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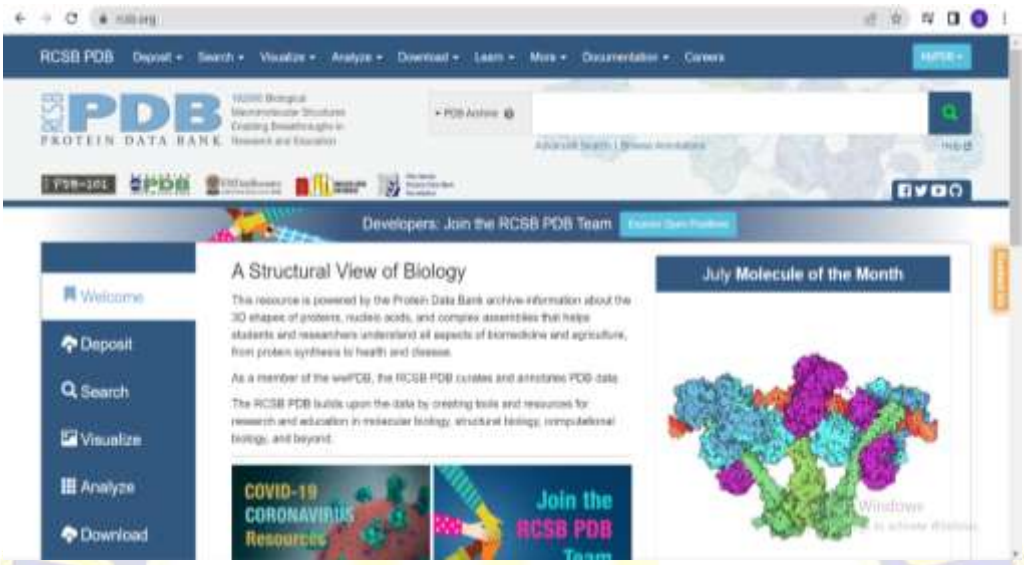
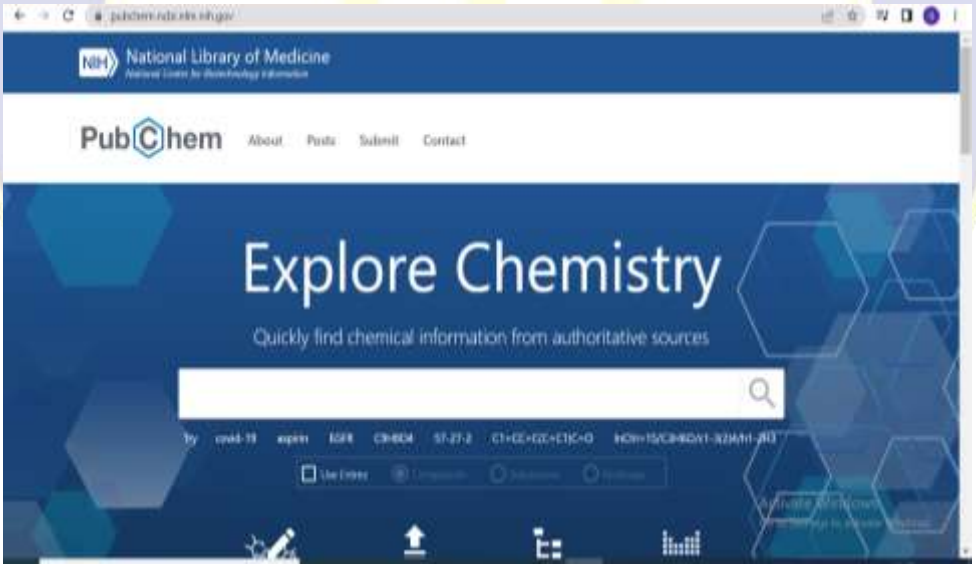
**LAMPIRAN 1**

