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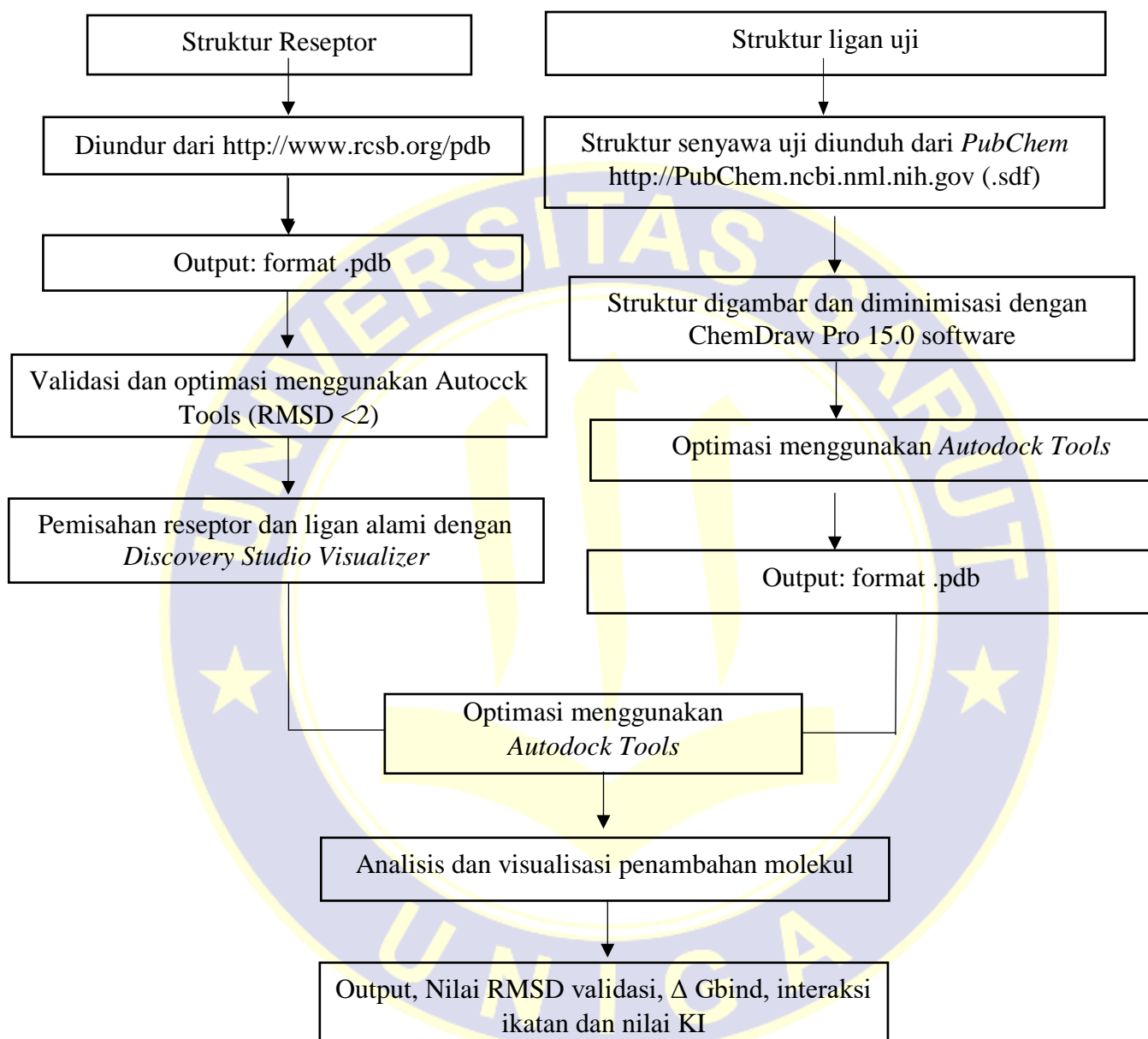
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## LAMPIRAN 1

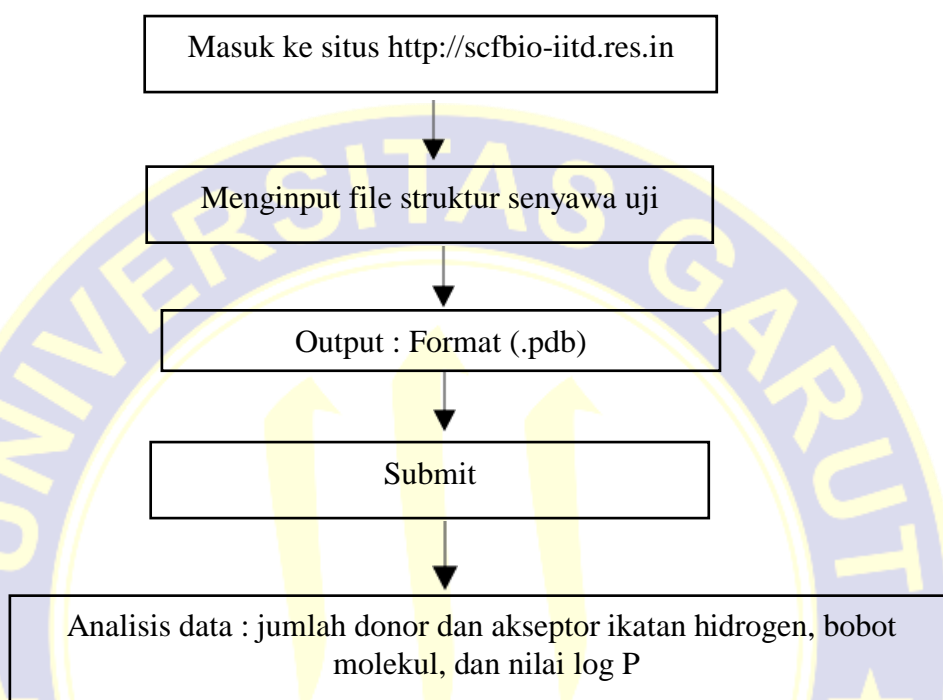
### ALUR PENELITIAN SIMULASI MOLEKULAR DOCKING



