquinic acid	- 7.82	3	PRO178, ASP180, ALA51	1840
17	p-coumaroylquinic-N-tryptophan	- 9.12	2	GLY177, ALA51,	205.02

LAMPIRAN 15

HASIL PENGUJIAN PREADMET

Tabel V.4. Hasil Uji Pre-ADMET

No	Nama Ligan	Absorbsi		Distribusi
		CaCo-2 (nm. Sec-1)	HIA (%)	PPB (%)
1	3,4-O-Dicaffeoylquinic Acid Malonyl	19.53	23.12	87.77
2	3,5-O-Dicaffeoylquinic Acid Malonyl	19.32	23.12	86.05
3	3-feruloyl-4-caffeoylquinic acid	18,66	39.17	80.29
4	3-feruloyl-5-caffeoylquinic acid	19.76	66.82	87.87
5	3-O-feruloylquinic acid	17.52	34.18	41.13
6	4,5-O-dicaffeoylquinic acid	19.55	23.13	86.7
7	4-O-feruloyl-5-caffeoylquinic acid	19.15	39.17	80.82
8	Caffeic Acid	21.11	82.30	40,29
9	Caffeine	21.26	93.82	14.07
10	N-Caffeoyltryptophan	17.43	79.28	92.19
11	Chlorogenic Acid	18,71	20.43	41.96
12	5-O-feruloylquinic acid	18.52	33.21	42.34
12	Cryptochlorogenic Acid	19.31	29,77	50.33
13	Neochlorogenic Acid	17.43	29.77	47.03
14	5-O-feruloylquinic acid	18.66	37.11	44.54
15	p-coumaroylquinic acid	18.71	20.42	41.96
16	p-coumaroylquinic-N-tryptophan	19.41	86.86	97.24

Keterangan: *in vitro CaCo-2 cell permeability (nm. Sec^{-1}): >70 higher permeability, 4-70 medium permeability, <4 low permeability; % human intestinal absorption (%HIA): 70-100% well absorbed, 20-70% moderately absorbed, 0-20% poorly absorbed; %plasma protein binding: >90% strongly bound, <90% weakly bound.*

LAMPIRAN 16

HASIL PENGUJIAN TOKSISITAS

Tabel V.5 Hasil Pengujian Toksisitas

No	Ligan	Cramer rules	Benigni/bosarulebase	Kroes TTC decission tree
1	3,4-O-Dicaffeoylquinic Acid Malonyl	3	8,9	1
2	3,5-O-Dicaffeoylquinic Acid Malonyl	3	8,9	1
3	3-feruloyl-4-caffeoylquinic acid	3	8,9	1
4	3-feruloyl-5-caffeoylquinic acid	3	8,9	1
5	3-O-feruloylquinic acid	2	8,9	1
6	4,5-O-dicaffeoylquinic acid	3	8,9	1
7	4-O-feruloyl-5-caffeoylquinic acid	3	8,9	1
8	Caffeic Acid	1	8,9	1
9	Caffeine	3	8,9	1
10	N-Caffeoyltryptophan	3	8,9	1
11	Chlorogenic Acid	2	8,9	1
12	Cryptochlorogenic Acid	1	8,9	1
13	Neochlorogenic Acid	2	8,9	1
14	5-O-feruloylquinic acid	2	8,9	1
15	p-coumaroylquinic acid	2	8,9	1
16	p-coumaroylquinic-N-tryptophan	3	8,9	1

Keterangan: *Cramer rules 1 Low class, 2 Intermediet class, 3 Hight class. Benigni/bose rulebase 2 (structural alert for non genotoxic carcinogenicity), 8 (negative for genotoxic carcinogenity), 9 (negative for non-genotoxic carcinogencity),. Kroes TTC decision tree 1(Subtance would not be expected to be a safety concern).*

LAMPIRAN 17

HASIL PREDIKSI BIOAVAILIBILITAS

Tabel V.6 Hasil Prediksi Bioavalibilitas

No	Ligan	BM	Log P	Ikatan Hidrogen		Keterangan
				Donor	Akseptor	
1	3,4-O-Dicaffeoylquinic Acid Malonyl	516	-0.269	7	9	Tidak Memenuhi Syarat
2	3,5-O-Dicaffeoylquinic Acid Malonyl	516	-0.91	7	9	Tidak Memenuhi Syarat
3	3-feruloyl-4-caffeoylquinic acid	530	0.175	6	9	Tidak Memenuhi Syarat
4	3-feruloyl-5-caffeoylquinic acid	530	0.355	6	9	Tidak Memenuhi Syarat
5	3-O-feruloylquinic acid	368	-1.433	5	7	Tidak Memenuhi Syarat
6	4,5-O-dicaffeoylquinic acid	602	-0.163	7	11	Tidak Memenuhi Syarat
7	4-O-feruloyl-5-caffeoylquinic acid	530	0.179	6	9	Tidak Memenuhi Syarat
8	Caffeic Acid	180	0.976	3	3	Memenuhi Syarat
9	Caffeine	194	-0.04	0	4	Memenuhi Syarat
10	N-Caffeoyltryptophan	366	1.971	5	5	Memenuhi Syarat
11	Chlorogenic Acid	354	-1.879	6	7	Tidak Memenuhi Syarat
12	Cryptochlorogenic Acid	354	-1.4	6	7	Tidak Memenuhi Syarat
13	Neochlorogenic Acid	354	-.1875	6	7	Tidak Memenuhi Syarat
14	5-O-feruloylquinic acid	370	-1.49	5	7	Memenuhi Syarat
15	p-coumaroylquinic acid	338	-1.282	5	6	Memenuhi Syarat
16	p-coumaroylquinic-N-tryptophan	338	-1.275	5	6	Memenuhi Syarat

Keterangan: BM (Berat molekul) <500 Dalton, Log P <5, Donor ikatan hidrogen <5 dan Akseptor ikatan hidrogen <10.

DAFTAR RIWAYAT HIDUP

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PKL Apotek ASy-Syifa Garut

PENGALAMAN ORGANISASI

SEKOLAH MENENGAH PERTAMA (SMP)

- Palang Merah Remaja (PMR) (Non Formal)

- Tim Basket (Non Formal)

SEKOLAH MENENGAH KEJURUAN

- Palang Merah Remaja (PMR) (Non Formal)

- Organisasi Siswa Intra Sekolah SMK Farmasi Purwakarta (Formal)

➢ Sebagai Divisi Dekorasi dan Dokumentasi 2014-2016