

DAFTAR PUSTAKA

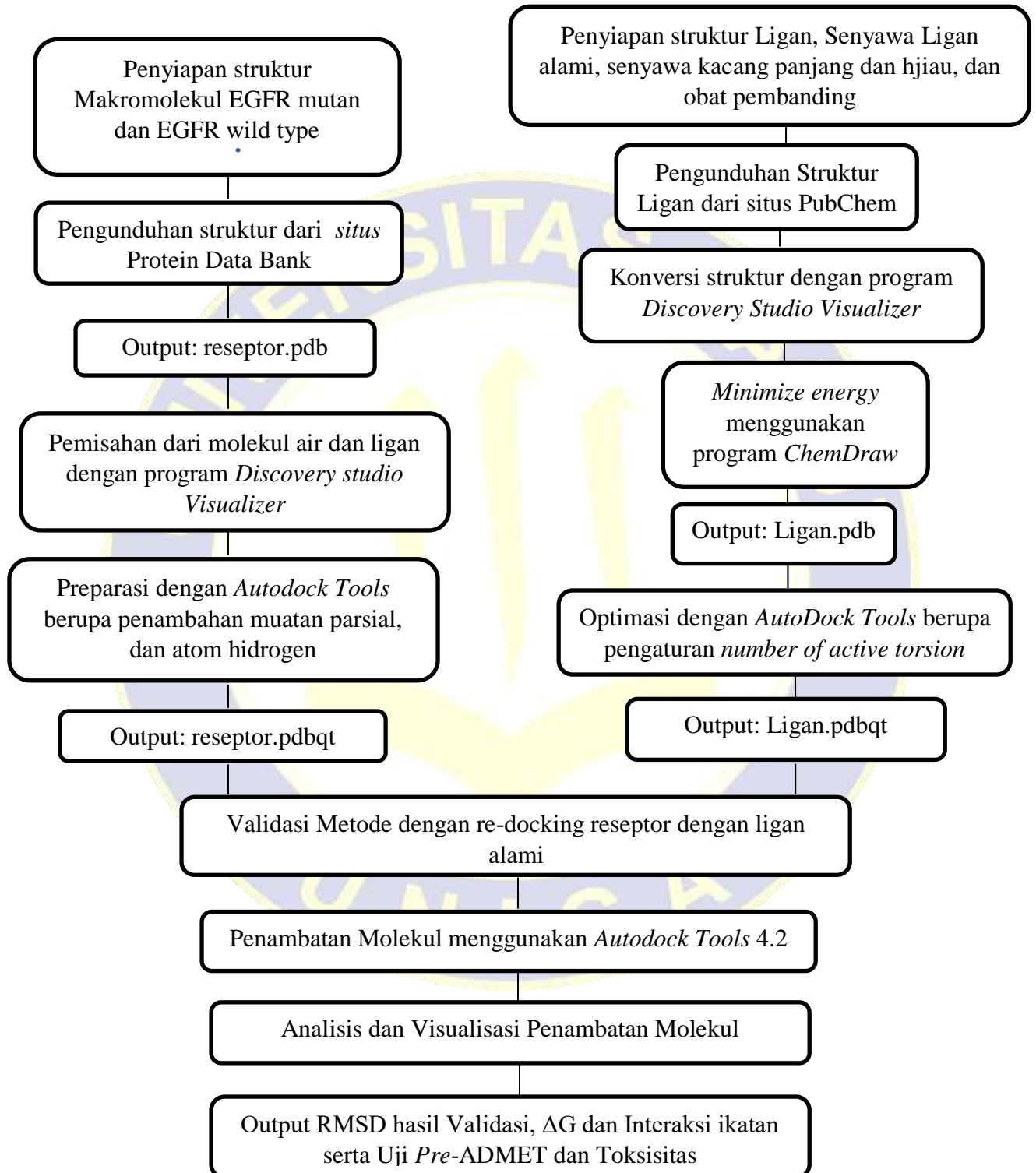
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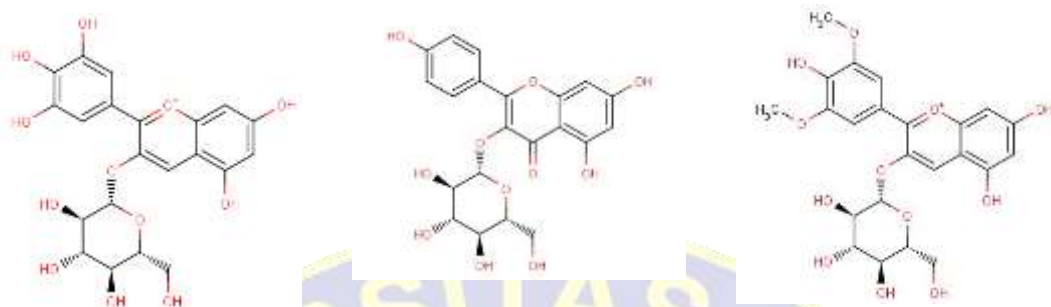
LAMPIRAN 1
ALUR PENELITIAN



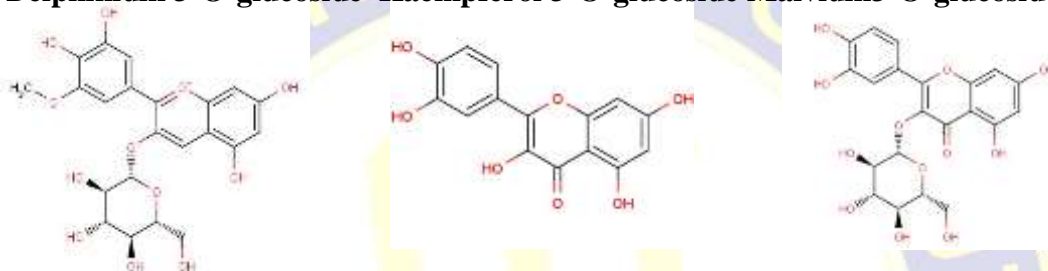
Gambar V.1 Alur penelitian

LAMPIRAN 2

SENYAWA KACANG PANJANG DAN SENYAWA KACANG HIJAU



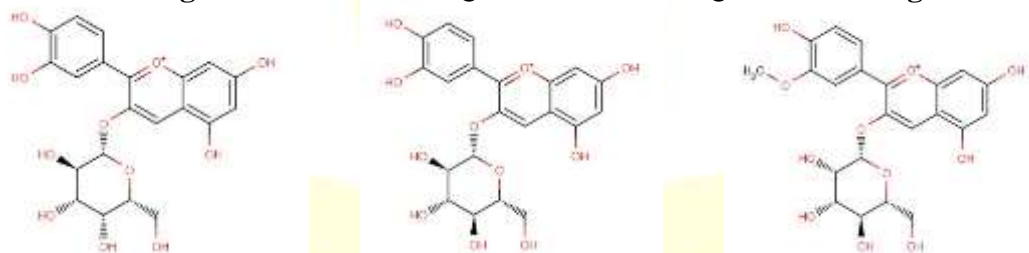
Delphinidin 3-O-glucoside Kaempferol 3-O-glucoside Malvidin 3-O-glucoside



Petunidin 3-O-glucoside

Quercetin

Quercetin 3-O-glucoside

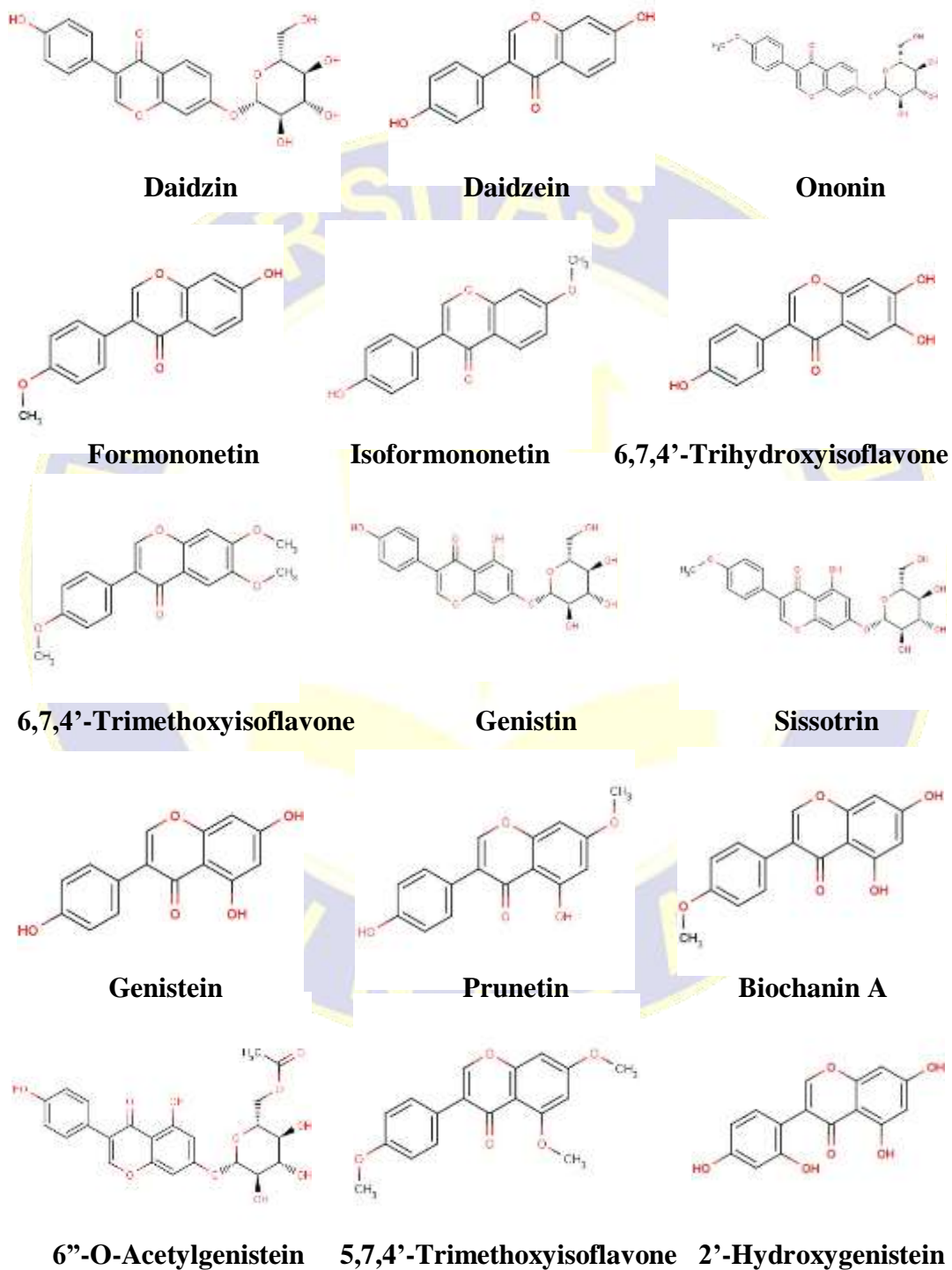


Cyanidin 3-O-galaktocide Cyanidin 3-O-glucoside Peonidin 3-O-glukoside

Gambar V.2 Struktur 2D Senyawa Kacang Panjang

LAMPIRAN 2
(LANJUTAN)