**Gambar IV.1** Alur penelitian simulasi *Molecular Docking*

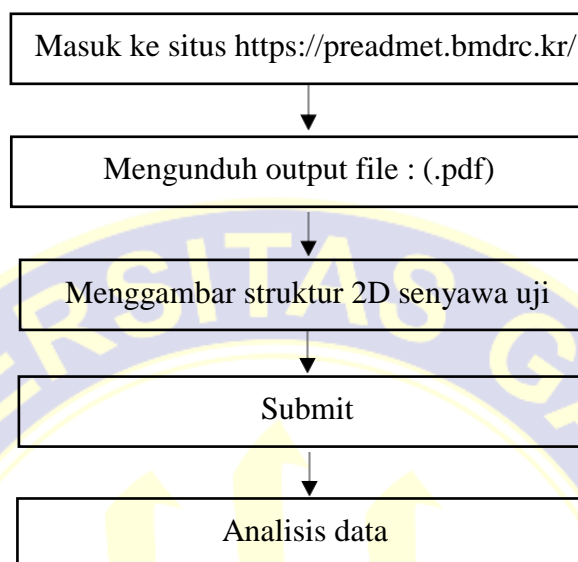
**LAMPIRAN 1  
(LANJUTAN)**

**ALUR PENELITIAN SIMULASI MOLEKULAR DOCKING**



**Gambar IV.2** Analisis fisikokimia berdasarkan *Lipinski Rule of Five*

**LAMPIRAN 1  
(LANJUTAN)  
ALUR PENELITIAN SIMULASI *MOLEKULAR DOCKING***



**Gambar IV.3** Analisis pre-ADME dan toksisitas

## LAMPIRAN 2

### SITUS DAN APLIKASI



Selamat datang

Menyetorkan

Mencari

Membayangkan

Menganalisa

#### Pandangan Struktural Biologi

Sumber daya ini didukung oleh informasi arsip Bank Data Protein tentang bentuk 3D protein, asam nukleat, dan rakitan kompleks yang membantu siswa dan peneliti memahami semua aspek biomedis dan pertanian, mulai dari sintesis protein hingga kesehatan dan penyakit.

Sebagai anggota wwPDB, PDB RCSB mengkurasi dan membubuhi keterangan data PDB.

RCSB PDB dibangun di atas data dengan menciptakan alat dan sumber daya untuk penelitian dan pendidikan dalam biologi molekuler, biologi struktural, biologi komputasi, dan seterusnya.

**COVID-19**

**CORONAVIRUS**

*Celebrating*

**PROTEIN**

#### Agustus Molekul Bulan

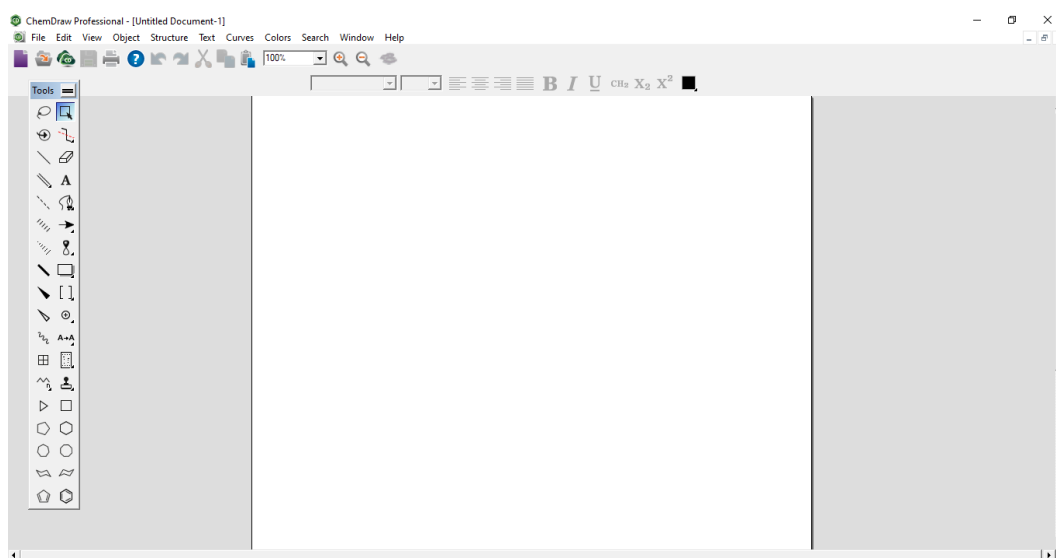
**Gambar IV.4** Tampilan situs *Protein Data Bank*



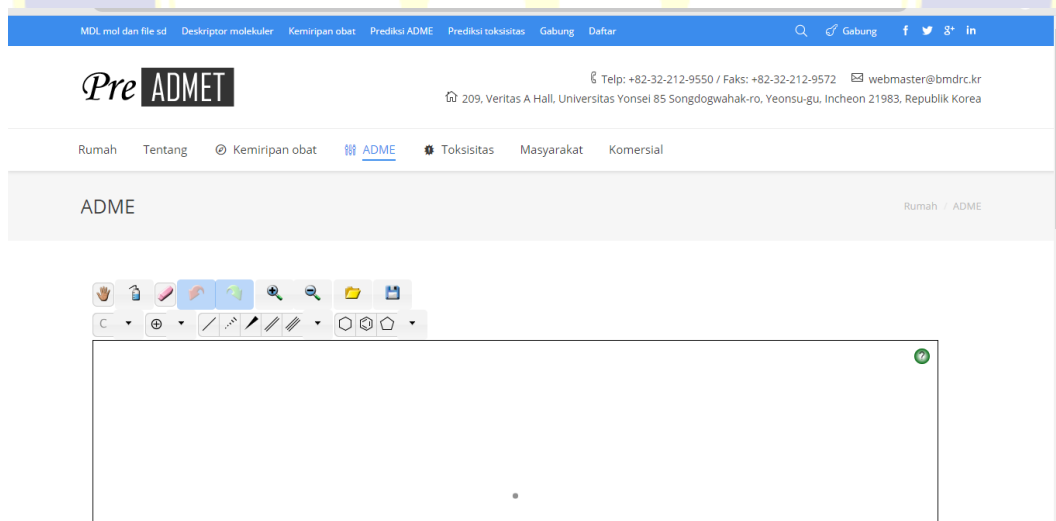
**Gambar IV.5** Tampilan situs *Pubchem*