**SITUS DAN APLIKASI**




**Gambar VII. 1**Tampilan situs Protein Data Bank (PDB)



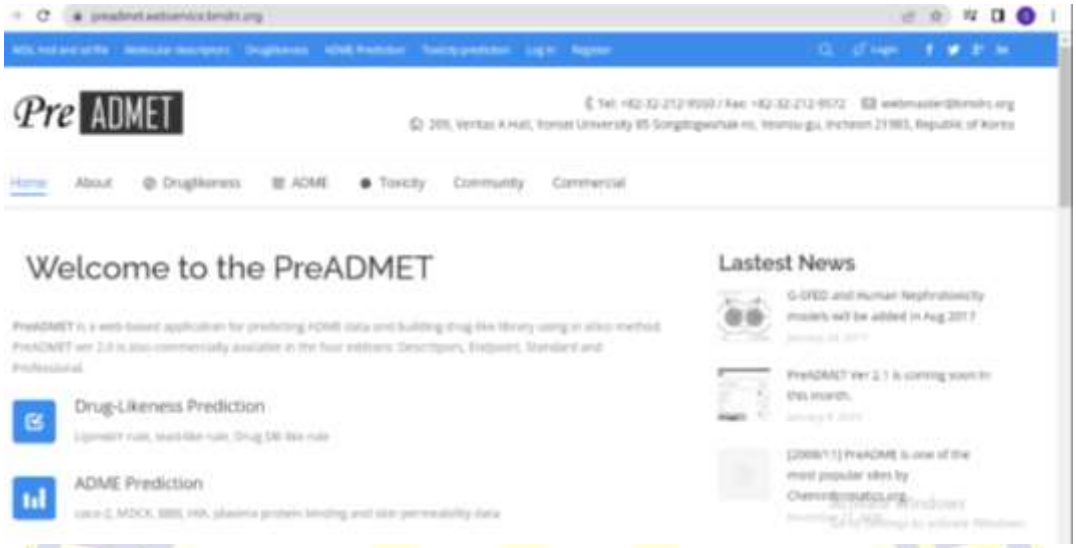

**Gambar VII. 2** Tampilan situs *Pubchem*

**LAMPIRAN 1**
**(LANJUTAN)**


**Gambar VII. 3** Tampilan situs Pass*Online*


**Gambar VII. 4** Tampilan situs *Lipinski Rule Of Five*

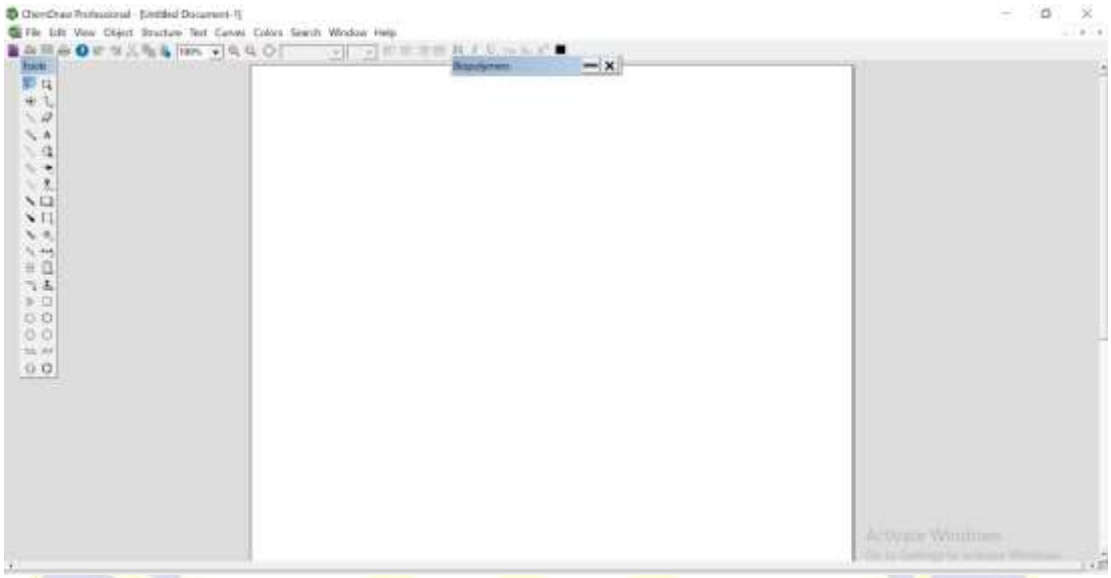
**LAMPIRAN 1**
**(LANJUTAN)**



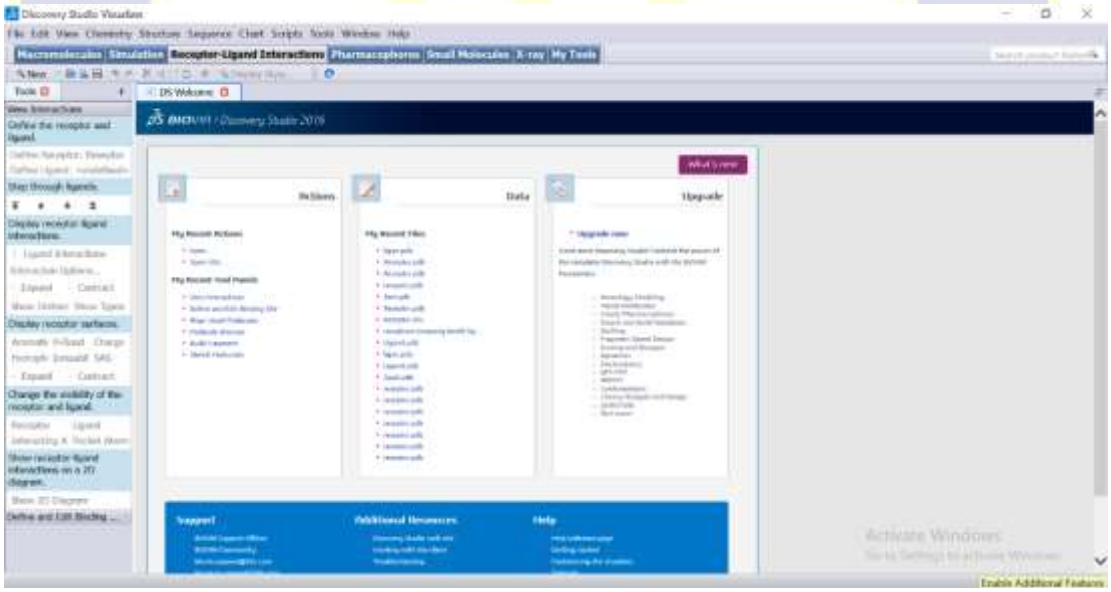

**Gambar VII. 5** Tampilan situs *PreAdmet*


**Gambar VII. 6** Tampilan aplikasi *Toxtree*

**LAMPIRAN 1**
**(LANJUTAN)**

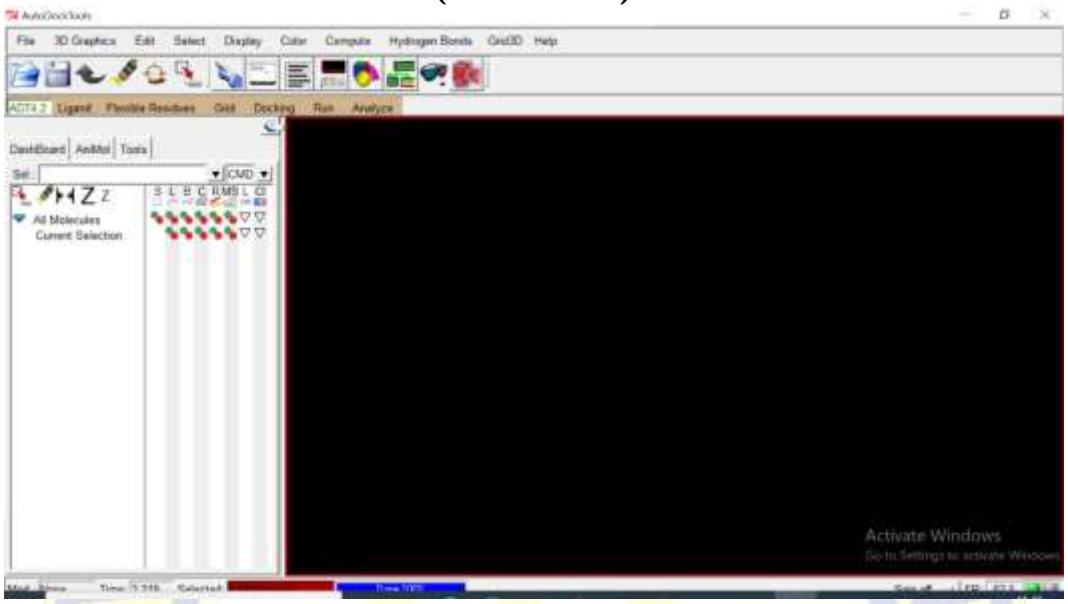


**Gambar VII. 7** Tampilan aplikasi *Chemdraw Profesional*

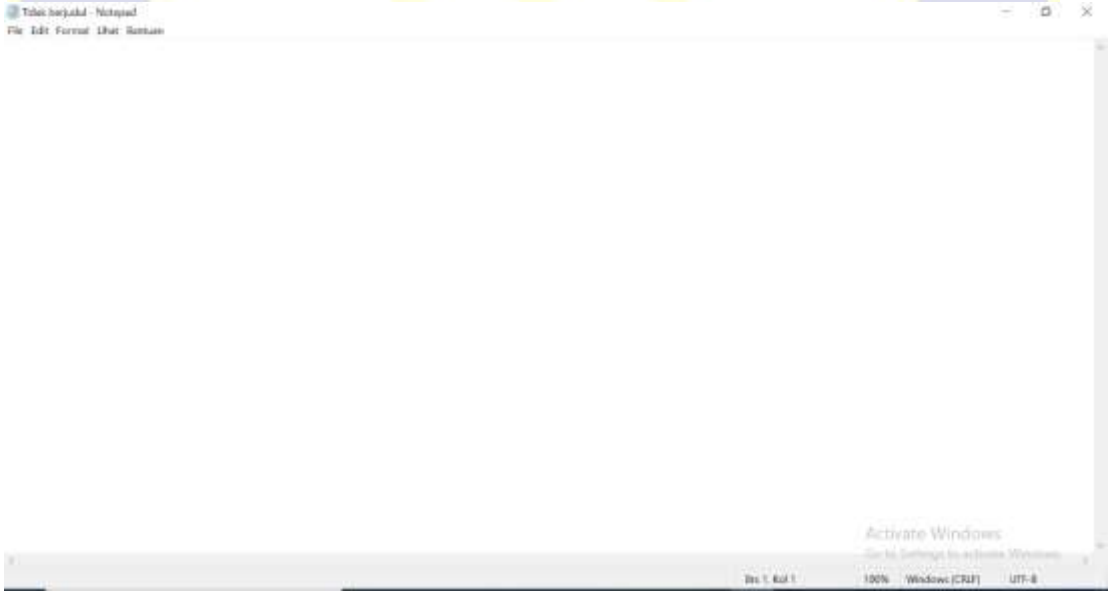


**Gambar VII. 8** Tampilan aplikasi *Discovery Studio Visualizer*

**LAMPIRAN 1**
**(LANJUTAN)**



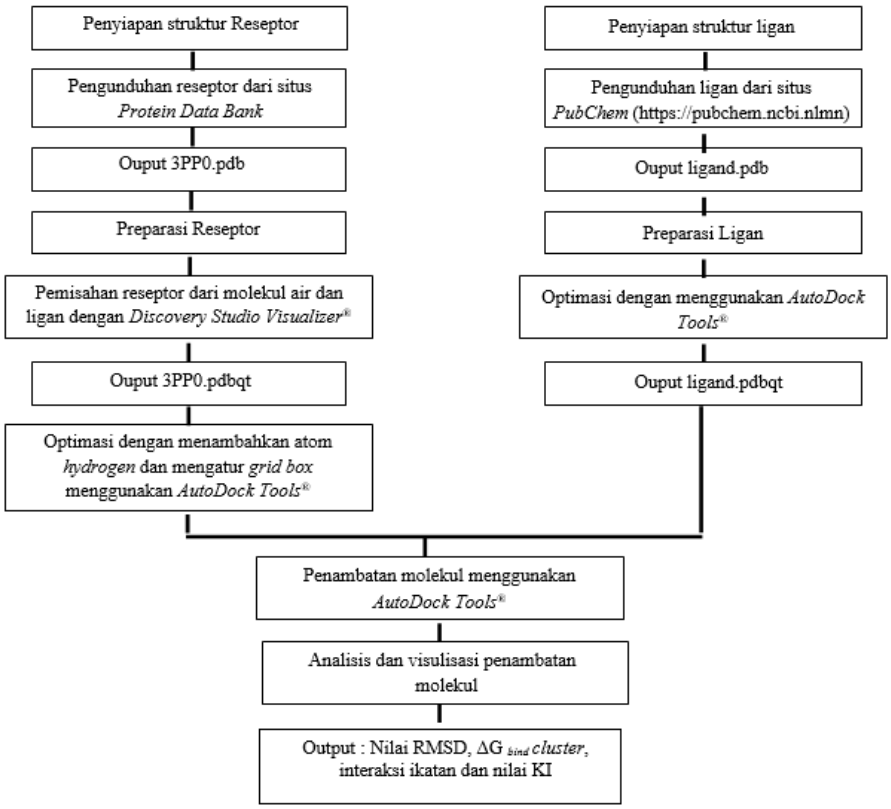

