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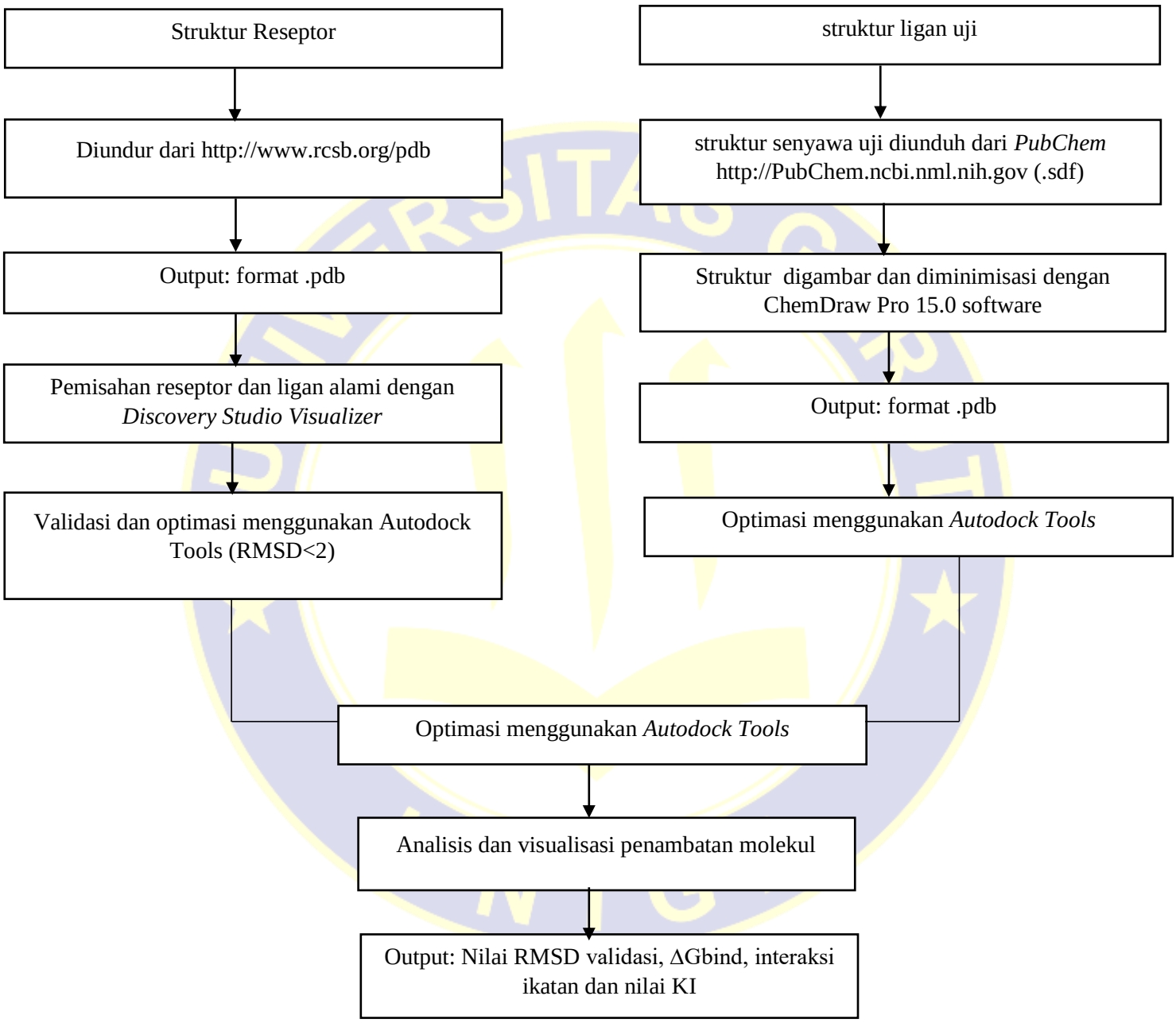
## LAMPIRAN 1