## LAMPIRAN 2 (LANJUTAN)

### SITUS DAN APLIKASI



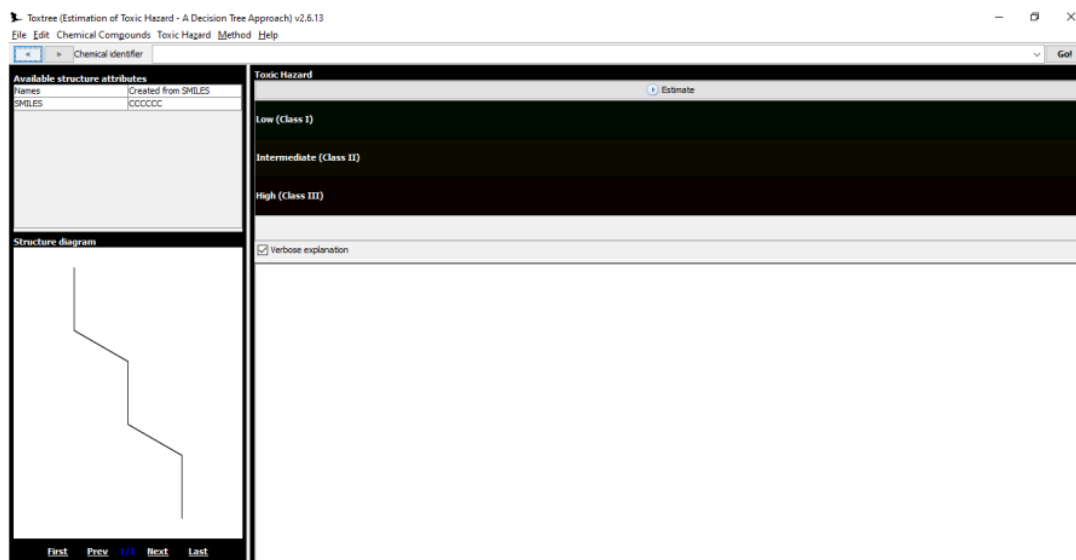
Gambar IV.6 Tampilan aplikasi *ChemDraw Professional 15.0*



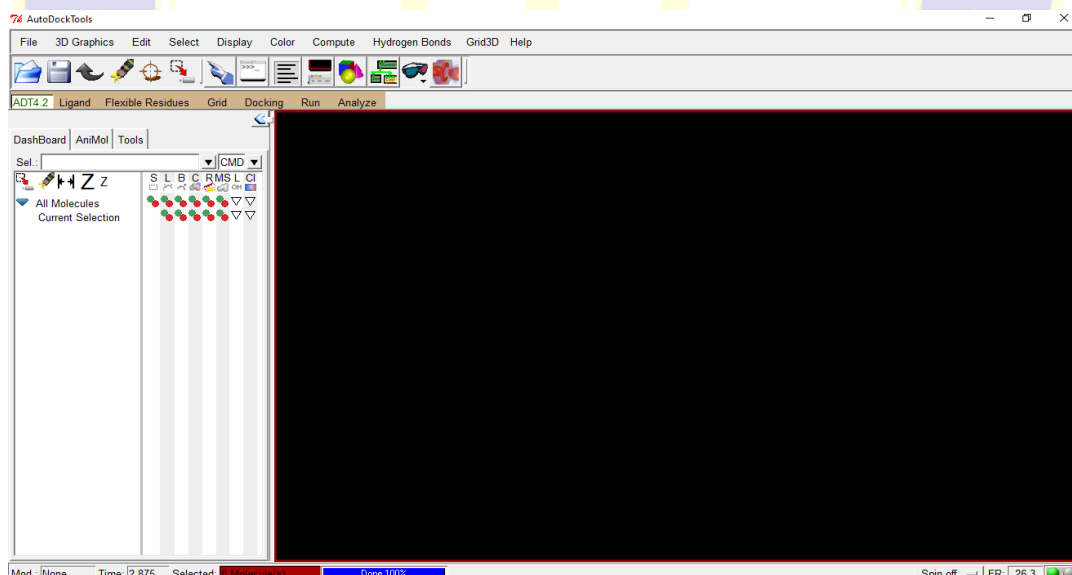
Gambar IV.7 Tampilan situs Pre-ADMET

## LAMPIRAN 2 (LANJUTAN)

### SITUS DAN APLIKASI



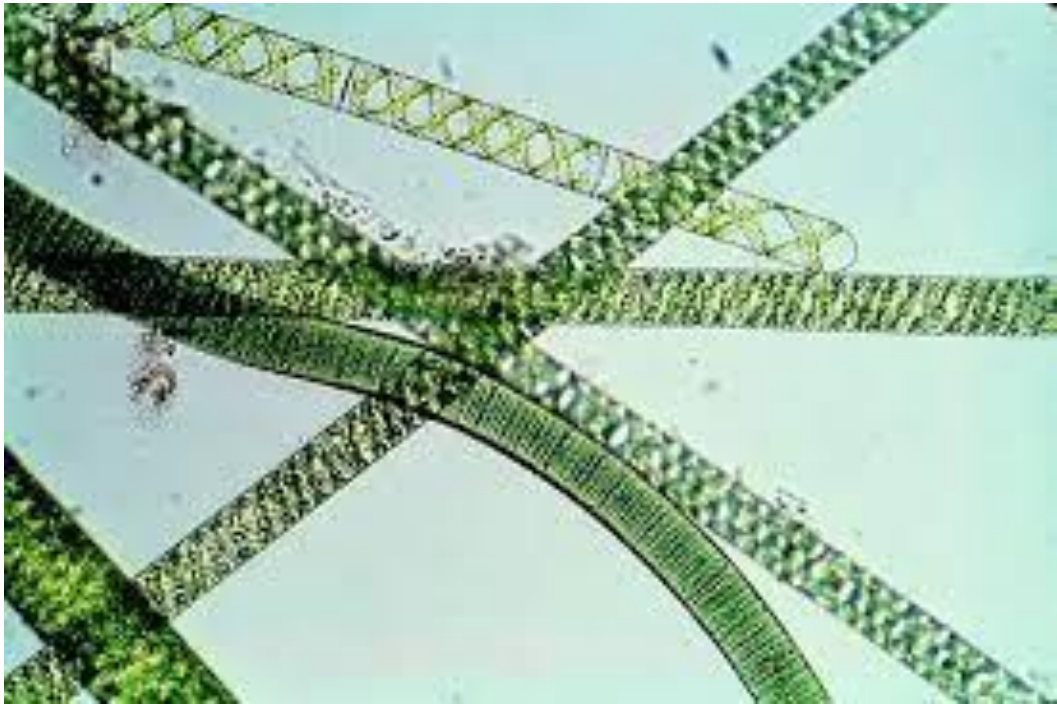
Gambar IV.8 Tampilan aplikasi *Toxtree*<sup>®</sup>