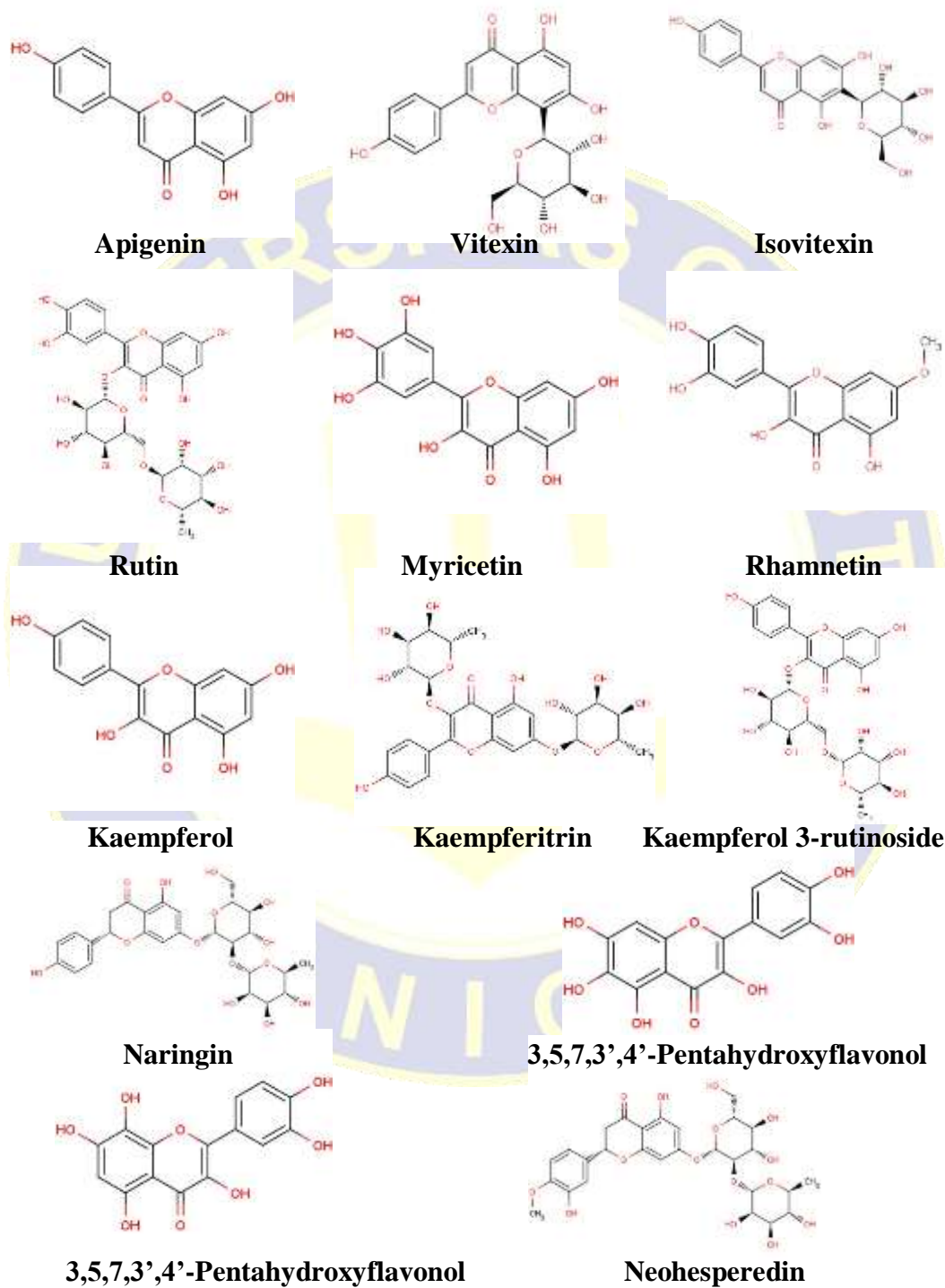
SENYAWA KACANG HIJAU



Gambar V.3 Struktur 2D Senyawa Kacang Hijau

**LAMPIRAN 2
(LANJUTAN)**

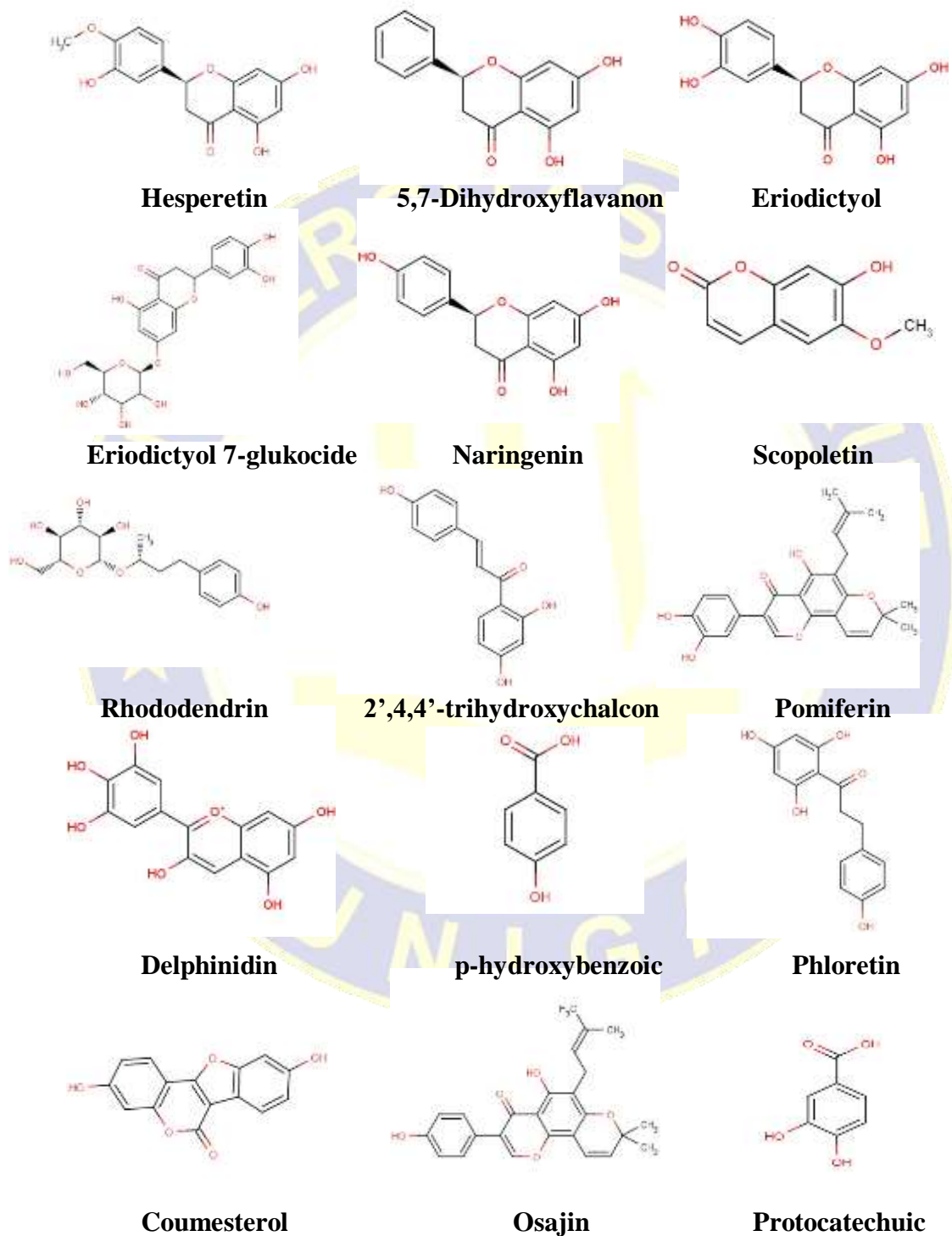
SENYAWA KACANG HIJAU



Gambar V.3 Struktur 2D Senyawa Kacang Hijau

**LAMPIRAN 2
(LANJUTAN)**

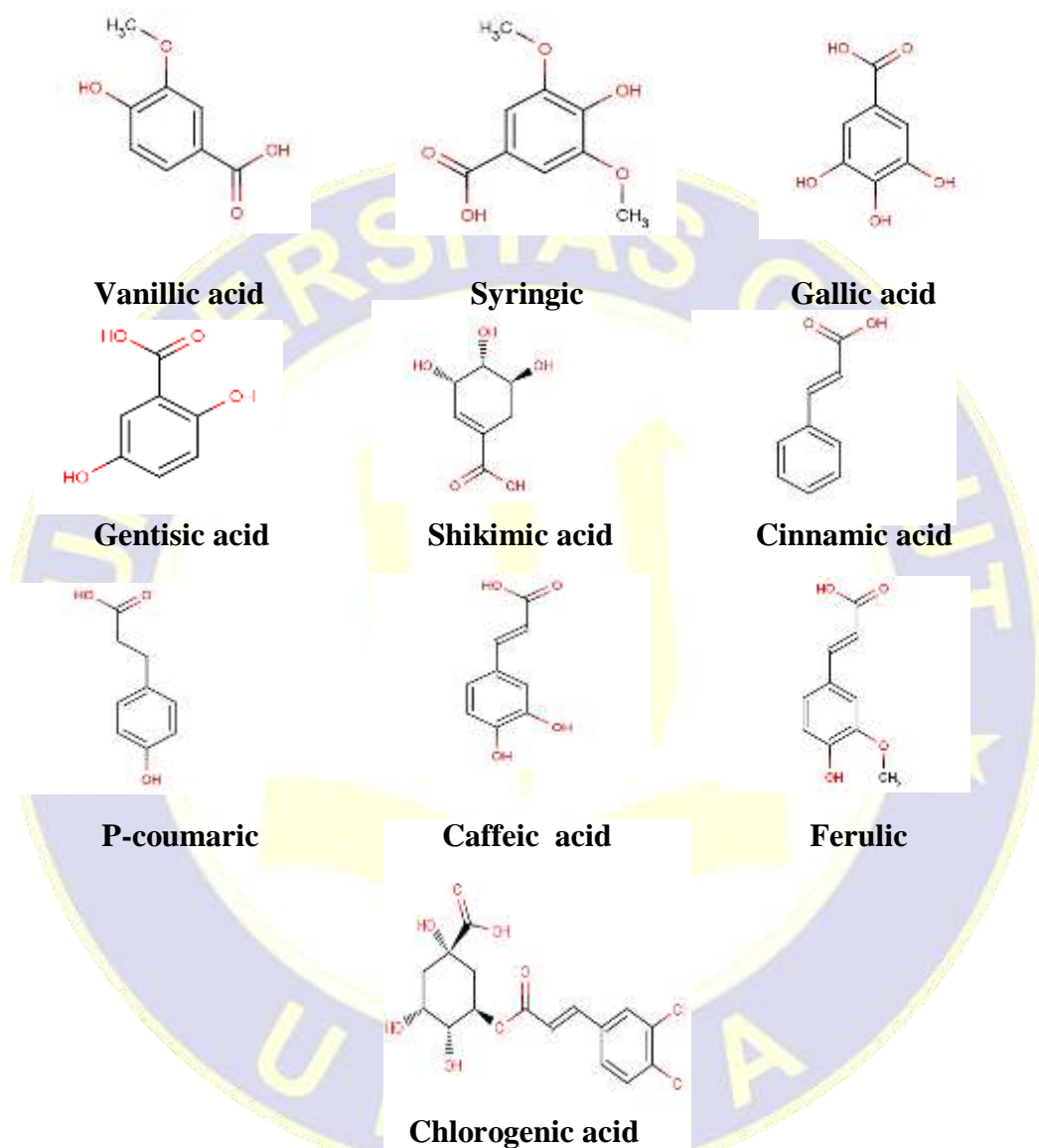
SENYAWA KACANG HIJAU



Gambar V.3 Struktur 2D Senyawa Kacang Hijau

**LAMPIRAN 2
(LANJUTAN)**

SENYAWA KACANG HIJAU