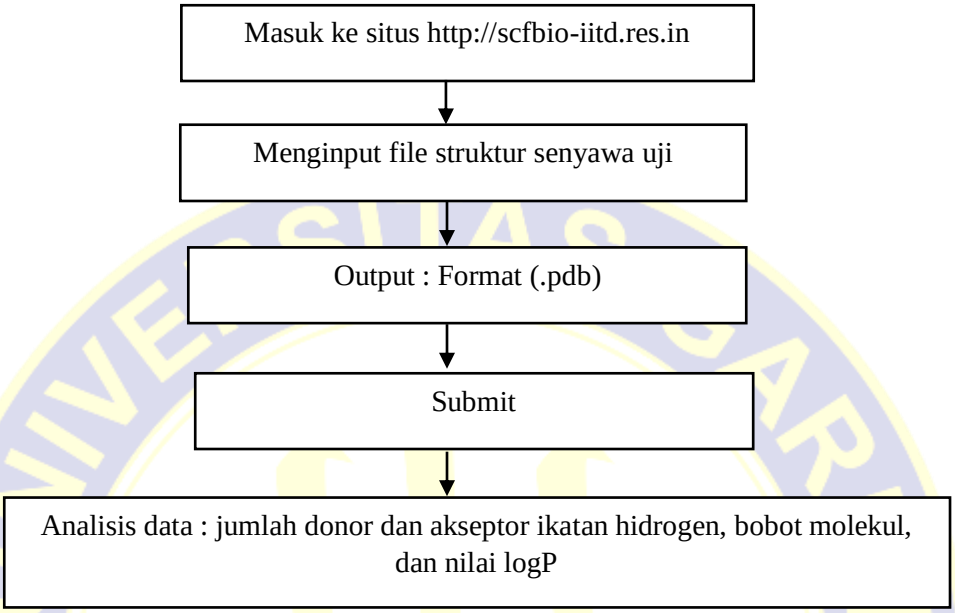
## ALUR PENELITIAN SIMULASI MOLEKULAR DOCKING