**Gambar VII. 9** Tampilan aplikasi *Autodock tools*




**Gambar VII. 10** Tampilan aplikasi *notepad*

# LAMPIRAN 2

## PROSEDUR DAN ALUR PENELITIAN




**Gambar VII. 11** *Molecular docking*

# LAMPIRAN 3

## HASIL PENELITIAN PREDIKSI *DRUGLIKENESS*

**Tabel VII. 1**
Hasil prediksi *druglikeness* menggunakan situs *online lipinski's rule of five*

| No | Ligan | BM (gr/mol) | Log P | Donor Ikatan | Akseptor Ikatan | Keterangan |
|---|---|---|---|---|---|---|
| 1 | 2-{2-[4-({5-chloro-6-[3-(trifluoromethyl) phenoxy]pyridin-3-yl} amino)-5H-pyrrolo [3,2-d]pyrimidin-5-yl] ethoxy}ethanol | 493 | 3,55 | 2 | 4 | Memenuhi |
| 2 | Trastuzumab | 493 | 2,35 | 2 | 6 | Memenuhi |
| 3 | 1,2-Ethandiol | 249 | 2,83 | 1 | 2 | Memenuhi |
| 4 | 1,3-Hexadiene | 82 | 1,69 | 0 | 0 | Memenuhi |
| 5 | 1-Eicosanol | 298 | 6,07 | 1 | 1 | Tidak Memenuhi |
| 6 | 1-Phenanthrenol | 194 | 2,18 | 1 | 1 | Memenuhi |
| 7 | 2,2,6,7-Tetramethyl | 435 | 2,89 | 1 | 4 | Memenuhi |
| 8 | 2,5-cyclohexadine | 258 | 3,52 | 0 | 2 | Memenuhi |
| 9 | 2,6,10-trimethylundecan | 214 | 4,26 | 1 | 1 | Memenuhi |
| 10 | 2-butanone | 72 | 1,12 | 0 | 1 | Memenuhi |
| 11 | 2-butenal | 70 | 0,76 | 0 | 1 | Memenuhi |
| 12 | 2-cyclohexenone | 96 | 1,28 | 0 | 1 | Memenuhi |

**LAMPIRAN 3**
**(LANJUTAN)**

**Tabel VII. 1**

| No | Ligan | BM (gr/mol) | Log P | Donor Ikatan | Akseptor Ikatan | Keterangan |
|---|---|---|---|---|---|---|
| 13 | 3,4-isopropylidene | 262 | 4,13 | 0 | 2 | Memenuhi |
| 14 | 6-isopropenyl | 168 | 2,41 | 0 | 2 | Memenuhi |