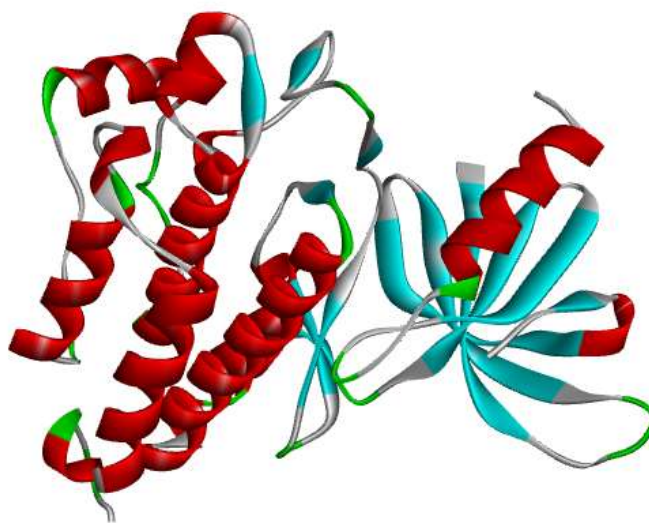
Gambar V.3 Struktur 2D Senyawa Kacang Hijau

LAMPIRAN 3
SITUS *PROTEIN DATA BANK*

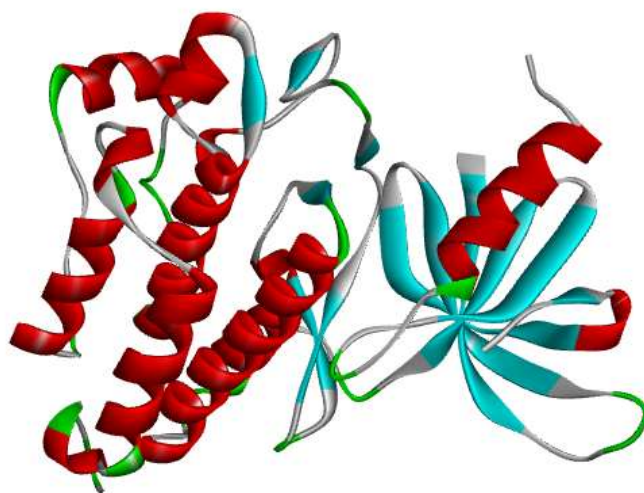


Gambar V.4 Program situs *protein data bank*

LAMPIRAN 4
STRUKTUR 3D RESEPTOR



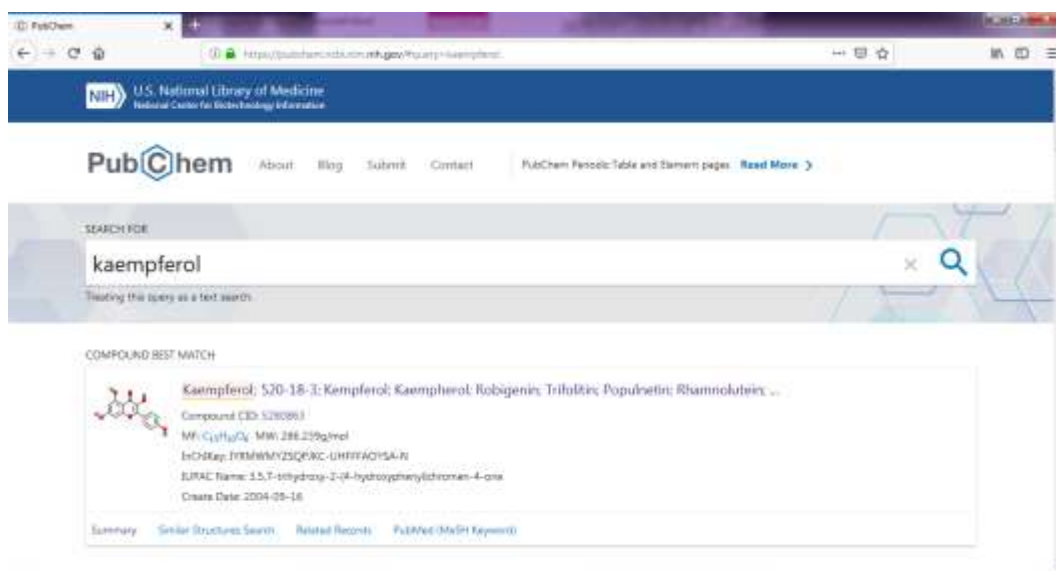
Gambar V.5 Struktur 3D reseptor EGRF *wildtype* (5UGC)



Gambar V.6 Struktur 3D reseptor EGFR mutan T790M-L858R-V948R (5HG7)