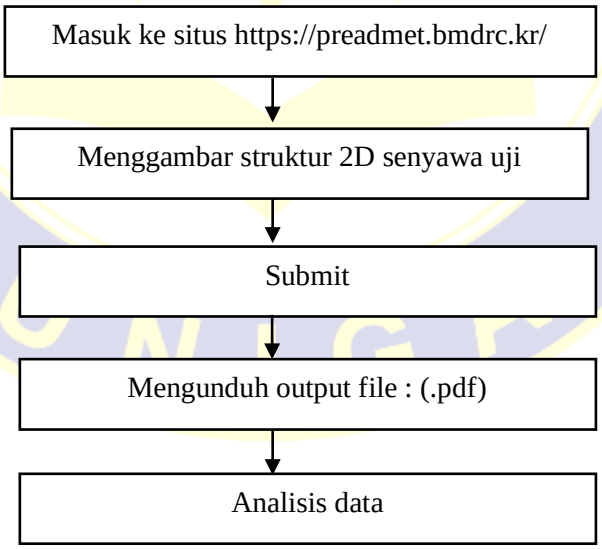

**Gambar VII. 1** Alur penelitian simulasi *molecular docking*

## LAMPIRAN 2

## ALUR PENELITIAN ANALISIS FISIKOKIMIA, ANALISIS FARMAKOKINETIKA, SERTA ANALISIS TOKSISITAS

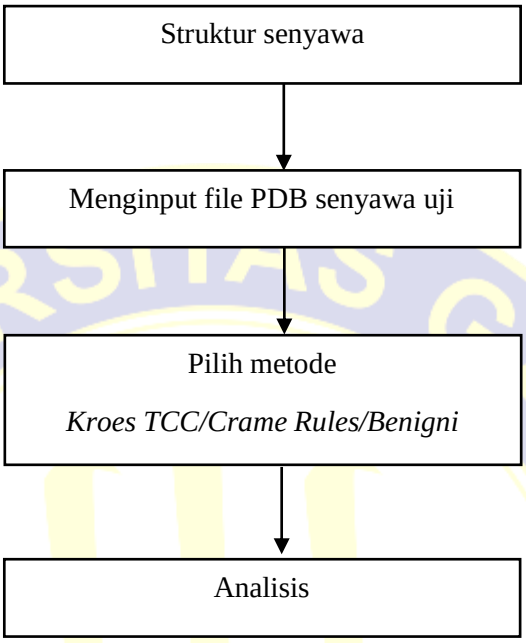



**Gambar VII. 2** Analisis fisikokimia berdasarkan *lipinski rule of five*




**Gambar VII. 3** Analisis farmakokinetik menggunakan situs *online* pre-ADMET

**LAMPIRAN 2**
**(Lanjutan)**

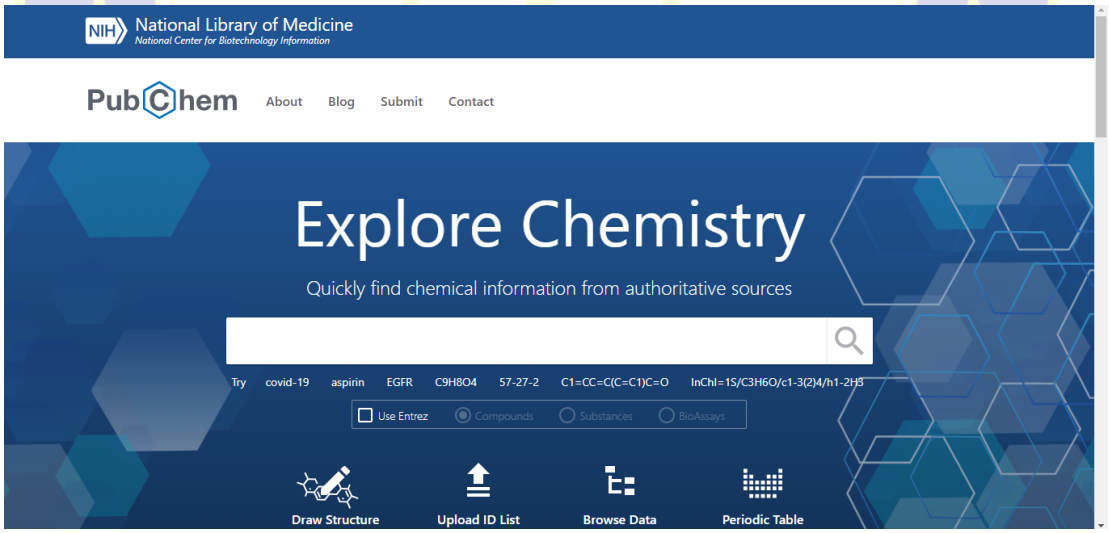