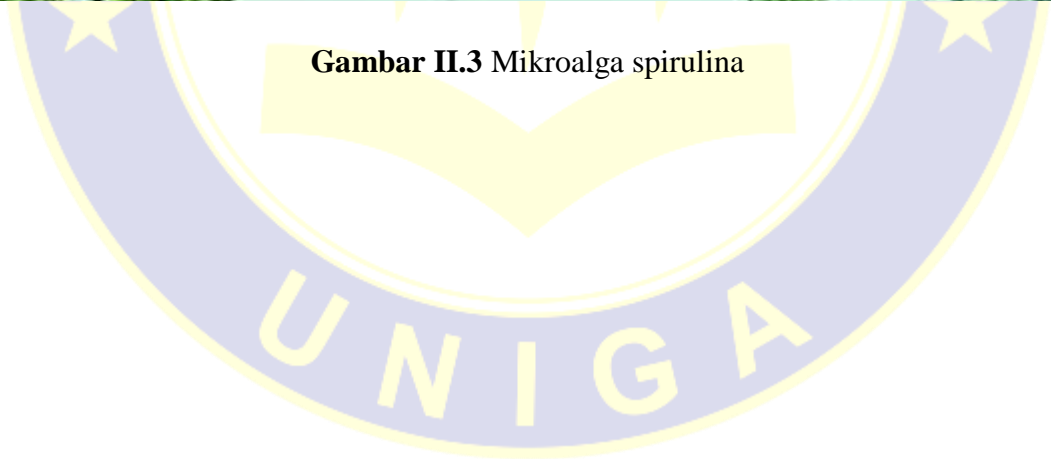
Gambar IV.9 Tampilan aplikasi *Autodock Tools*<sup>®</sup>

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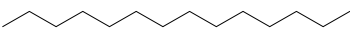
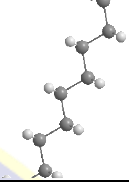
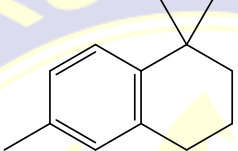
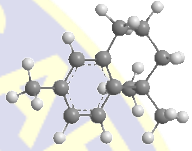
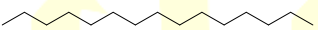
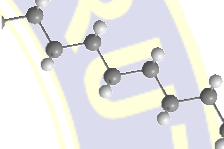
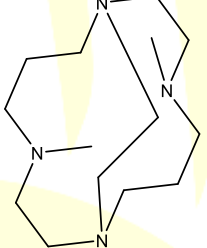
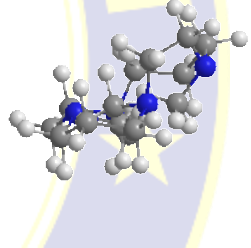
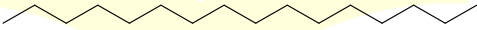
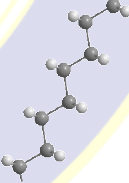

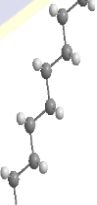
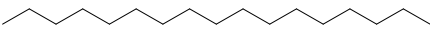
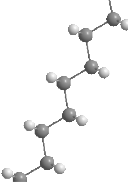
**MIKROALGA SPIRULINA**




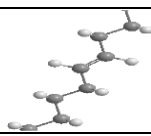
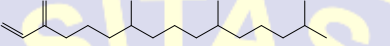
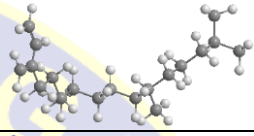
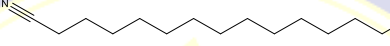
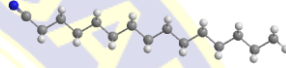
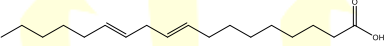
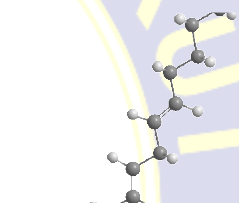
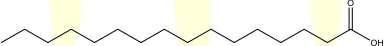
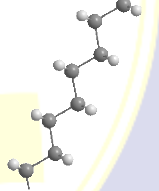
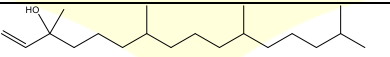
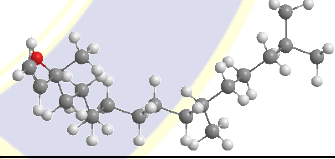
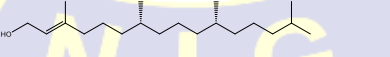
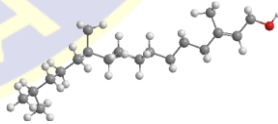
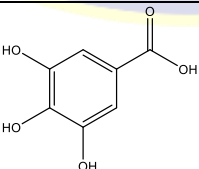
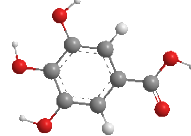
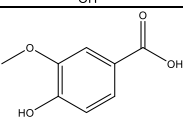
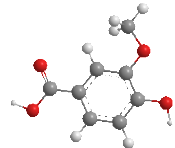
**Gambar II.3** Mikroalga spirulina



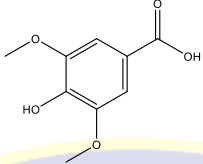
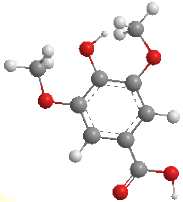
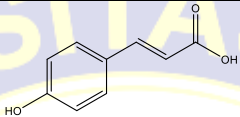
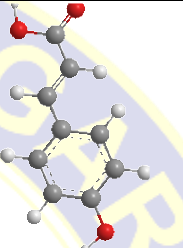
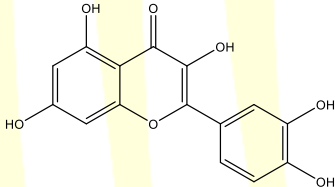
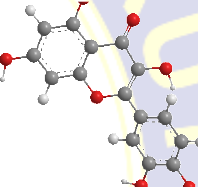
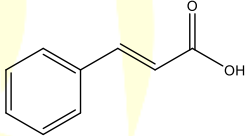
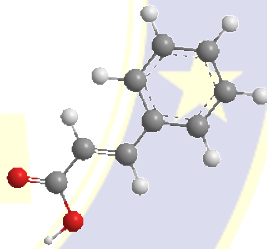
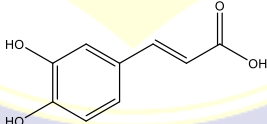
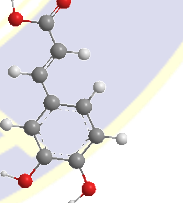
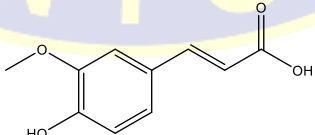
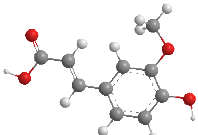
**LAMPIRAN 4**  
**STRUKTUR SENYAWA**