| 15 | 9-octadecenoic acid | 282 | 4,73 | 1 | 2 | Memenuhi |
| 16 | Benzofuran | 118 | 1,49 | 0 | 1 | Memenuhi |
| 17 | Cadinene | 206 | 4,20 | 0 | 0 | Memenuhi |
| 18 | Calarene | 204 | 3,96 | 0 | 0 | Memenuhi |
| 19 | caryophyllene oxide | 220 | 3,48 | 0 | 1 | Memenuhi |
| 20 | cyclohexane | 84 | 1,83 | 0 | 0 | Memenuhi |
| 21 | cyclohexene | 82 | 1,63 | 0 | 0 | Memenuhi |
| 22 | gamma-gurjunene | 204 | 3,98 | 0 | 0 | Memenuhi |
| 23 | Hexadecane | 336 | 5,14 | 0 | 0 | Tidak Memenuhi |
| 24 | Isopropenyl | 201 | 1,76 | 0 | 1 | Memenuhi |
| 25 | Ledene | 204 | 3,96 | 0 | 0 | Memenuhi |
| 26 | Longifolenaldehyde | 220 | 3,81 | 0 | 1 | Memenuhi |
| 27 | Longiverbenone | 218 | 3,41 | 0 | 1 | Memenuhi |
| 28 | Naphthalene | 128 | 1,94 | 0 | 0 | Memenuhi |