**Gambar VII. 4** Alur prediksi toksisitas menggunakan aplikasi *toxtree*

# LAMPIRAN 3

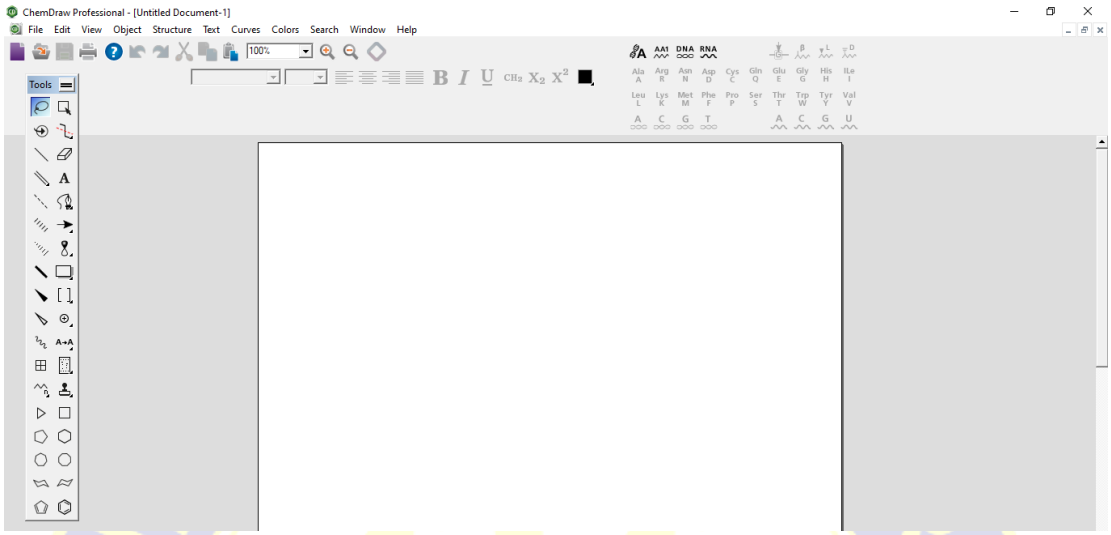
# SITUS DAN APLIKASI


**Gambar VII. 5** Tampilan *situs protein data bank*

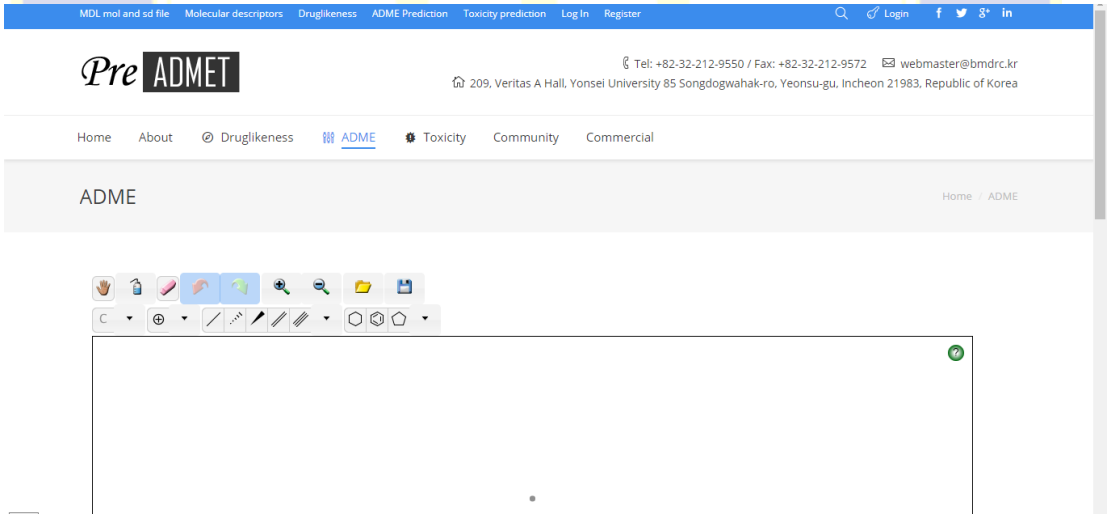



**Gambar VII. 6** Tampilan situs *pubchem*

**LAMPIRAN 3**
**(Lanjutan)**

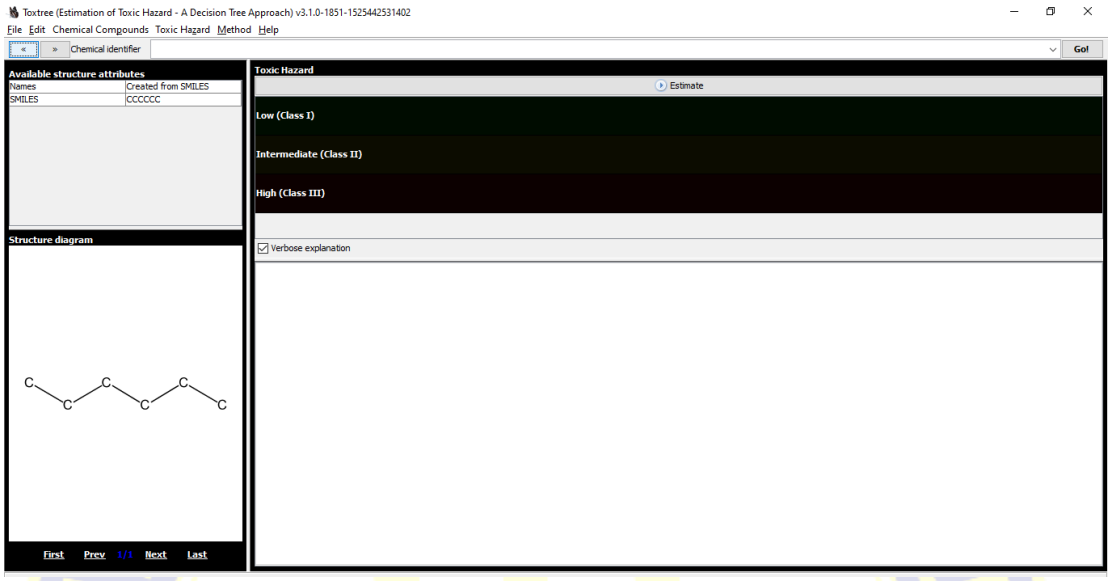



**Gambar VII. 7** Tampilan aplikasi *chemdraw professional* 15.0®

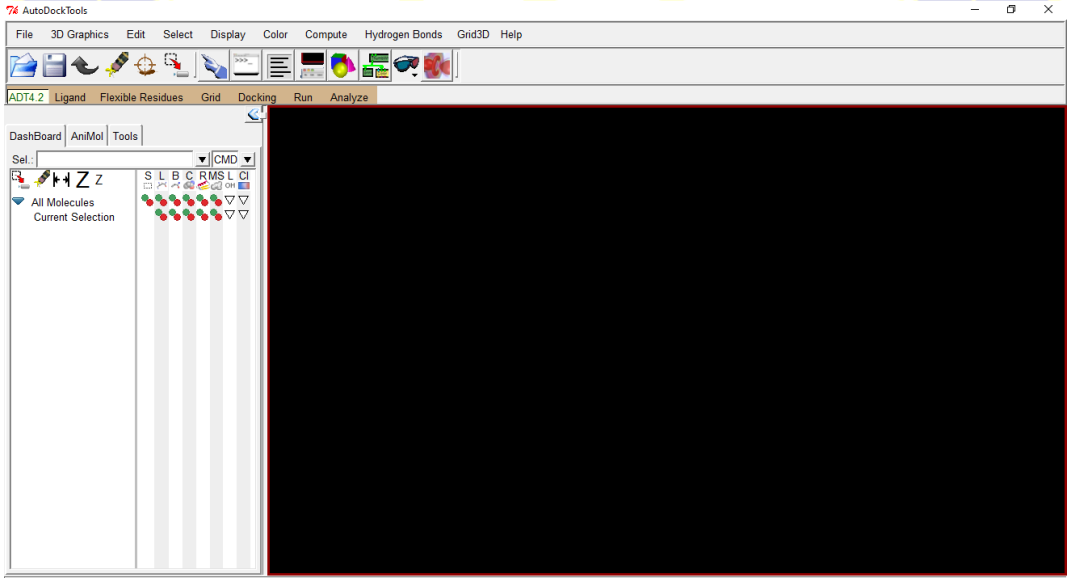



**Gambar VII. 8** Tampilan situs *pre*-ADMET

# LAMPIRAN 3
# (Lanjutan)

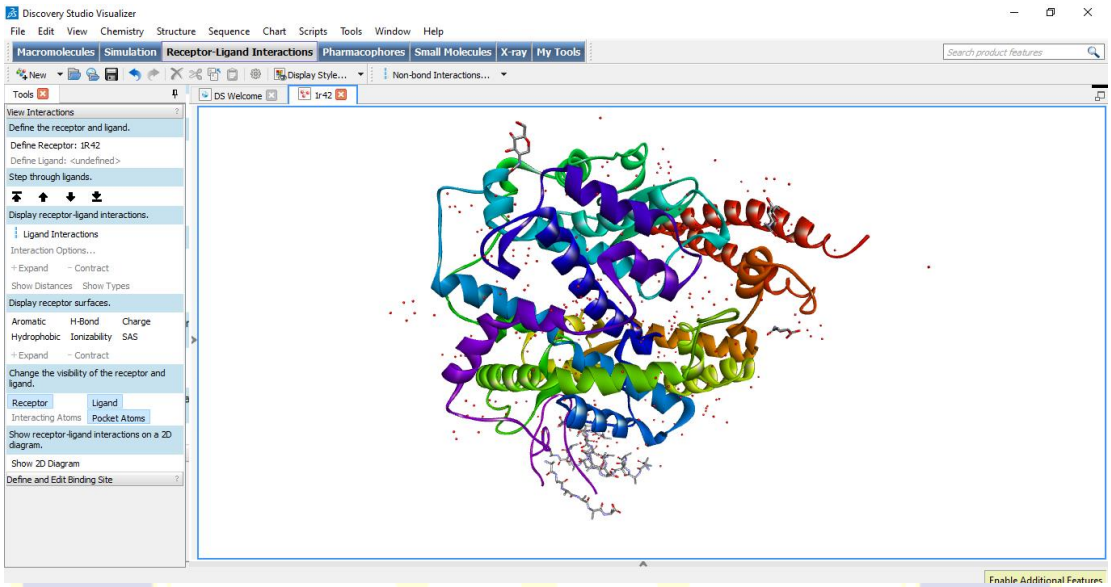