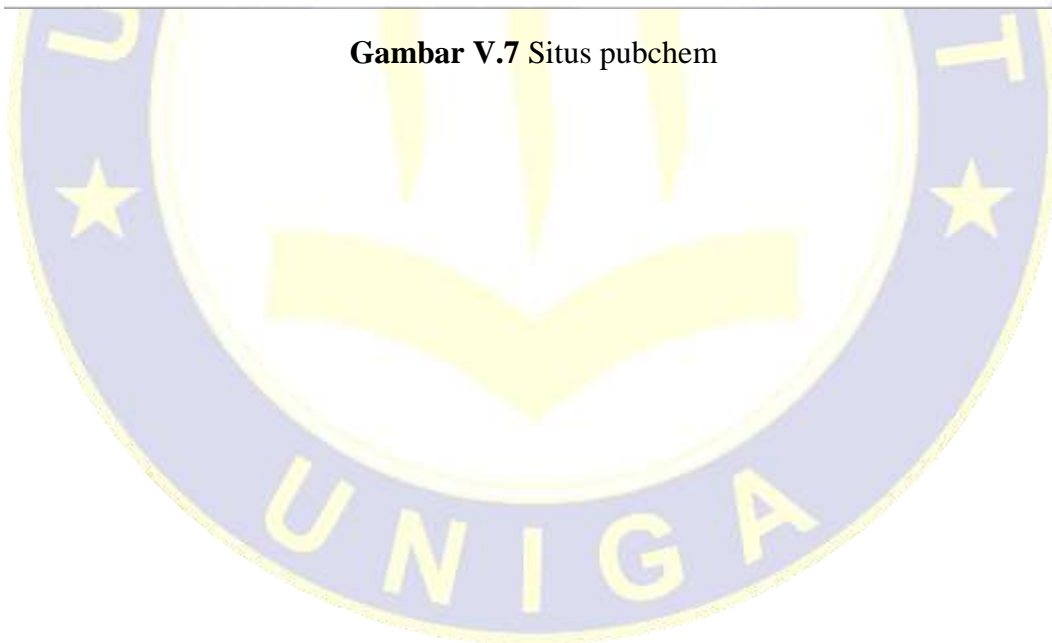
LAMPIRAN 5

SITUS PUBCHEM



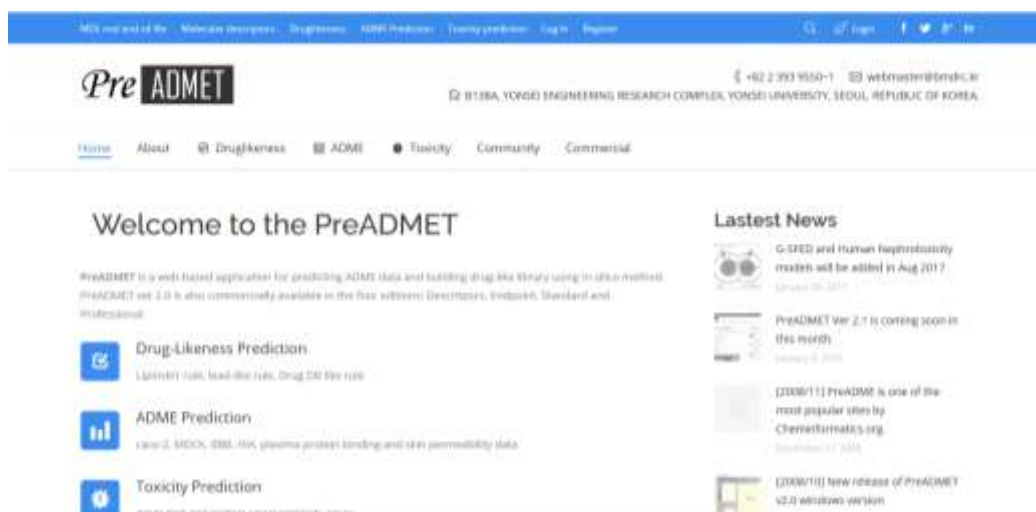
The screenshot displays the PubChem website interface. At the top, the NIH logo and "U.S. National Library of Medicine" are visible. The main navigation bar includes "PubChem", "About", "Blog", "Submit", "Contact", and "PubChem Periodic Table and Element pages". A search bar contains the text "kaempferol". Below the search bar, the results section is titled "COMPOUND BEST MATCH" and features a chemical structure of kaempferol. The text next to the structure lists synonyms: "Kaempferol; 5,7-O-3; Kempferol; Kaempferol; Robigenin; Trifollicin; Populnetin; Rhamnolutein; ...". Below this, technical details are provided: "Compound CID: 5280863", "MF: C₁₅H₁₀O₆, MW: 286.25g/mol", "InChIKey: DIRMWNYZCQKAC-UHFFFAQISA-N", "EPA Name: 3,5,7-trihydroxy-2-(4-hydroxyphenyl)chromen-4-one", and "Create Date: 2004-05-18". At the bottom of the results box, there are links for "Summary", "Similar Structures Search", "Related Records", and "PubMed (MeSH Keyword)".

Gambar V.7 Situs pubchem



LAMPIRAN 6

SITUS PRE-ADMET



The screenshot shows the homepage of the PreADMET website. At the top, there is a blue navigation bar with links for 'MOL and mol file', 'Molecule Descriptors', 'Drug-likeness', 'ADME Prediction', 'Toxicity Prediction', 'Log in', and 'Register'. Below this is the 'PreADMET' logo and contact information: '+82 2 393 9550-7' and 'webmaster@medic.or.kr'. A secondary navigation bar includes 'Home', 'About', 'Drug-likeness', 'ADME', 'Toxicity', 'Community', and 'Commercial'. The main content area features a 'Welcome to the PreADMET' section with a brief description of the application and its availability. To the right, there is a 'Lastest News' section with three articles. The bottom of the page is partially obscured by a large, semi-transparent watermark of the UNIGA logo.

MOI mol and file Molecule Descriptors Drug-likeness ADME Prediction Toxicity Prediction Log in Register

PreADMET +82 2 393 9550-7 webmaster@medic.or.kr
B118A, YONSEI ENGINEERING RESEARCH COMPLEX, YONSEI UNIVERSITY, SEJUL, REPUBLIC OF KOREA

Home About Drug-likeness ADME Toxicity Community Commercial

Welcome to the PreADMET

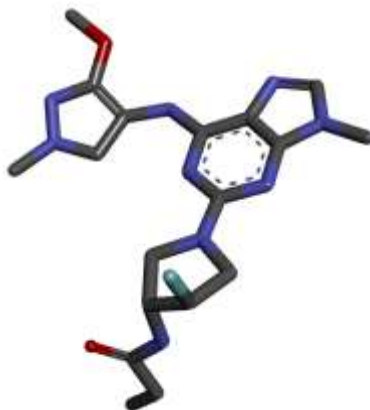
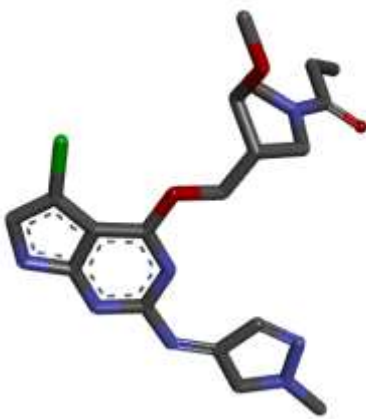
PreADMET is a web-based application for predicting ADME data and building drug like library using in silico method. PreADMET ver 2.0 is also commercially available in the four versions: Desktop, Web, Standard and Professional.

- Drug-Likeness Prediction**
Learn the rule, lead the rule, Drug DO the rule
- ADME Prediction**
can predict MDCK, Caco-2, P-glyc, plasma protein binding and skin permeability data
- Toxicity Prediction**
AMES test and rodent carcinogenicity assay

Lastest News

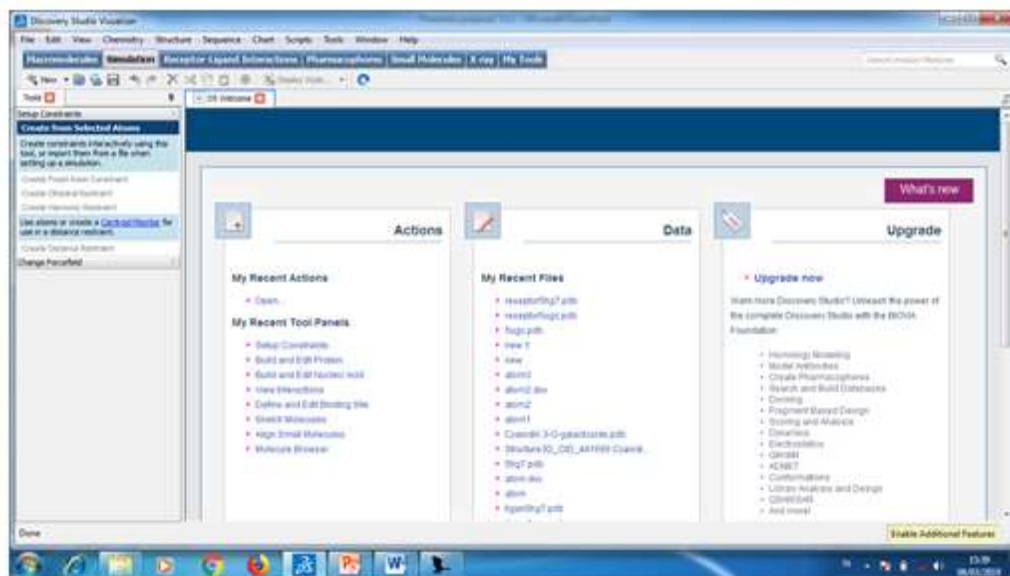
- G-SPED and human hepatotoxicity models will be added in Aug 2017
[press 06.2017]
- PreADMET ver 2.1 is coming soon in the month
[press 01.2018]
- [[2008/11]] PreADMET is one of the most popular sites by Cheminformatics.org
[November 11, 2008]
- [[2008/10]] New release of PreADMET v2.0 windows version

Gambar V.8 situs PreADMET

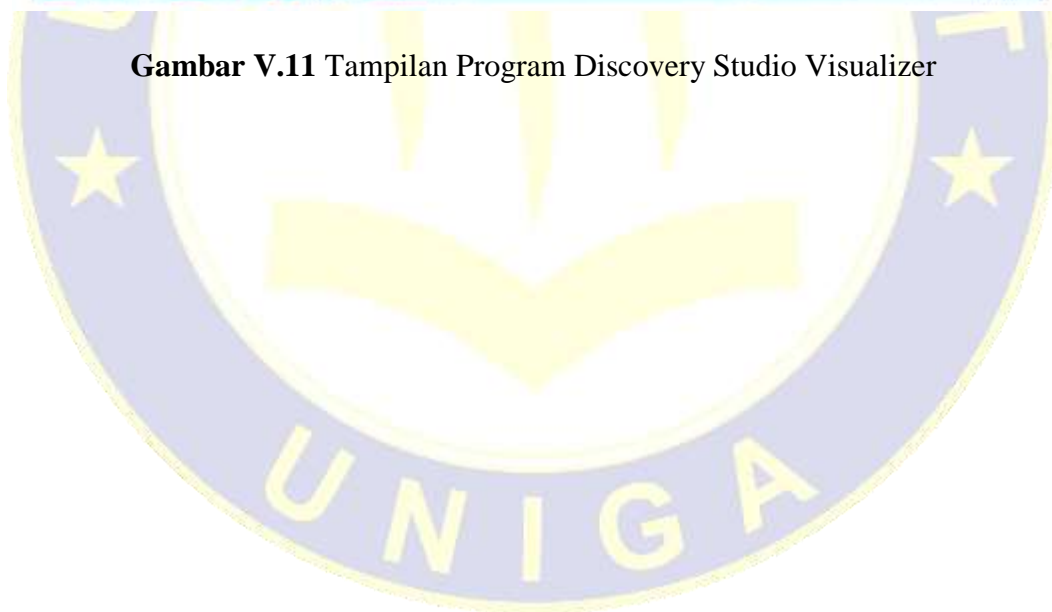
LAMPIRAN 7**LIGAN ALAMI 5UGC DAN 5HG7****Gambar V.9** Ligan Alami 5UGC**Gambar V.10** Ligan Alami 5HG7