**LAMPIRAN 3**
**(LANJUTAN)**

**Tabel VII. 1**

| No | Ligan | BM (gr/mol) | Log P | Donor Ikatan H | Akseptor Ikatan H | Keterangan |
|---|---|---|---|---|---|---|
| 29 | Nootkatane | 218 | 3,62 | 0 | 1 | Memenuhi |
| 30 | nootkatone | 218 | 3,62 | 0 | 1 | Memenuhi |
| 31 | Sesquirosefuran | 218 | 3,69 | 0 | 1 | Memenuhi |
| 32 | Spathulenol | 220 | 3,67 | 1 | 1 | Memenuhi |
| 33 | Tetralone | 146 | 1,93 | 0 | 1 | Memenuhi |
| 34 | Zierone | 218 | 3,59 | 0 | 1 | Memenuhi |

## LAMPIRAN 4

## HASIL PENELITIAN PREDIKSI FARMAKOKINETIKA

**Tabel VII. 2**
Hasil prediksi farmakokinetika menggunakan situs *online Pre-ADMET*

| No | Ligan | Absorbsi | | Distribusi | Metabolisme dan Ekskresi | | | |
|---|---|---|---|---|---|---|---|---|
| | | HIA (%) | Caco-2 cell (nm sec) | Plasma Protein Binding (%) | CYP 2C19 | CYP2 C9 | CYP 2D6 | CYP 3A4 |
| 1 | 2-{2-[4-({5-chloro-6-[3-(trifluoromethyl)phenoxy ]pyridin-3-yl}amino)-5H-pyrrolo[3,2-d]pyrimidin-5-yl]ethoxy}ethanol | 95,56[a] | 36.18[b] | 90.99 [a] | non | Inh | non | Inh |
| 2 | Trastuzumab | 93.22[a] | 19.04 [b] | 68.94 [b] | non | non | non | Inh |
| 3 | 1,2-Ethandiol | 93.56 [a] | 1.88 [c] | 92.68 | Inh | Inh | non | non |
| 4 | 1,3-Hexadiene | 100 [a] | 23.39 [b] | 51.08 [b] | Inh | Inh | non | non |
| 5 | 1-Eicosanol | 100 [a] | 47.02 [b] | 100 [a] | Inh | Inh | non | Inh |
| 6 | 1-Phenanthrenol | 100 [a] | 29.99 [b] | 100 [a] | Inh | Inh | non | Inh |
| 7 | 2,2,6,7-Tetramethyl | 98.99 [a] | 50.19 [b] | 91.00 [a] | non | non | non | non |
| 8 | 2,5-cyclohexadine | 99.14 [a] | 46.90 [b] | 100 [a] | Inh | Inh | non | non |
| 9 | 2,6,10-trimethylundecan | 100 [a] | 31.08 [b] | 100 [a] | Inh | Inh | non | Inh |
| 10 | 2-butanone | 100 [a] | 34.22 [b] | 69.47 [b] | Inh | Inh | non | Inh |
| 11 | 2-butenal | 100 [a] | 28.38 [b] | 71.16 [b] | Inh | Inh | non | non |
| 12 | 2-cyclohexenone | 100 [a] | 34.40 [b] | 89.98 [b] | Inh | Inh | non | non |
| 13 | 3,4-isopropylidene | 100 [a] | 45.12 [b] | 100 [a] | non | Inh | non | non |
| 14 | 6-isopropenyl | 100 [a] | 33.86 [b] | 98.85 [a] | Inh | Inh | non | Inh |
| 15 | 9-octadecenoic acid | 98.43 [a] | 28.19 [b] | 100 [a] | Inh | Inh | non | Inh |
| 16 | Benzofuran | 100 [a] | 53.25 [b] | 100 [a] | Inh | Inh | non | Inh |
| 17 | Cadinene | 100 [a] | 23.40 [b] | 100 [a] | Inh | Inh | non | non |
| 18 | Calarene | 100 [a] | 23.63 [b] | 100 [a] | non | Inh | non | non |
| 19 | Caryophyllene oxide | 100 [a] | 56.34 [b] | 90.84 [a] | non | Inh | non | non |
| 20 | Cyclohexane | 100 [a] | 22.29 [b] | 100 [a] | Inh | Inh | non | Inh |
| 21 | Cyclohexene | 100 [a] | 23.39 [b] | 93.74 [a] | Inh | Inh | non | non |
| 22 | Gamma-gurjunene | 100 [a] | 23.64 [b] | 100 [a] | Inh | Inh | non | Inh |
| 23 | Hexadecane | 100 [a] | 22.19 [b] | 100 [a] | Inh | Inh | non | Inh |
| 24 | Isopropenyl | 100 [a] | 11.29 [b] | 87.60 [b] | Inh | Inh | non | Inh |