No	Nama senyawa	2D	3D
1	Tetradecane		
2	$\alpha$ -Ionene		
3	Pentadecane		
4	2-hexadecane		
5	Hexadecane		
6	hexadecanenitrile		
7	<i>Heptadecane</i>		

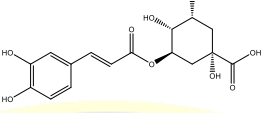
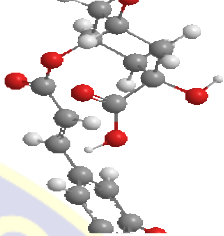
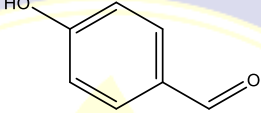
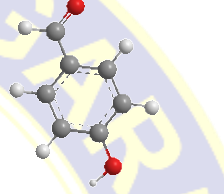
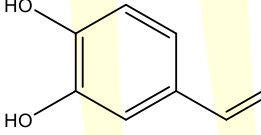
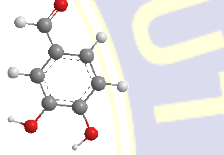
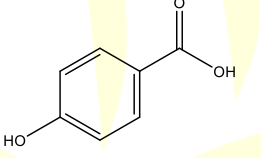
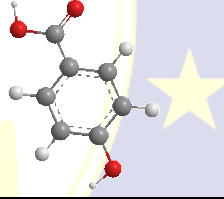
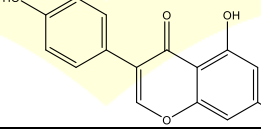
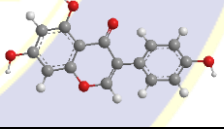
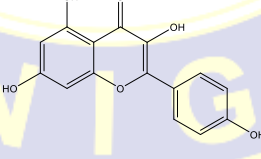
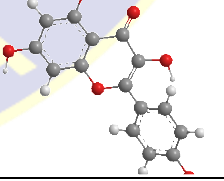
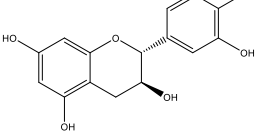
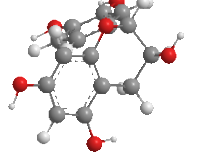
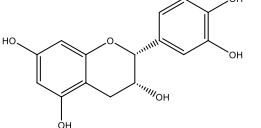
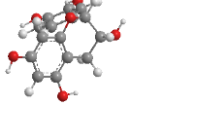
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(LANJUTAN)**

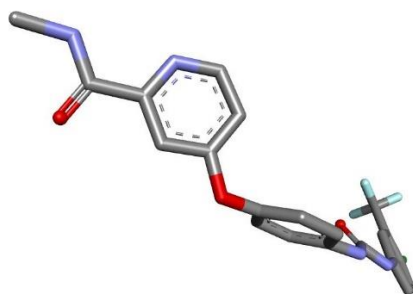
NO	Nama senyawa	2D	3D
8	8-heptadecane		
9	Neophytadiene		
10	pentadecanenitrile		
11	9,12-octadecadienoic acid		
12	Hexadecenoic acid		
13	Isophytol		
14	Phytol		
15	Gallic acid		
16	Vanillic acid		

**LAMPIRAN 4  
(LANJUTAN)**

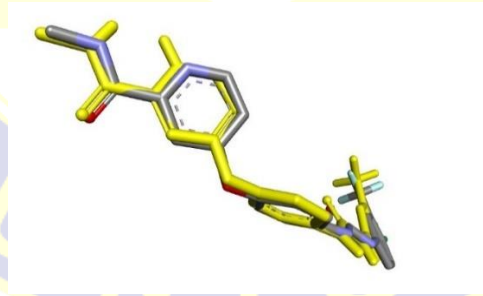
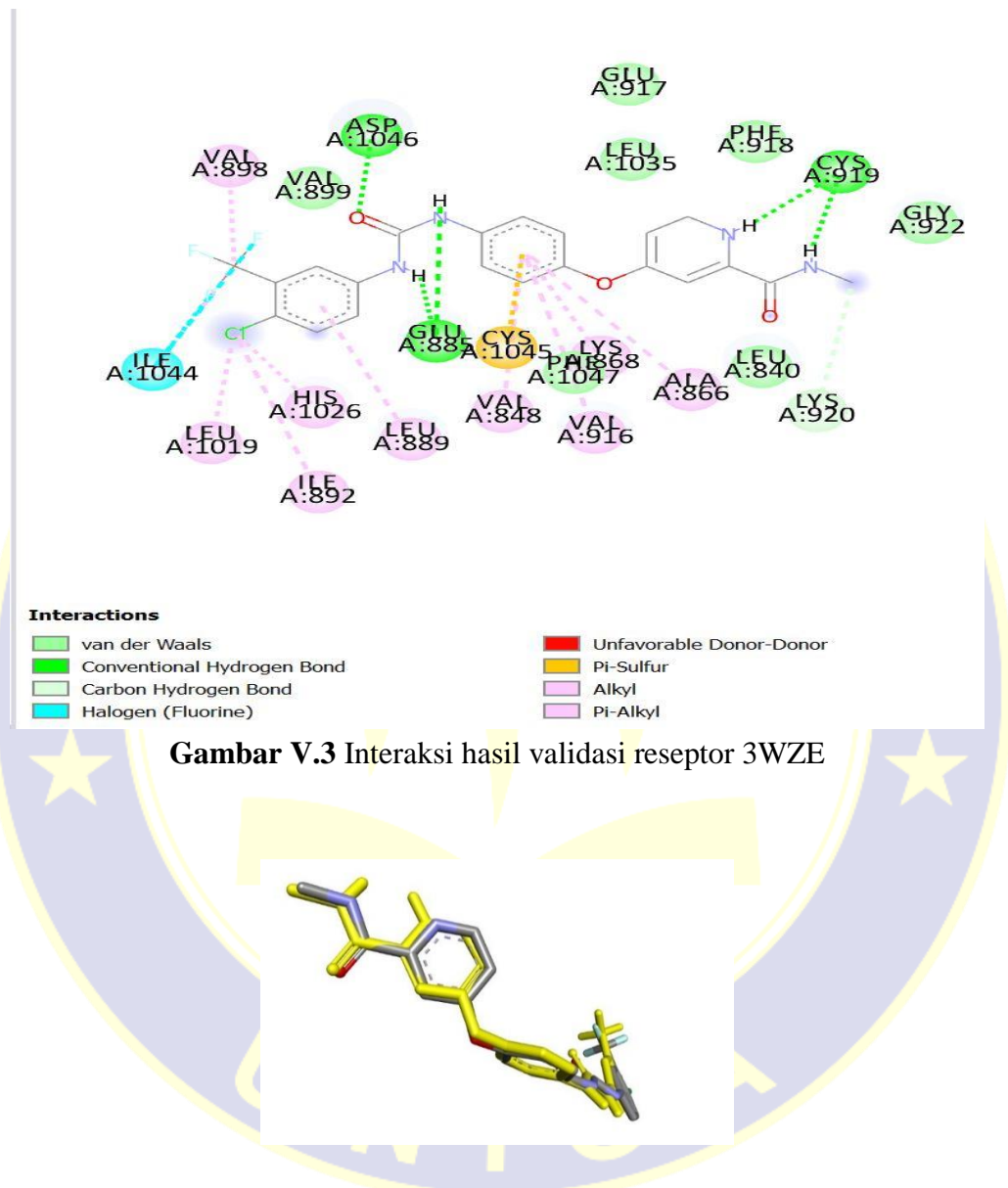
NO	Nama senyawa	2D	3D
17	<i>Syringic acid</i>		
18	<i>p-coumaric acid</i>		
19	<i>Quercetin</i>		
20	<i>Cinnamic acid</i>		
21	<i>Caffeic acid</i>		
22	<i>Ferulic acid</i>		