LAMPIRAN 8

PERANGKAT LUNAK DISCOVERY STUDIO VISUALIZER



Gambar V.11 Tampilan Program Discovery Studio Visualizer



LAMPIRAN 9

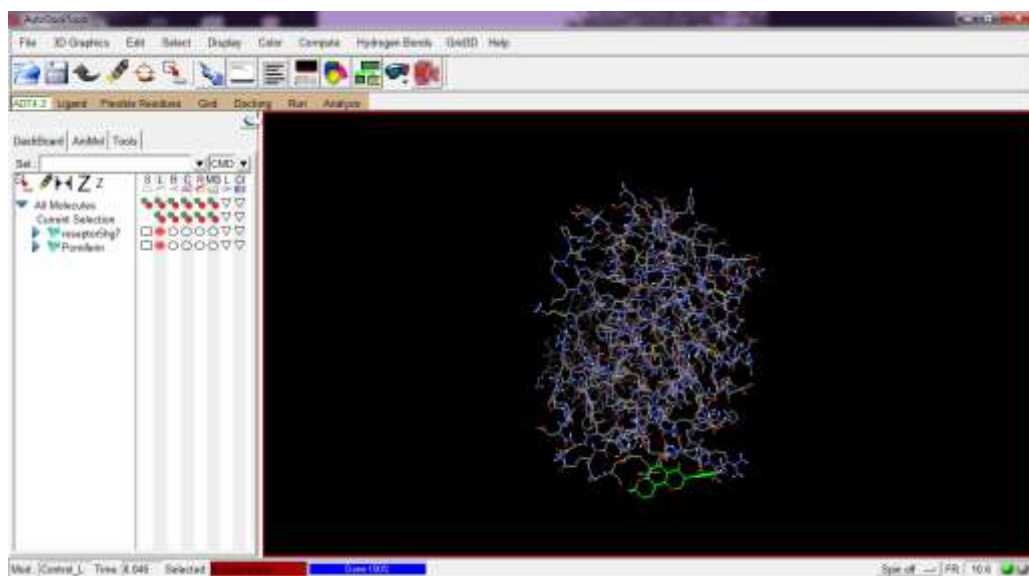
SITUS LIPINSKI'S RULE OF FIVE



The screenshot shows the web interface for the Lipinski Rule of Five tool. At the top, it identifies the Supercomputing Facility for Bioinformatics & Computational Biology at IIT Delhi. The main heading is "Lipinski Rule of Five". Below this, a paragraph explains the tool's purpose: to distinguish between drug-like and non-drug-like molecules based on five criteria. These criteria are listed in a bulleted format: molecular mass <math>< 350</math> Daltons, high lipophilicity (expressed as $\text{LogP} < 5</math>), less than 5 hydrogen bond donors, less than 10 hydrogen bond acceptors, and molar refractivity between 40-130. A note states that these filters help in early preclinical development and can help avoid costly late-stage failures. The interface is divided into three steps: Step 1: Input Drug File, which includes a file selection button and a "No file selected" message; Step 2: Input pH Value, with a text input field containing "7" and a range indicator "[Value ranges from 0.0 to 14.0]"; and Step 3: Click on 'Submit' to submit your job, featuring "Submit" and "Reset" buttons. A "How to Use the Tool" section at the bottom provides "OPTION 1:-" and a note that the input file should be in specific formats like *.pdb, *.mol, *.mcd, *.xyz, *.cif, *.mol.$

Gambar V.12 situs lipinski's rule of five

LAMPIRAN 10
PERANGKAT LUNAK AUTODOCK TOOLS

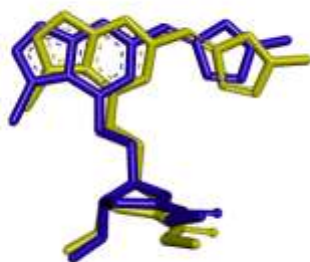


Gambar V.13 Tampilan Program Autodock Tools

LAMPIRAN 11
VALIDASI METODE



Gambar V.14 Visualisasi tumpang tindih ligan alami 5UGC (Biru) dengan ligan hasil *redocking* (kuning)



Gambar V.15 Visualisasi tumpang tindih ligan alami 5HG7 (Biru) dengan ligan hasil *redocking* (kuning)

Tabel V.1

Grid Box, RMSD, Nilai Ikatan Energi, dan Validasi Metode Ligan Alami

Kode PDB	<i>Grid Box</i>	RMSD	Ikatan Energi Ligan Alami (kkal/mol)
5UGC	X : -13,881 Y : 13,823 Z : -24,926	1,328Å	-7,87
5HG7	X : -13,599 Y : 15,359 Z : -25,243	1,917Å	-8,34

LAMPIRAN 12

SIFAT FISIKOKIMIA SENYAWA KACANG PANJANG DAN KACANG HIJAU BERDASARKAN ATURAN LIPINSKI'S RULE OF FIVE

Tabel V.2

Sifat Fisikokimia Senyawa Kacang Panjang berdasarkan aturan Lipinski's Rule Of Five

No	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	Akseptor Hidrogen	Ket
1	Delphinidin 3-O-glucoside	465	-0,10	9	12	Tidak Memenuhi
2	Kaempferol 3-O-glucoside	448	-0,44	7	11	Tidak Memenuhi
3	Malvidin 3-O-glucoside	493	0,50	7	12	Tidak Memenuhi
4	Petunidin 3-O-glucoside	479	0,20	8	12	Tidak memenuhi
5	Quercetin	302	2,01	5	7	Memenuhi
6	Quercetin 3-O-glucoside	464	-0,73	8	12	Tidak memenuhi
7	Cyanidin 3-O-galactocide	449	0,19	8	11	Tidak memenuhi
8	Cyanidin 3-O-glucoside	449	0,19	8	11	Tidak Memenuhi
9	Peonidin 3-O-glucoside	463	0,49	7	11	Tidak Memenuhi

**LAMPIRAN 12
(LANJUTAN)**

Tabel V.3

Sifat Fisikokimia Senyawa Kacang Hijau Berdasarkan aturan Lipinski's Rule Of Five

No	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	Akseptor Hidrogen	Ket
1	Daidzin	416	0,18	5	9	Memenuhi
2	Daidzein	254	2,71	2	4	Memenuhi
3	Ononin	430	0,49	4	9	Memenuhi
4	Formononetin	268	3,02	1	4	Memenuhi
5	Isoformononetin	268	3,02	1	4	Memenuhi
6	6,7,4'- trihydroxyisoflavon	270	2,42	3	5	Memenuhi
7	6,7,4'- trimethoxyisoflavon	312	3,32	0	5	Memenuhi
8	Genistin	432	-0,11	6	10	Tidak Memenuhi
9	Sissotrin	446	0,19	5	10	Memenuhi
10	Genistein	270	2,42	3	5	Memenuhi
11	Prunetin	284	2,72	2	5	Memenuhi
12	Biochanin A	284	2,72	2	5	Memenuhi
13	6''-O-acetylgenistin	474	0,46	5	11	Tidak Memenuhi
14	5,7,4'- trimethoxyisoflavon	312	3,33	0	5	Memenuhi
15	2'-hydroxygenistein	286	2,12	4	6	Memenuhi

**LAMPIRAN 12
(LANJUTAN)**

Tabel V.3

Sifat Fisikokimia Senyawa Kacang Hijau Berdasarkan aturan Lipinski's Rule Of Five

No	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	Akseptor Hidrogen	Ket
16	Apigenin	270	2,42	3	5	Memenuhi
17	Vitexin	432	-0,06	7	10	Tidak Memenuhi
18	Isovitexin	432	-0,06	7	10	Tidak Memenuhi
19	Rutin	610	-1,87	10	16	Tidak Memenuhi
20	Kaempferol	286	2,31	4	6	Memenuhi
21	Myricetin	318	1,72	6	8	Tidak Memenuhi
22	Rhamnetin	316	2,31	4	7	Memenuhi
23	Kaempferitrin	578	-0,19	8	14	Tidak Memenuhi
24	Kaempferol 3-rutinoside	594	-1,58	9	15	Tidak Memenuhi
25	3,5,7,3',4'-pentahydroxyflavonol	318	1,72	6	8	Tidak Memenuhi
26	3,7,8,3',4'-pentahydroxyflavonol	318	1,72	6	8	Tidak Memenuhi
27	Naringin	580	-1,16	8	14	Tidak Memenuhi
28	Neohesperidin	610	-1,16	8	15	Tidak Memenuhi

LAMPIRAN 12
(LANJUTAN)

Tabel V.3

Sifat Fisikokimia Senyawa Kacang Hijau Berdasarkan aturan Lipinski's Rule Of Five