**Gambar VII 9** Tampilan aplikasi *toxtree*®

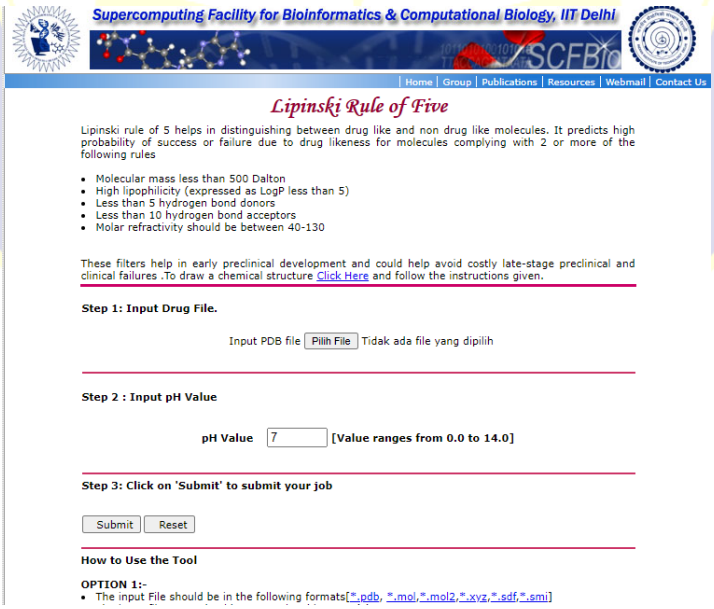



**Gambar VII 10** Tampilan aplikasi *autodock tools*®

**LAMPIRAN 3**
**(Lanjutan)**




**Gambar VII. 11** Tampilan aplikasi *discovery studio visualizer®*

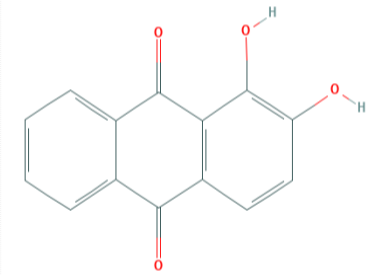
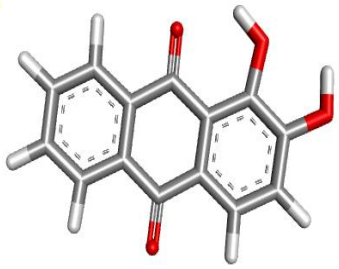
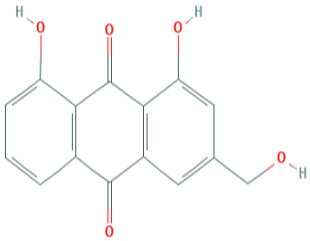
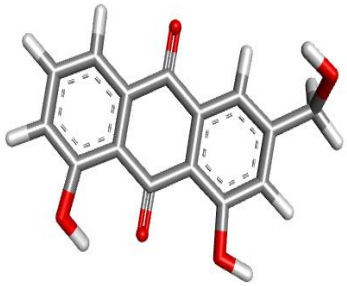
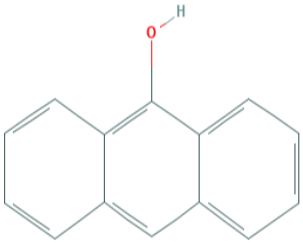
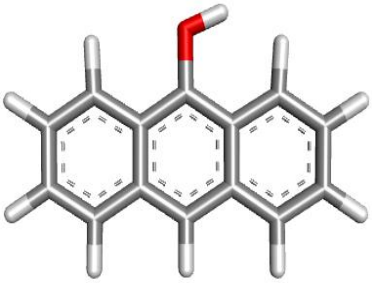