**LAMPIRAN 4  
(LANJUTAN)**

NO	Nama senyawa	2D	3D
23	<i>Chlorogenic acid</i>		
24	<i>4-hydroxybenzaldehyde</i>		
25	<i>3,4-dihydroxybenzaldehyde</i>		
26	<i>p-hydroxybenzoic acid</i>		
27	<i>Genistein</i>		
28	<i>Kaemferol</i>		
29	<i>Catechin</i>		
30	<i>Epicatechin</i>		

**LAMPIRAN 5****RESEPTOR DAN STRUKTUR LIGAN ALAMI****Gambar V.1** Reseptor 3WZE**Gambar V.2** Struktur ligan alami sorafenib 3WZE

**LAMPIRAN 6**  
**HASIL VALIDASI METODE**



**Gambar V.4** Tumpang tindih ligan alami 3WZE dengan ligan hasil *redocking*

## LAMPIRAN 7

## HASIL PENAMBATAN MOLEKUL SENYAWA UJI

Tabel V.1

Hasil Penambatan Pada Reseptor 3WZE

NO.	SENYAWA	$\Delta G$ (kcal/Mol)	ki ( $\mu$ molar)	ASAM AMINO
1.	4-hydroxybenzaldehyde	-4.82	293.21	GLU:885, CYS:1045, ASP:1046, CYS:868, VAL:989, LEU:889, VAL:899, HIS:1026
2.	Vanillic acid	-5.00	217.44	CYS:1045, GLU:885, ASP:1046
3.	Syringic acid	-5.03	206.36	GLU:917, CYS:919
4.	Gallic acid	-5.21	152.58	CYS:1045, ASP:1046, GLU:885
5.	P – hydroxybenzoic acid	-5.93	127.92	ASP:1046, CYS:1045, GLU:885
6.	Tetradecane	-5.60	78.70	CYS:919, GLU:917, CYS:1045, GLU:885
7.	9,12-octadecadienoic acid	-5.69	68.04	GLU:885, ASP:1046, CYS:1045, 919
8.	Hexadecane	-5.89	47.83	CYS:919, CYS:1045, ASP:1046, GLU:885, GLU:917
9.	Pentadecane	-5.93	45.32	CYS:1045, ASP:1046, CYS:919, GLU:917
10.	Cinnamic acid	-5.98	596.65	GLU:917, CYS:1045, CYS:919, ASP:1046
11.	Heptadecane	-6.16	30.48	GLU:885, ASP:1046, CYS:1045, CYS:919
12.	8-heptadecane	-6.26	25.95	GLU:885, ASP:1046, CYS:1045, CYS:919
13.	Pentadecanenitrile	-6.44	19.12	CYS:1045, ASP:1046, GLU:917, CYS:919, GLU:885
14.	Ferulic acid	-6.98	7.71	CYS:919, CYS:1045, ASP:1046, GLU:885
15.	3,4- dihydroxybenzaldehyde	-6.28	25.12	<b>CYS:1045, GLU:885, ASP:1046</b>

**LAMPIRAN 7  
(LANJUTAN)**

NO.	SENYAWA	$\Delta G$ (kcal/Mol)	$k_i$ ( $\mu$ molar)	ASAM AMINO
16.	<i>Hexadecanenitrile</i>	-6.50	17.30	ASP:1046, GLU:885, CYS:919, CYS:1045
17.	p-coumaric acid	-6.51	16.79	GLU:917, CYS:919, CYS:1045, ASP:1046, GLU:885
18.	Hexadecenoic acid	-6.52	16.17	GLU:917, CYS:919, CYS:1045, GLU:885, ASP:1046
19.	Caffeic acid	-6.63	13.94	CYS:1045, ASP:1046
20.	$\alpha$ -Ionene	-6.72	11.95	GLU:885, CYS:1045, ASP:1046
21.	Epicatechin	-7.03	7.024	GLU:885, ASP:1046, CYS:1045, CYS:919, GLU:917
22.	Phytol	-7.49	3.24	GLU:885, GLU:917, CYS:919, ASP:1046
23.	Neophytadiene	-7.58	2.79	GLU:885, CYS:919, GLU:917, CYS:1045, ASP:1046
24.	Ishophytol	-7.66	2.43	CYS:919, GLU:917, CYS:1045, ASP:1046, GLU:885
25.	Catechin	-7.83	1.81	CYS:1045, GLU:885, GLU:917, CYS:919, ASP:1046,
26.	Genistein	-8.37	152.58	GLU:917, CYS:1045, GLU:885, ASP:1046, CYS:919
27.	Chlorogenic acid	-8.49	596.65	ASP:1046, CYS:1045, GLU:885, CYS:868, GLU:917, CYS:919,
28.	Quercetin	-9.21	176.35	GLU:885, CYS:1045, GLU:917, CYS:919, ASP:1046
29.	Kaempferol	-9.23	172.40	CYS:919, GLU:917, CYS:1045, ASP:1046, GLU:885,
30.	2-hexadecane	10.37	25.22	CYS:1045, GLU:885, ASP:1046
#	<i>Sorafenib ( Ligan Pemanding )</i>	-12.38	844.58	CYS:919, GLU:885, ASP:1046