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

**Tabel VII. 2**

| No | Ligan | Absorbsi | | Distribusi | Metabolisme dan Ekskresi | | | |
|---|---|---|---|---|---|---|---|---|
| | | HIA (%) | Caco-2 cell (nm sec) | Plasma Protein Binding (%) | CYP 2C19 | CYP 2C9 | CYP 2D6 | CYP 3A4 |
| 25 | Ledene | 100 [a] | 22.32 [b] | 100 [a] | non | Inh | non | Inh |
| 26 | Longifolenaldehyde | 100 [a] | 23.30 [b] | 81.11 [b] | non | Inh | non | Inh |
| 27 | Longiverbenone | 100 [a] | 39.18 [b] | 99.05 [a] | non | Inh | non | non |
| 28 | Naphthalene | 100 [a] | 23.44 [b] | 100 [a] | Inh | Inh | non | Inh |
| 29 | Nootkatane | 100 [a] | 15.97 [b] | 100 [a] | non | Inh | non | non |
| 30 | Nootkatone | 100 [a] | 15.97 [b] | 100 [a] | non | Inh | non | non |
| 31 | Sesquirosefuran | 100 [a] | 31.06 [b] | 100 [a] | Inh | Inh | non | Inh |
| 32 | Spathulenol | 100 [a] | 54.42 [b] | 82.88 [b] | non | Inh | non | Inh |
| 33 | Tetralone | 100 [a] | 34.71 [b] | 54.85 [b] | Inh | Inh | non | Inh |
| 34 | Zierone | 100 [a] | 43.18 [b] | 100 [a] | Inh | Inh | non | Inh |

Keterangan :

HIA : 70 - 100 penyerapan baik[a]

20 – 70 terserap cukup[b]

< 20 kurang terserap[c]

CaCo-2 (nm-sec) : >70 permeabilitas tinggi[a]

4 – 70 permeabilitas sedang[b]

< 4 permeabilitas rendah[c]

PPB (%) : > 90 terikat kuat[a]

< 90 terikat lemah[b]

## LAMPIRAN 5

## HASIL PENELITIAN PREDIKSI TOKSISITAS

**Tabel VII. 3**
Hasil prediksi toksisitas menggunakan aplikasi *toxtree*

| No | Ligan | Cramer Rules | Karsinogenik | | Kroes TCC |
|---|---|---|---|---|---|
| | | | Genotoxic | Non genotoxic | |
| 1 | 2-{2-[4-({5-chloro-6-[3-(trifluoromethyl)phenoxy]pyridin-3-yl}amino)-5H-pyrrolo[3,2-d]pyrimidin-5-yl]ethoxy}ethanol | 3 | - | - | 1 |
| 2 | Trastuzumab | 3 | + | - | 2 |
| 3 | 1,2 ethandiol | 1 | - | - | 1 |
| 4 | 1,3-hexadiene | 1 | - | - | 1 |
| 5 | 1-eicosanol | 1 | - | - | 1 |
| 6 | 1-phenanthrenol | 3 | + | - | 2 |
| 7 | 2,2,6,7-tetramethyl | 3 | - | - | 1 |
| 8 | 2,5-cyclohexadine | 2 | - | + | 2 |
| 9 | 2,6,10-trimethylundecan | 1 | - | + | 1 |
| 10 | 2-butanone | 1 | - | - | 1 |
| 11 | 2-butenal | 1 | + | - | 2 |
| 12 | 2-cyclohexenone | 2 | + | - | 2 |
| 13 | 3,4-isopropylidene | 3 | - | - | 1 |
| 14 | 6-isopropenyl | 1 | - | - | 1 |
| 15 | 9-octadecenoic acid | 1 | - | - | 1 |
| 16 | Benzofuran | 3 | - | - | 1 |
| 17 | Cadinene | 1 | - | - | 1 |
| 18 | Calarene | 1 | - | - | 1 |
| 19 | Caryophyllene oxide | 3 | + | + | 2 |
| 20 | Cyclohexane | 1 | - | - | 1 |
| 21 | Cyclohexene | 1 | - | - | 1 |
| 22 | Gamma-gurjunene | 1 | - | - | 1 |
| 23 | Hexadecane | 1 | - | - | 1 |
| 24 | Isopropenyl | 1 | + | - | 2 |
| 24 | Ledene | 1 | - | - | 1 |
| 26 | Longifolenaldehyde | 1 | + | - | 2 |
| 27 | Longiverbenone | 3 | + | - | 2 |
| 28 | Naphthalene | 3 | - | - | 1 |
| 29 | Nootkatane | 3 | + | - | 2 |