**Gambar VII. 12** Tampilan situs *lipinski rule of five*

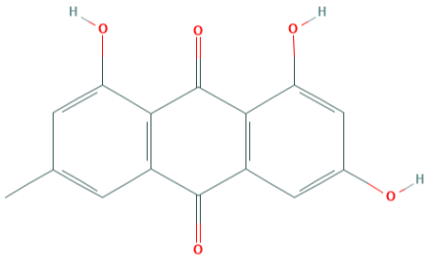
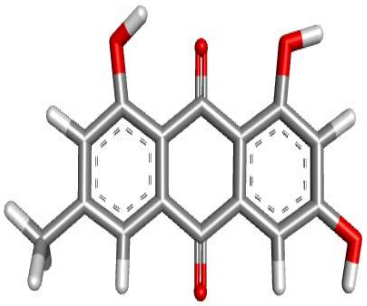
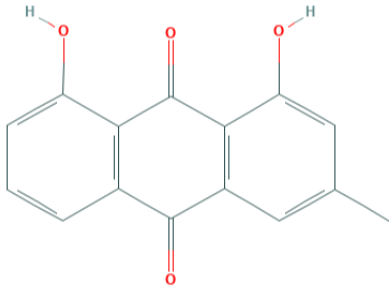
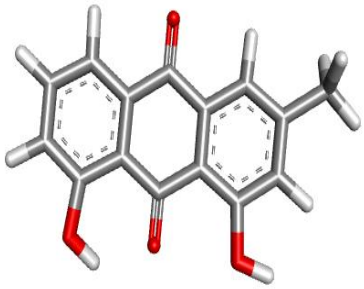
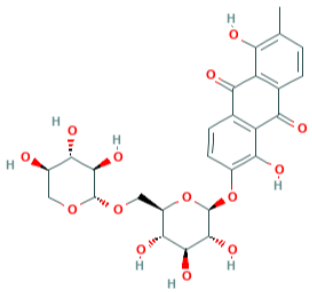
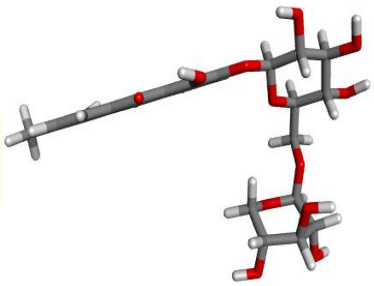
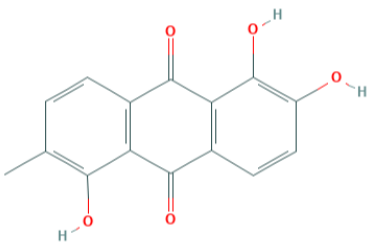
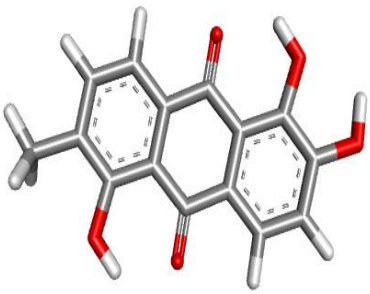
## LAMPIRAN 4

## STRUKTUR SENYAWA ANTRAKUINON

**Tabel VII.1**
Struktur 2D dan 3D Senyawa Antrakuinon

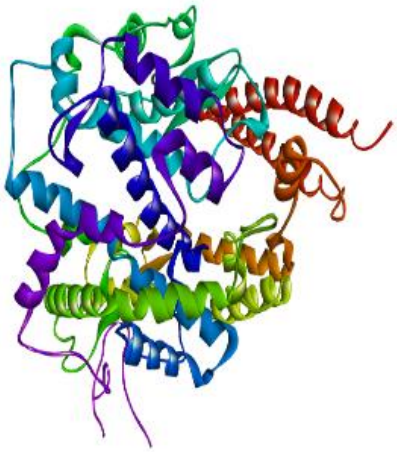
| No. | Senyawa | Struktur 2D | Struktur 3D |
|---|---|---|---|
| 1. | Alizarin |  |  |
| 2. | Aloe-emodin |  |  |
| 3. | Anthranol |  |  |