## LAMPIRAN 8

HASIL PREDIKSI *DRUG LIKENESS*

Tabel V.2

Hasil prediksi *drug likeness* berdasarkan aturan *Lipinski Rule of Five*

NO.	SENYAWA	BM	Log P	Ikatan hidrogen		Keterangan
				Donor	Akseptor	
1.	4-hydroxybenzaldehyde	122	0,79	1	1	Memenuhi Syarat
2.	Vanillic acid	168	0,63	2	4	Memenuhi Syarat
3.	Syringic acid	198	0,86	2	5	Memenuhi Syarat
4.	Gallic acid	170	0,18	4	5	Memenuhi Syarat
5.	P – hydroxybenzoic acid	510	3,32	5	7	Memenuhi Syarat
6.	Tetradecane	198	4,53	0	0	Tidak Memenuhi Syarat
7.	9,12-octadecadienoic acid	280	4,59	1	2	Memenuhi Syarat
8.	Hexadecane	226	5,14	0	0	Tidak Memenuhi Syarat
9.	Pentadecane	212	4,84	0	0	Tidak Memenuhi Syarat
10.	Cinnamic acid	148	0,74	1	2	Memenuhi Syarat
11.	Heptadecane	240	5,45	0	0	Tidak Memenuhi Syarat
<b>12.</b>	<b><i>8-heptadecane</i></b>	<b>238</b>	<b>5,24</b>	<b>0</b>	<b>0</b>	<b>Tidak Memenuhi Syarat</b>

**LAMPIRAN 8  
(LANJUTAN)**

NO.	SENYAWA	BM	Log P	Ikatan hidrogen		Keterangan
				Donor	Akseptor	
13.	Pentadecanenitrile	223	4,51	0	1	Memenuhi Syarat
14.	Ferulic acid	194	0,55	2	4	Memenuhi Syarat
15.	3,4-dihydroxybenzaldehyde	138	0,67	2	3	Memenuhi Syarat
16.	Hexadecanenitrile	237	4,82	0	1	Tidak Memenuhi Syarat
17.	p-coumaric acid	164	0,15	2	3	Memenuhi Syarat
18.	Hexadecenoic acid	254	3,63	1	2	Memenuhi Syarat
19.	Caffeic acid	180	0,03	3	4	Memenuhi Syarat
20.	$\alpha$ -Ionene	174	3,13	0	0	Tidak Memenuhi Syarat
21.	Epicatechin	290	1,09	5	6	Memenuhi Syarat
22.	Phytol	294	5,72	1	1	Memenuhi Syarat
23.	Neophytadiene	278	5,96	0	0	Tidak Memenuhi Syarat
24.	Ishophytol	296	5,91	1	1	Memenuhi Syarat
25.	Catechin	290	1,09	5	6	Memenuhi Syarat
26.	Genistein	270	0,94	3	5	Memenuhi Syarat
27.	Chlorogenic acid	354	1,28	6	9	Tidak Memenuhi Syarat
28.	Quercetin	302	0,52	5	7	Memenuhi Syarat

NO.	SENYAWA	BM	Log P	Ikatan hidrogen		Keterangan
				Donor	Akseptor	
29.	Kaempferol	286	0,64	4	6	Memenuhi Syarat
30.	2-hexadecane	254	2,61	0	0	Tidak Memenuhi Syarat

**Keterangan :** BM < 500 Dalton, Log P <5, Donor Ikatan Hidrogen <5, dan

Aseptor Ikatan Hidrogen <10.



**LAMPIRAN 9**  
**HASIL PREDIKSI TOKSISITAS**

**Tabel V.3**  
Hasil prediksi toksisitas ligan pembanding dan senyawa aktif mikroalga spirulina  
(*Artoshpira plantesis*)

NO	SENYAWA	CRAME RULES	KROSS TTC	BENIGNI
1.	4-hydroxybenzaldehyde	1	2	8,9
2.	Vanillic acid	2	1	8,9
3.	Syringic acid	2	1	8,9
4.	Gallic acid	2	1	8,9
5.	P – hydroxybenzoic acid	2	1	8,9
6.	Tetradecane	2	1	8,9
7.	9,12-octadecadienoic acid	2	1	8,9
8.	Hexadecane	2	1	8,9
9.	Pentadecane	2	1	8,9
10.	Cinnamic acid	2	1	8,9
11.	Heptadecane	2	1	8,9
12.	8-heptadecane	2	1	8,9
13.	Pentadecanenitrile	2	1	8,9
14.	Ferulic acid	2	1	8,9
15.	3,4-dihydroxybenzaldehyde	1	2	1,9

**LAMPIRAN 9  
(LANJUTAN)**

<b>NO</b>	<b>SENYAWA</b>	<b>CRAME RULES</b>	<b>KROSS TTC</b>	<b>BENIGNI</b>
16.	<i>Hexadecanenitrile</i>	2	1	8,9
17.	p-coumaric acid	2	1	8,9
18.	Hexadecenoic acid	2	1	8,9
19.	Caffeic acid	2	1	8,9
20.	$\alpha$ -Ionene	2	1	8,9
21.	Epicatechin	2	1	8,9
22.	Phytol	2	1	8,9
23.	Neophytadiene	2	1	8,9
24.	Ishophytol	2	1	8,9
25.	Catechin	2	1	8,9
26.	Genistein	2	1	8,9
27.	Chlorogenic acid	2	1	8,9
28.	Quercetin	1	1	8,9
29.	Kaempferol	2	1	8,9
30.	<i>2-hexadecane</i>	2	1	8,9