No	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	Akseptor Hidrogen	Ket
29	Hesperetin	302	2,52	3	6	Memenuhi
30	5,7-dihydroxyflavanon	312	-0,05	5	6	Memenuhi
31	Eriodictyol 7-glucoside	450	-0,31	7	11	Tidak Memenuhi
32	Eriodictyol	288	2,21	4	6	Memenuhi
33	Naringenin	272	2,51	3	5	Memenuhi
34	Rhododendrin	328	-0,47	5	7	Memenuhi
35	Scopoletin	192	1,33	1	4	Memenuhi
36	Pomiferin	420	5,11	3	6	Tidak Memenuhi
37	Delphinidin	303	2,42	6	7	Tidak Memenuhi
38	2',4,4-trihydroxychalcon	256	2,70	3	4	Memenuhi
39	Phloretin	274	2,32	4	5	Memenuhi
40	Coumestrol	268	3,04	2	5	Memenuhi
41	Osajin	404	5,40	2	5	Tidak Memenuhi
42	p-hydroxybenzoic	138	1,09	2	3	Memenuhi
43	protocatechuic	154	0,79	3	4	Memenuhi
44	Syringic	198	1,11	2	5	Memenuhi

LAMPIRAN 12
(LANJUTAN)

Tabel V.3

Sifat Fisikokimia Senyawa Kacang Hijau Berdasarkan aturan Lipinski's Rule Of Five

No	Senyawa	BM (g/mol)	Log P	Donor Hidrogen	Akseptor Hidrogen	Ket
45	Gallic acid	170	0,50	4	5	Memenuhi
46	Vanillic acid	168	1,09	2	4	Memenuhi
47	Gentisic acid	154	0,79	3	4	Memenuhi
48	Shikimic acid	174	-1,52	4	5	Memenuhi
49	p-coumaric	166	1,41	2	3	Memenuhi
50	Caffeic acid	180	1,19	3	4	Memenuhi
51	Cinnamic acid	148	1,78	1	2	Memenuhi
52	Ferulic	194	1,49	2	4	Memenuhi
53	Chlorogenic acid	354	-0,64	6	9	Tidak Memenuhi

Syarat : 1. Berat molekul kurang dari 500; 2. Memiliki tidak lebih dari 5 gugus hidrogen donor; 3. Memiliki tidak lebih dari 10 gugus hidrogen akseptor; 4. Nilai log P tidak lebih dari 5

LAMPIRAN 13
HASIL PENAMBATAN MOLEKUL

Tabel V.4
Hasil Penambatan Molekuler Ligan Alami, Senyawa Kacang Panjang dan Obat
Pembanding pada Reseptor EGFR *wildtype* (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1	Ligan Alami	-7,87	2	PRO794, MET793	1710
2	Gefitinib (pembanding)	-9,05	1	MET793	233,39
3	Quercetin 3-O-Glucoside	-9,31	7	CYS797, GLN791, MET793, LEU718, THR854, ASP800, PRO794	148,77
4	Quercetin	-9,17	5	GLN791, THR854, MET793, LEU718, CYS77	188,85
5	Delphinidin 3-O-glucoside	-8,56	6	GLN791, LEU718, MET793, ASP800, PRO794, CYS797	530,09

LAMPIRAN 13
(LANJUTAN)

Tabel V.4

Hasil Penambatan Molekuler Senyawa Kacang Panjang pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
6	Peonidin 3-O-glucoside	-8,33	5	CYS775, GLN791, MET793, THR854, SER720	779,15
7	Kaempferol 3-O-glucoside	-8,19	5	GLN791, LEU718, ARG841, CYS775, PRO794	995,54
8	Malvidin 3-O-Glucoside	-8,01	5	GLN791, MET793, PRO794, CYS797, ASP800	1350
9	Cyanidin 3-O-galaktocide	-7,94	4	GLN791, MET793, LEU718, PRO794	1520
10	Cyanidin 3-O-glucoside	-7,85	5	GLU804, MET793, ASP800, LYS716, PRO794	1760

LAMPIRAN 13
(LANJUTAN)

Tabel V.4

Hasil Penambatan Molekuler Senyawa Kacang Panjang pada Reseptor EGFR *wildtype* (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
11	Petunidin 3-O-glucoside	-7,85	5	ASP800, CYS775, GLN791, MET793, PRO794	1770

LAMPIRAN 13
(LANJUTAN)

Tabel V.4
Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1	Osajin	-10,28	1	PRO794	29,31
2	Pomiferin	-10,17	3	LYS716, LYS728, MET793	34,86
3	Kaempferol 3- retinoside	-9,36	7	ASP800, CYS775, CYS797, GLN791, GLU804, PHE795, PRO794	136,96
4	Coumestrol	-9,13	3	LYS745, MET793, THR854	204,61
5	Ononin	-9,08	2	ASP800, GLU804	220,62
6	Apigenin	-8,98	4	LEU718, GLN791, MET793, THR854	260,85

**LAMPIRAN 13
(LANJUTAN)**

Tabel V.4
Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
7	Kaempferol	-8,93	5	ASP855, LEU718, LYS745, MET793, THR854	285,85
8	Genistin	-8,87	5	CYS775, GLN791, GLU804, MET793, PHE795	315,14
9	Chlorogenic acid	-8,83	5	ASP800, LYS745, GLN791, MET793, THR854	337,61
10	Rhamnetin	-8,83	4	ASP800, CYS797, GLN791, MET793	336,42
11	Naringenin	-8,70	6	CYS775, GLN791, LEU718, LYS745, MET793, THR854	418,83

**LAMPIRAN 13
(LANJUTAN)**

Tabel V.4

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
12	Eriodictyol	-8,69	6	CYS775, GLN791, MET793, THR854, LEU718, LYS745	426,90
13	Myricetin	-8,65	5	CYS775, LEU718, GLN791, MET793, THR854	453,88
14	5,7-Dihydroxyflavanon	-8,61	3	GLN791, MET793, THR854	490,27
15	Formononetin	-8,57	3	LYS745, MET793, THR854	522,40
16	Daidzin	-8,55	5	CYS797, LYS745, THR854, PRO794, PHE795	535,96

LAMPIRAN 13
(LANJUTAN)

Tabel V.4

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
17	2',4,4'- Trihydroxychalcon	-8,52	5	GLN791, LEU718, MET793, LYS745, THR854	567,30
18	Genistein	-8,49	5	CYS775, GLN791, MET793, THR854, PRO794	601,41
19	3,5,7,3',4'- Pentahydroxyflavonol	-8,47	5	CYS775, CYS797, GLN791, MET793, ASP800	619,11
20	Vitexin	-8,45	3	LYS745, MET793, THR854	635,66
21	6,7,4'- Trimethoxyisoflavon	-8,42	1	MET793	674,17
22	Isoformononetin	-8,39	4	ASP855, LYS745,	707,42

LAMPIRAN 13
(LANJUTAN)

Tabel V.4

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
				MET793, THR854	
23	Daidzein	-8,36	4	ASP855, MET793, LYS745, THR854	749,60
24	Biochanin A	-8,34	4	GLN791, LYS745, MET793, THR854	775,92
25	Sissotrin	-8,34	4	ASP800, GLU804, CYS797, CYS775	768,05
26	Prunetin	-8,28	4	ASP855, LYS745, MET793, THR854	846,46
27	6''-O-Acetylgenistin	-8,18	4	LYS716, LYS745, MET793, THR854	1000
28	5,7,4'-Trimethoxyisoflavon	-8,15	1	MET793	1060

**LAMPIRAN 13
(LANJUTAN)**

Tabel V.4
Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
29	3,7,8,3',4'- Pentahydroxyflavonol	-7,93	3	GLN791, PRO794	1550
30	Phloretin	-7,88	5	GLN791, LYS745, MET793, THR854, LEU718	1670
31	Neohesperidin	-7,84	4	CYS797, GLU804, MET793, PRO794	1790
32	Delphinidin	-7,85	5	CYS797, GLN791, MET793, CYS775, THR854	1750
33	2'-Hydroxygenistein	-7,85	3	MET793, LYS745, THR854	1770
34	Naringin	-7,81	7	ASP855, ASP800, CYS797, GLU804, LYS745, MET793,	1900

LAMPIRAN 13
(LANJUTAN)

Tabel V.4

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
35	Isovitexin	-7,81	5	ASP800, CYS775, GLN791, GLU804, PHE795	1870
36	6,7,4'- Trihydroxyisoflavon	-7,74	3	MET793, PRO794, THR854	2120
37	Hesperetin	-7,30	3	ASP800, CYS797, MET793	4490
38	Caffeic acid	-7,21	3	LYS745, MET793, THR854	5200
39	Kaempferitrin	-7,02	3	ASP800, GLN791, PRO794	7140
40	Rhododendrin	-6,90	3	LYS745, THR854, PRO794	8730
41	Ferulic	-6,79	4	ASP855, LYS745,	10610

LAMPIRAN 13
(LANJUTAN)

Tabel V.4
Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
				MET793, THR854	
42	Scopoletin	-6,65	4	LYS745, THR854, MET793, GLN791	13400
43	Cinnamic acid	-6,62	2	LYS745, THR854	14100
44	<i>P</i> -coumaric	-6,59	4	ASP855, LYS745, MET793, THR854	14720
45	Rutin	-6,54	2	ASP800, MET793	15990
46	<i>P</i> -hydroxybenzoic	-6,34	2	GLN791, THR854	22650
47	Eriodictyol 7-Glucoside	-6,28	4	ARG841, ASP800, CYS797, LEU718	24930
48	Vanillic acid	-6,01	2	LYS745, THR854	39120
49	Protocatechuic	-5,50	3	CYS775, GLN791, THR854	93,15

**LAMPIRAN 13
(LANJUTAN)**

Tabel V.4
Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR
wildtype (5UGC)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
50	Gentisic acid	-5,43	2	LYS728, MET793,	105180
51	Gallic acid	-5,36	3	LYS716, LYS728, MET793	118210
52	Shikimic acid	-5,16	3	LYS716, LYS728, MET793	163960
53	Syringic	-4,66	2	GLN791, MET793	380900