**LAMPIRAN 4**
**(LANJUTAN)**

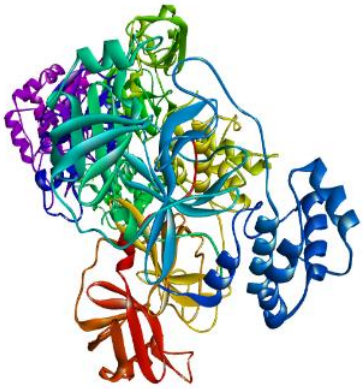
| No. | Senyawa | Struktur 2D | Struktur 3D |
|---|---|---|---|
| 4. | Emodin |  |  |
| 5. | Krisofanol |  |  |
| 6. | Morindin |  |  |
| 7. | Morindone |  |  |

**LAMPIRAN 5**

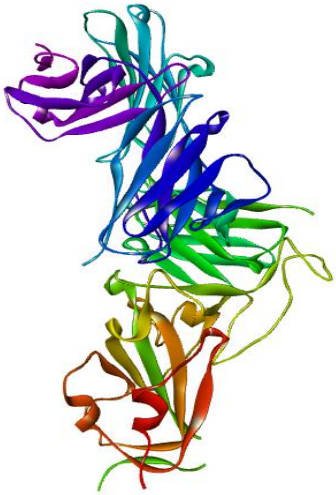
**Reseptor**



**Reseptor 1R42**



**Reseptor 6M2N**



**Reseptor 7BZ5**

# LAMPIRAN 6

## HASIL PENAMBATAN MOLEKUL SENYAWA UJI

**TABEL VII. 2**
Hasil Penambatan pada Reseptor 6M2N

| NO. | SENYAWA | ΔG (kcal/Mol) | ki (µmolar) | ASAM AMINO |
|---|---|---|---|---|
| 1. | Morindin | +6.65 | - | CYS:145,HIS:41:164,GLN:189, ASN:142,ASP:187 |
| 2. | Anthranol | -6.21 | 27.95 | MET:165:49,CYS:145:44, HIS:41,GLN:189 |
| 3. | Aloe-emodin | -7.10 | 6.27 | GLY:143,GLU:166,MET:165, CYS:145,HIS:41,ASN:142 |
| 4. | Alizarin | -7.19 | 5.37 | GLY:143,LEU:141,GLU:166, MET:165,CYS:145,HIS:41, SER:144 |
| 5. | Emodin | -7.21 | 5.22 | GLY:143,GLU:166,MET:165:49, CYS:145:44,HIS:41,GLN:189 |
| 6. | Krisofanol | -7.24 | 4.93 | GLY:143,GLU:166,MET:165, CYS:145,HIS:41,ASN:142 |

**LAMPIRAN 6**
**(LANJUTAN)**

**TABEL VII. 2**
Lanjutan

| No. | Senyawa | ΔG (kcal/Mol) | ki (µmolar) | ASAM AMINO |
|---|---|---|---|---|
| 7. | Morindone | -7.48 | 3.27 | GLY:143,LEU:141,GLU:166, CYS:145,HIS:41,SER:144, GLN:189,MET:49 |
| 8. | Favipiravir (ligan pembanding) | -3.44 | 3220 | GLY:143,GLU:166,CYS:145, HIS:163,SER:144,ASN:142 |
| 9. | **5,6,7-trihydroxy-2-phenyl-4H-chromen-4-one (ligan alami)** | -.8.45 | 0.635 | GLY:143,LEU:141,GLU:166, ASN:142,MET:165:49, CYS:44:145,HIS:41 |

**LAMPIRAN 6**
**(LANJUTAN)**

**TABEL VII. 3**
Hasil Penambatan Molekul Reseptor 1R42

| NO. | SENYAWA | ΔG (kcal/Mol) | ki (mMolar) | ASAM AMINO |
|---|---|---|---|---|
| 1. | Krisofanol | +7.36 | - | SER:420:545:317, ASN:546,HIS:417 |
| 2. | Morindone | +2.93 | - | SER:420,ASN:546 |
| 3. | Emodin | +2.72 | - | SER:420:317:545, ASN:546 |
| 4. | Morindin | +2.46 | - | SER:420:545,ASN:546, HIS:417 |
| 5. | Aloe-emodin | +1.74 | - | SER:420,ASN:546 |
| 6. | Alizarin | -1.82 | 46.28 | SER:420,ASN:546 |
| 7. | Anthranol | -2.57 | 12.99 | SER:420 |
| 8. | Favipiravir (ligan pembanding) | -1.64 | 63.30 | SER:420:545,ASN:546, HIS:417,ASP:543 |
| 9. | **2-acetamido-2-deoxy-beta-D-glucopyranose (ligan alami)** | -2.08 | 29.99 | SER:420,ASN:546 |