**LAMPIRAN 9  
(LANJUTAN)**

**Keterangan :**

**Cramer rules:**

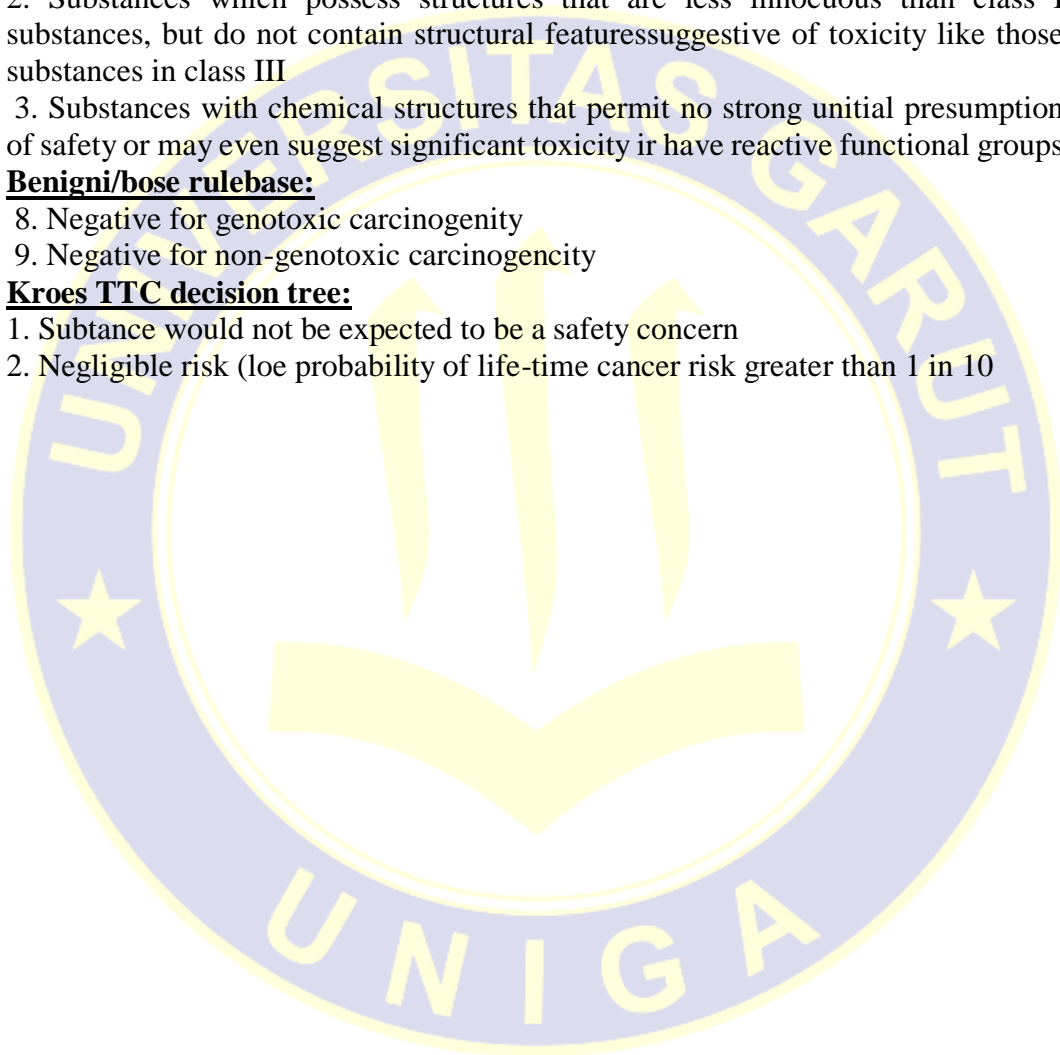
1. Substances with simple chemical structures and few which efficient modes of metabolism exist, suggesting a low order of oral toxicity
2. Substances which possess structures that are less innocuous than class I substances, but do not contain structural features suggestive of toxicity like those substances in class III
3. Substances with chemical structures that permit no strong initial presumption of safety or may even suggest significant toxicity if they have reactive functional groups

**Benigni/bose rulebase:**

8. Negative for genotoxic carcinogenicity
9. Negative for non-genotoxic carcinogenicity

**Kroes TTC decision tree:**

1. Substance would not be expected to be a safety concern
2. Negligible risk (low probability of life-time cancer risk greater than 1 in 10)



## LAMPIRAN 10

## HASIL PREDIKSI PROFIL ABSORBSI DAN DISTRIBUSI

Tabel V.4

Hasil prediksi profil absorpsi dan distribusi ligan pembanding dan senyawa aktif mikroalga spirulina (*Arthospira Plantesis*)

NO	SENYAWA	HIA	CaCo-2	Protein Plasma Binding (PPB)
1.	4-hydroxybenzaldehyde	94.087***	20.52**	61.00%
2.	Vanillic acid	85.369***	19.93**	52.10**%
3.	Syringic acid	82.027***	18.83**	69.77**%
4.	Gallic acid	53.6968**	13.84**	65.38**%
5.	P – hydroxybenzoic acid	87.974**	20.19**	84.01**%
6.	Tetradecane	100.0***	22.19**	100***%
7.	9,12-octadecadienoic acid	98.370***	28.08**	100***%
8.	Hexadecane	100.000***	22.19**	100***%
9.	Pentadecane	100.000***	21.03**	100***%
10.	Cinnamic acid	97.845***	22.03**	60.85**%
11.	Heptadecane	100.00***	22.19**	100***%
12.	8-heptadecane	100.000***	23.19**	100***%
13.	Pentadecanenitrile	100.000**	37.85**	100***%
14.	Ferulic acid	90.603***	21.11**	50.41%
15.	3,4-dihydroxybenzaldehyde	86.677***	19.19**	23.72%
16.	Hexadecanenitrit	100.000***	39.08**	100***%

**LAMPIRAN 10  
(LANJUTAN)**

NO	SENYAWA	HIA	CaCo-2	Protein Plasma Binding (PPB)
17.	p-coumaric acid	92.095***	21.10**	63.05*%
18.	Hexadecenoic acid	98.420***	25.96**	100***%
19.	Caffeic acid	82.301***	21.10**	40.29*%
20.	$\alpha$ -Ionene	100.00***	23.45**	100***%
21.	Epicatechin	66.7079**	0.65696*	100***%
22.	Phytol	100.00***	37.61**	100***%
23.	Neophytadiene	100.000***	23.15**	100***%
24.	Ishophytol	100.000***	28.33**	100***%
25.	Catechin	66.707**	0,65*	100***%
26.	Genistein	88.122***	5.747**	89.73***%
27.	Chlorogenic acid	63.4852**	3.412*	93.23***%
28.	Quercetin	63.4852**	3.412*	93.23*%
29.	Kaempferol	79.439***	9.57***	89.60*%
30.	<i>2-hexadecane</i>	100.000***	16.925*	94.38*%

**LAMPIRAN 10  
(LANJUTAN)**

**Keterangan:**

HIA (%) : \*\*\* : > 70 (terserap baik) \*\* : 20 - 70 (terserap cukup) \* : < 20 (kurang terserap).

CaCo-2 Cell (nm sec) : \*\*\* : > 70 (permeabilitas tinggi) \*\* : 4-70 (permeabilitas sedang) \* : < 4 (permeabilitas rendah).

Protein Plasma Binding (%) : \*\* : > 90 (terikat kuat) \* : < 90 (terikat lemah).