LAMPIRAN 13
HASIL PENAMBATAN MOLEKUL

Tabel V.5
Hasil Penambatan Molekuler Ligan Alami, Senyawa Kacang Panjang dan Obat
Pembanding pada Reseptor EGFR *mutan* (5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1	Ligan Alami	-8,34	2	CYS797, MET793	768,85
2	Gefitinib (pembanding)	-7,00	1	MET793	7370
3	Quercetin 3-O-Glucoside	-8,64	5	CYS775, GLN791, MET793, LEU718, SER720	467,66
4	Quercetin	-8,26	5	GLN791, THR854, MET793, ASP800, CYS797	875,53
5	Petunidin 3-O-glucoside	-7,78	6	ASP800, ARG841, CYS797, GLN791, LEU718, MET793	1990

LAMPIRAN 13
(LANJUTAN)

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Panjang pada Reseptor EGFR
mutan (5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
6	Malvidin 3-O-Glucoside	-7,73	6	GLN791, LEU718, MET793, ARG841, CYS797, ASP800	2150
7	Kaempferol 3-O-glucoside	-7,71	4	GLN791, LEU718, MET793, SER720	2240
8	Cyanidin 3-O-glucoside	-7,68	5	GLN791, MET793, ASP800, ARG841, CYS797	2350
9	Cyanidin 3-O-galaktocide	-7,41	5	ASP800, CYS797, GLN791, MET793, SER720	3700
10	Delphinidin 3-O-glucoside	-7,13	6	GLN791, LEU718, MET793, ASP800, ARG841, CYS797	5910

**LAMPIRAN 13
(LANJUTAN)****Tabel V.5**Hasil Penambatan Molekuler Senyawa Kacang Panjang pada Reseptor EGFR
mutan (5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
11	Peonidin 3-O-glucoside	-7,31	5	ASP800, CYS797, GLN791, MET793, SER720	4400

LAMPIRAN 13
(LANJUTAN)

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan*
(5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
1	Pomiferin	-9,09	3	CYS775, LYS745, THR854	215,63
2	Osajin	-8,99	2	LYS745, THR854	255,16
3	Kaempferol	-8,75	6	ASP855, GLN791, LEU718, LYS745, MET793, THR854	382,42
4	Coumestrol	-8,57	4	ASP855, LYS745, MET793, THR854	521,54
5	Biochanin A	-8,55	5	GLN791, LYS745, MET793, CYS775, THR854	538,21
6	Rhamnetin	-8,30	4	ASP800, CYS797, GLN791, MET793	820,88

**LAMPIRAN 13
(LANJUTAN)**

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan*
(5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
7	Naringin	-8,24	5	ASP800, GLN791, LEU718, MET793, SER720	906,52
8	Eriodictyol	-8,13	5	ASP800, CYS797, GLN791, MET793, THR854	1090
9	Daidzein	-8,12	4	ASP855, MET793, LYS745, THR854	1110
10	Apigenin	-7,88	4	LYS745, LEU718, MET793, THR854	1680
11	Myricetin	-8,08	5	ASP800, CYS797, GLN791, MET793, THR854	1200
12	Formononetin	-8,03	3	LYS745, MET793,	1300

LAMPIRAN 13
(LANJUTAN)

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan*
(5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
				THR854	
13	Prunetin	-7,98	4	ASP855, LYS745, MET793, THR854	1420
14	Vitexin	-7,97	5	ARG841, CYS797, LYS745, MET793, THR854	1450
15	Hesperetin	-7,92	3	ASP800, MET793, SER720	1560
16	Daidzin	-7,91	4	ASP800, CYS797, LYS745, THR854	1590
17	Apigenin	-7,88	4	LYS745, LEU718, MET793, THR854	1680
18	Naringenin	-7,88	6	CYS775, GLN791,	1670

LAMPIRAN 13
(LANJUTAN)

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan*
(5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
				LEU718, LYS745, MET793, THR854	
19	3,5,7,3',4'- Pentahydroxyflavonol	-7,82	4	CYS797, GLN791, MET793, ASP800	1840
20	Isoformononetin	-7,70	3	LYS745, MET793, THR854	2280
21	6,7,4'- Trimethoxyisoflavon	-7,68	1	MET793	2350
22	5,7- Dihydroxyflavanon	-7,66	4	CYS775, GLN791, MET793, THR854	2410
23	2',4,4'- Trihydroxychalcon	-7,65	4	LEU718, MET793, LYS745, THR854	2480
24	5,7,4'- Trimethoxyisoflavon	-7,62	4	CYS775, GLN791, MET793, THR854	2580

**LAMPIRAN 13
(LANJUTAN)**

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan*
(5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
25	2'-Hydroxygenistein	-7,55	5	CYS775, GLN791, MET793, LYS745, THR854	2910
26	Kaempferol 3-retinoside	-7,55	5	ARG841, ASN842, ASP800, GLN791, LEU718	2910
27	6,7,4'-Trihydroxyisoflavon	-7,53	3	GLN791, MET793, SER720	3040
28	Delphinidin	-7,48	5	ASP800, CYS797, GLN791, LEU718, MET793	3300
29	Genistein	-7,30	3	GLN791, MET793, SER720	4470
30	Kaempferitrin	-7,30	6	ARG841, ASN824,	4480

**LAMPIRAN 13
(LANJUTAN)**

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan*
(5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
				ASP800, GLN791, MET793, PRO794	
31	Isovitexin	-7,14	5	ASP800, CYS775, CYS797, GLN791, LEU718,	5860
32	Ononin	-7,14	2	CYS797, GLU804	5830
33	Genistin	-7,12	4	CYS775, GLN791, MET793, PHE795	6000
34	3,7,8,3',4'- Pentahydroxyflavon ol	-7,10	3	GLN791, LEU718, PRO794	6230
35	Caffeic acid	-7,09	4	GLN791, LYS745, MET793, THR854	6410
36	6''-O-Acetylgenistin	-6,89	2	GLN791, MET793	8910

LAMPIRAN 13
(LANJUTAN)

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan*
(5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
37	Phloretin	-6,77	6	CYS775, GLN791, LYS745, MET793, THR854, PRO794	10900
38	Chlorogenic acid	-6,58	3	CYS775, LYS745, THR854	15000
39	Sissotrin	-6,56	3	ARG841, GLN791, MET793	15500
40	Cinnamic acid	-6,30	2	LYS745, THR854	24000
41	Neohesperidin	-6,11	3	ASP800, CYS797, SER720	33020
42	Eriodictyol 7-Glucoside	-6,08	3	ARG841, CYS797, LEU718	34740
43	<i>P</i> -coumaric	-6,02	4	LYS745, GLN791, MET793, THR854	38680

LAMPIRAN 13
(LANJUTAN)

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan*
(5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
44	Rutin	-5,93	4	ARG841, LEU718, GLN791, PRO794	44800
45	Rhododendrin	-5,87	3	GLN791, MET793, SER720	49640
46	<i>P</i> -hydroxybenzoic	-5,75	3	ASP855, GLN791, THR854	61460
47	Scopoletin	-5,64	3	CYS775, THR854, MET793	73330
48	Protocatechuic	-5,33	3	ASP855, GLN791, THR854	124060
49	Gallic acid	-5,22	3	LYS716, LYS728, MET793	150110
50	Vanillic acid	-5,14	2	LYS745, THR854	169470
51	Syringic	-4,54	2	GLN791, MET793	468280

LAMPIRAN 13
(LANJUTAN)

Tabel V.5

Hasil Penambatan Molekuler Senyawa Kacang Hijau pada Reseptor EGFR *mutan* (5HG7)

No	Senyawa	Ikatan Energi (ΔG)	Jumlah Ikatan Hidrogen	Residu Asam Amino	KI (nM)
52	Gentisic acid	-4,53	2	GLN791, MET793,	479510
53	Shikimic acid	-4,13	2	MET793, PRO794	939110

LAMPIRAN 14
UJI PREAMMET

Tabel V.6
Uji PreADMET (Absorpsi dan Distribusi) Senyawa Senyawa Kacang Panjang dan Obat Pemanding

No	Senyawa	Caco-2 (nm.sec ⁻¹)	HIA (%)	Plasma Protein Binding (%)
1	Gefitinib	54,15 ^b	96,62 ^a	80,77 ^b
2	Cyanidin 3-O-galactocide	3,65 ^c	17,86 ^c	80,20 ^b
3	Cyanidin 3-O-glucoside	5,92 ^b	19,72 ^c	79,61 ^b
4	Delphinidin 3-O-glucoside	4,86 ^b	8,81 ^c	80,18 ^b
5	Kaempferol 3-O-glucoside	11,21 ^b	24,98 ^b	60,6 ^b
6	Malvidin 3-O-Glucoside	7,36 ^b	30,95 ^b	55,49 ^b
7	Peonidin 3-O-glucoside	6,85 ^b	35,22 ^b	65,41 ^b
8	Petunidin 3-O-glucoside	13,42 ^b	64,23 ^b	65,99 ^b
9	Quercetin	3,41 ^c	93,23 ^a	63,48 ^b
10	Quercetin 3-O-Glucoside	9,44 ^b	11,77 ^c	59,16 ^b

LAMPIRAN 14
(LANJUTAN)

Tabel V.6

Uji PreADMET (Absorpsi dan Distribusi) Senyawa Senyawa Kacang Hijau

No	Senyawa	Caco-2 (nm.sec ⁻¹)	HIA (%)	Plasma Protein Binding (%)
1	2'-Hydroxygenistein	3,58 ^c	79,43 ^a	96,23 ^a
2	2',4,4'-Trihydroxychalcon	20,16 ^b	88,31 ^a	98,25 ^a
3	3,5,7,3',4'- Pentahydroxyflavonol	0,99 ^c	40,94 ^b	98,33 ^a
4	3,7,8,3',4'- Pentahydroxyflavonol	10,59 ^b	44,06 ^b	80,47 ^b
5	5,7-Dihydroxyflavanon	2,47 ^c	92,35 ^a	98,45 ^a
6	5,7,4'-Trimethoxyisoflavon	47,53 ^b	97,92 ^a	84,5 ^b
7	6''-O-Acetylgenistin	9,66 ^b	55,08 ^b	65,25 ^b
8	6,7,4'-Trihydroxyisoflavon	3,75 ^c	88,11 ^a	96,64 ^a
9	6,7,4'-Trimethoxyisoflavon	45,21 ^b	97,92 ^a	85,64 ^b
10	Apigenin	10,55 ^b	88,12 ^a	97,25 ^a
11	Biochanin A	3,40 ^c	93,04 ^a	85,01 ^b
12	Caffeic acid	21,11 ^b	79,21 ^a	47,92 ^b