**LAMPIRAN 6**
**(LANJUTAN)**

**TABEL VII. 4**
Hasil Penambatan Molekul Reseptor 7BZ5

| NO. | SENYAWA | ΔG (kcal/Mol) | ki (mMolar) | ASAM AMINO |
|---|---|---|---|---|
| 1. | Emodin | +6.20 | - | ASN:343 |
| 2. | Morindin | +1.93 | - | GLY:339,ASN:343, LEU:368,SER:371:373, VAL:367 |
| 3. | Morindone | -2.23 | 23.22 | GLY:339,LEU:368,PHE:342 |
| 4. | Aloe-emodin | -2.29 | 21.03 | GLY:339 |
| 5. | Krisofanol | -2.56 | 13.23 | GLY:339,ASN:343, LEU:368,PHE:342:374:338 |
| 6. | Alizarin | -2.67 | 11.09 | ASN:343 |
| 7. | Anthranol | -2.90 | 7.49 | ASN:343 |
| 8. | Favipiravir (ligan pembanding) | -2.13 | 27.28 | ASN:343 |
| 9. | **2-acetamido-2-deoxy-beta-D-glucopyranose** | -2.02 | 32.92 | GLY:339,ASN:343, LEU:368,PHE:342:338 |

# LAMPIRAN 7

## TABEL VII. 5

Hasil Prediksi *Drug Likeness* Berdasarkan Aturan *Lipinski Rule Of Five*

| No | Senyawa | BM | Log P | Ikatan hidrogen | | Keterangan |
|---|---|---|---|---|---|---|
| | | | | Donor | Akseptor | |
| 1. | Alizarin | 240 | 1.873 | 2 | 4 | Memenuhi syarat |
| 2. | Aloe-emodin | 270 | 1.365 | 3 | 5 | Memenuhi syarat |
| 3. | Anthranol | 194 | 3.698 | 1 | 1 | Memenuhi syarat |
| 4. | Emodin | 270 | 1.88 | 3 | 5 | Memenuhi syarat |
| 5. | Krisofanol | 254 | 2.181 | 2 | 4 | Memenuhi syarat |
| 6. | Morindin | 564 | -2.176 | 8 | 14 | Tidak Memenuhi syarat |
| 7. | Morindone | 270 | 1.887 | 3 | 5 | Memenuhi syarat |

# LAMPIRAN 8

## TABEL VII. 6

Hasil Prediksi Toksisitas Ligan Pembanding dan Senyawa Antrakuinon

| No. | Senyawa | Crame Rules | Kross TTC | Benigni |
|---|---|---|---|---|
| 1. | Alizarin | 3 | 2 | 1,9 |
| 2. | Aloe-emodin | 3 | 2 | 1,9 |
| 3. | Anthranol | 3 | 2 | 1,9 |
| 4. | Emodin | 3 | 2 | 1,9 |
| 5. | Krisofanol | 3 | 2 | 1,9 |
| 6. | Morindin | 3 | 2 | 1,9 |
| 7. | Morindone | 3 | 2 | 1,9 |

**LAMPIRAN 8**
**(LANJUTAN)**

**TABEL VII. 6**

Lanjutan (Keterangan Tabel)

Keterangan :

*Cramer rules* = *(1) Substances with sample chemical structures and fix which efficient modes of meabolism 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 unitial presumption of safety or may even suggest significant toxicity it have reactive functional groups.*

*Benigni/Bossa rulebase* = *(1) Structural Alert for genotoxic carcinogenicity.*

*(2) Structural Alert for nongenotoxic carcinogenicity.*

*(3) Negative for genotoxic carcinogenicity.*

*(4) Negative for nongenotoxic carcinogenicity.*

*Kroes TTC* = *(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 106)*

# LAMPIRAN 9

## TABEL VII. 7

Hasil Prediksi Profil Absorbsi dan Distribusi Ligan Pembanding dan Senyawa Antrakuinon

| No. | Senyawa | HIA | Caco-2 | Protein Plasma Binding |
|---|---|---|---|---|
| 1. | Alizarin | 92.336 | 0.335 | 98.049 |
| 2. | Aloe-emodin | 87.270 | 5.761 | 87.567 |
| 3. | Anthranol | 100.00 | 29.994 | 100.00 |
| 4. | Emodin | 87.006 | 20.274 | 97.775 |
| 5. | Krisofanol | 92.598 | 16.336 | 96.497 |
| 6. | Morindin | 19.207 | 17.092 | 44.121 |
| 7. | Morindone | 86.996 | 20.890 | 96.675 |

**LAMPIRAN 10**

**TABEL V.II 7**

Lanjutan (Keterangan Tabel)

Keterangan :

*% Human Intestinal Absorbsi (% HIA) = (1) 70-100% well absorbed*

*(2) 20-70% moderately absorbed*

*(3) 0-20% poorly absorbed*

*In Vitro Caco-2 cell permeability (nm sec-1)* = *(1) >70 higher permeability*

*(2) 4-70 medium permeability*

*(3) <4 low permeability*

*Plasma Protein Binding* = *(1) >90 strongly bound*

*(2) >90 weakly bound*