LAMPIRAN 14
(LANJUTAN)

Tabel V.6

Uji PreADMET (Absorpsi dan Distribusi) Senyawa Senyawa Kacang Hijau

No	Senyawa	Caco-2 (nm.sec ⁻¹)	HIA (%)	Plasma Protein Binding (%)
13	Chlorogenic acid	9,18 ^b	43,55 ^b	60,86 ^b
14	Cinnamic acid	21,01 ^b	97,84 ^a	60,85 ^b
15	Coumestrol	1,72 ^c	92,53 ^a	95,78 ^a
16	Daidzein	7,72 ^b	92,64 ^a	88,70 ^b
17	Daidzin	8,93 ^b	65,77 ^b	42,38 ^b
18	Delphinidin	0,37 ^c	54,22 ^b	100 ^a
19	Eriodictyol	4,53 ^b	77,43 ^a	100 ^a
20	Eriodictyol 7-Glucoside	4,86 ^b	21,74 ^b	71,63 ^b
21	Ferulic	21,12 ^b	90,60 ^a	50,41 ^b
22	Formononetin	7,60 ^b	95,55 ^a	85,09 ^b
23	Gallic acid	13,84 ^b	53,69 ^b	65,38 ^b
24	Genistein	5,74 ^b	88,12 ^a	89,74 ^b
25	Genistin	8,21 ^b	47,10 ^b	65,18 ^b
26	Gentisic acid	18,30 ^b	74,75 ^a	69,61 ^b

LAMPIRAN 14
(LANJUTAN)

Tabel V.6

Uji PreADMET (Absorpsi dan Distribusi) Senyawa Senyawa Kacang Hijau

No	Senyawa	Caco-2 (nm.sec ⁻¹)	HIA (%)	Plasma Protein Binding (%)
27	Hesperetin	7,00 ^b	87,19 ^a	96,79 ^a
28	Isoformononetin	14,76 ^b	95,55 ^a	86,11 ^b
29	Isovitexin	6,91 ^b	31,37 ^b	61,48 ^b
30	Kaempferitrin	5,18 ^b	13,76 ^c	42,73 ^b
31	Kaempferol	9,57 ^b	79,44 ^a	89,61 ^b
32	Kaempferol 3-retinoside	9,13 ^b	6,28 ^c	42,37 ^b
33	Myricetin	0,99 ^c	40,96 ^b	96,78 ^a
34	Naringenin	4,65 ^b	92,57 ^a	98,65 ^a
35	Naringin	10,39 ^b	4,86 ^c	50,65 ^b
36	Neohesperidin	7,16 ^b	6,06 ^c	39,31 ^b
37	Ononin	7,27 ^b	82,49 ^a	65,01 ^b
38	Osajin	23,19 ^b	94,87 ^a	94,92 ^a
39	<i>P</i> -coumaric	21,11 ^b	90,67 ^a	61,73 ^b
40	<i>P</i> -hydroxybenzoic	20,31 ^b	88,14 ^a	8,04 ^b

LAMPIRAN 14
(LANJUTAN)

Tabel V.6

Uji PreADMET (Absorpsi dan Distribusi) Senyawa Senyawa Kacang Hijau

No	Senyawa	Caco-2 (ngnm.sec ⁻¹)	HIA (%)	Plasma Protein Binding (%)
41	Phloretin	18,10 ^b	78,98 ^a	100 ^a
42	Pomiferin	14,70 ^b	92,47 ^a	95,21 ^a
43	Protocatechuic	18,30 ^b	74,75 ^a	27,11 ^b
44	Prunetin	7,07 ^b	93,04 ^a	86,28 ^b
45	Rhamnetin	9,33 ^b	88,18 ^a	83,47 ^b
46	Rhododendrin	11,02 ^b	51,11 ^b	68,02 ^b
47	Rutin	5,31 ^b	10,61 ^c	61,76 ^b
48	Scopoletin	0,27 ^c	93,92 ^a	29,42 ^b
49	Shikimic acid	14,22 ^b	43,06 ^b	23,79 ^b
50	Sissotrin	6,53 ^b	65,89 ^b	60,54 ^b
51	Syringic	18,83 ^b	82,03 ^a	69,77 ^b
52	Vanillic acid	19,93 ^b	85,37 ^a	52,11 ^b
53	Vitexin	5,48 ^b	31,37 ^b	61,48 ^b

Keterangan :

%HIA = (a) 70-100% well absorbed, (b) 20-70% moderately absorbed, (c) 0-20% poorly absorbed.

In Vitro caco-2 cell permeability = (a) >70 higher permeability, (b) 4-70 medium permeability, (c) < 4 low permeability.
% PPB = (a) >90% strongly bond, (b) < 90% weakly bond.



LAMPIRAN 15

UJI TOKSISITAS

Tabel V.7

Uji Toksisitas Senyawa Kacang Panjang dan Obat Perbandingan

No	Senyawa Ligan	Mutagenik	Karsinogenik
1	Gefitinib	Mutagen	Negatif
2	Cyanidin 3-O-galaktocide	Non-Mutagen	Positif
3	Cyanidin 3-O-glucoside	Non-Mutagen	Positif
4	Delphinidin 3-O-glucoside	Non-Mutagen	Positif
5	Kaempferol 3-O-glucoside	Non-Mutagen	Negatif
6	Malvidin 3-O-Glucoside	Non-Mutagen	Negatif
7	Peonidin 3-O-glucoside	Non-Mutagen	Negatif
8	Petunidin 3-O-glucoside	Non-Mutagen	Positif
9	Quercetin	Mutagen	Negatif
10	Quercetin 3-O-Glucoside	Non-Mutagen	Negatif

LAMPIRAN 15
(LANJUTAN)

Tabel V.7
Uji Toksisitas Senyawa Kacang Hijau

No	Senyawa Ligan	Mutagenik	Karsinogenik
1	2'-Hydroxygenistein	Mutagen	Negatif
2	2',4,4'-Trihydroxychalcon	Mutagen	Positif
3	3,5,7,3',4'- Pentahydroxyflavonol	Mutagen	Negatif
4	3,7,8,3',4'- Pentahydroxyflavonol	Mutagen	Negatif
5	5,7-Dihydroxyflavanon	Mutagen	Negatif
6	5,7,4'-Trimethoxyisoflavon	Mutagen	Negatif
7	6''-O-Acetylgenistin	Non-Mutagen	Positif
8	6,7,4'-Trihydroxyisoflavon	Non-Mutagen	Positif
9	6,7,4'-Trimethoxyisoflavon	Mutagen	Negatif
10	Apigenin	Mutagen	Positif
11	Biochanin A	Mutagen	Negatif
12	Caffeic acid	Mutagen	Negatif
13	Chlorogenic acid	Mutagen	Positif

**LAMPIRAN 15
(LANJUTAN)**

Tabel V.7
Uji Toksisitas Senyawa Kacang Hijau

No	Senyawa Ligan	Mutagenik	Karsinogenik
14	Cinnamic acid	Mutagen	Negatif
15	Coumestrol	Mutagen	Negatif
16	Daidzein	Mutagen	Negatif
17	Daidzin	Mutagen	Positif
18	Delphinidin	Mutagen	Negatif
19	Eriodictyol	Mutagen	Negatif
20	Eriodictyol 7-Glucoside	Non-Mutagen	Negatif
21	Ferulic	Mutagen	Negatif
22	Formononetin	Mutagen	Negatif
23	Gallic acid	Mutagen	Negatif
24	Genistein	Mutagen	Negatif
25	Genistin	Non-Mutagen	Positif
26	Gentisic acid	Mutagen	Negatif
27	Hesperetin	Mutagen	Negatif

LAMPIRAN 15
(LANJUTAN)

Tabel V.7
Uji Toksisitas Senyawa Kacang Hijau

No	Senyawa Ligan	Mutagenik	Karsinogenik
28	Isoformononetin	Mutagen	Negatif
29	Isovitexin	Mutagen	Positif
30	Kaempferitrin	Non-Mutagen	Negatif
31	Kaempferol	Mutagen	Negatif
32	Kaempferol 3-retinoside	Non-Mutagen	Negatif
33	Myricetin	Mutagen	Negatif
34	Naringenin	Mutagen	Negatif
35	Naringin	Non-Mutagen	Positif
36	Neohesperidin	Non-Mutagen	Negatif
37	Ononin	Mutagen	Positif
38	Osajin	Non-Mutagen	Negatif
39	<i>P</i> -coumaric	Mutagen	Negatif
40	<i>P</i> -hydroxybenzoic	Mutagen	Negatif

LAMPIRAN 15
(LANJUTAN)

Tabel V.7
Uji Toksisitas Senyawa Kacang Hijau

No	Senyawa Ligan	Mutagenik	Karsinogenik
41	Phloretin	Mutagen	Negatif
42	Pomiferin	Non-Mutagen	Negatif
43	Protocatechuic	Mutagen	Negatif
44	Prunetin	Mutagen	Negatif
45	Rhamnetin	Mutagen	Negatif
46	Rhododendrin	Mutagen	Negatif
47	Rutin	Non-Mutagen	Negatif
48	Scopoletin	Mutagen	Negatif
49	Shikimic acid	Mutagen	Positif
50	Sissotrin	Non-Mutagen	Positif
51	Syringic	Mutagen	Negatif
52	Vanillic acid	Mutagen	Negatif
53	Vitexin	Non-Mutagen	Positif