**LAMPIRAN 5**
**(LANJUTAN)**

**Tabel VII. 3**

| No | Ligan | Cramer Rules | Karsinogenik | | Kroes TCC |
|---|---|---|---|---|---|
| | | | Genotoxic | Non genotoxic | |
| 30 | Nootkatone | 3 | + | - | 2 |
| 31 | Sesquirosefuran | 3 | - | - | 1 |
| 32 | Spathulenol | 3 | - | - | 1 |
| 33 | Tetralone | 1 | - | - | 1 |
| 34 | Zierone | 3 | + | - | 2 |

**Keterangan** : *Kroes TTC decission tree 1 (Subtance would not be expected to be a safety concern), 2 (Negligible risk (low probability of a life time cancer risk greater than 1 in 10^6 ), cramer rules : class 1 : low, class 2 : intermediet, class 3 : high*

## LAMPIRAN 6

## ENERGI BEBAS DAN RESIDU ASAM AMINO RESEPTOR 3PP0

**Tabel VII. 4**
Energi bebas dan residu asam amino simulasi molecular *docking* senyawa minyak atsiri terhadap reseptor HER-2 ID 3PP0

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 1 | 2-{2-[4-({5-chloro-6-[3-(trifluoromethyl)phenoxy]pyridin-3-yl}amino)-5H-pyrrolo[3,2-d]pyrimidin-5-yl]ethoxy}ethanol | -9.95 | 51.27 | ALA730, GLY729, ASP863, VAL734, THR862, PHE864, MET774, LEU785, SER783, LYS753, LEU796, ARG784, THR798, LEU786, GLN799, ILE752, ALA751, VAL797, MET801, LEU800, LEU852, LEU726, GLY804, ARG849, CYS805, ASN850 |
| 2 | Trastuzumab | -10.76 | 12.99 | LEU785, LEU796, THR798, ARG784, SER783, MET774, PHE864, ASP863, SER728, ALA730, ASN850, GLY729, THR862, CYS805, ARG849, GLY804, LEU726, LEU800, MET801, ALA751, LEU852, VAL734, LYS753 |
| 3 | 1,2-Ethandiol | -2.18 | 25.05 | ASP863, GLU770, GLY865, LEU755, LYS753, LEU796 PHE864 |

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

**Tabel VII. 4**

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 4 | 1,3-Hexadiene | -3.75 | 1.78 | THR798, SER783, ARG784, MET774, PHE864, GLU770, LEU785, ALA771, LEU796 |
| 5 | 1-Eicosanol | -6.73 | 11.71 | LYS753, VAL734, LEU800, PRO802, MET801, GLY804, LEU726, ALA751, LEU852, THR798, ASP863, THR862, PHE864,, SER783, ARG784, LEU785, MET774, GLU770, ALA771, ILE767 LEU796 |
| 6 | 1-Phenanthrenol | -7.76 | 2.05 | ARG784, THR798, THR862, SER783, ASP863, ALA771, GLU770, PHE864, MET774, LEU785, LYS753, LEU796 |
| 7 | 2,2,6,7-Tetramethyl | -10.63 | 16.26 | LEU796, THR862, ALA730, LYS753, GLY729, ASP863, SER728, ASN850, ALA751, ARG849, LEU852, LEU726, GLN799, LEU800, CYS805, MET801, GLY804, THR798, VAL734 |

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

**Tabel VII. 4**

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 8 | 2,5-cyclohexadine | -8.72 | 408.66 | GLU770, SER783, ASP,863, THR862, VAL734, ALA751, THR798, LEU852, LYS753, VAL797, ILE752, ILE767, PHE864, LEU785, LEU796, ALA771, MET774 |
| 9 | 2,6,10-trimethylundecan | -6.65 | 13.31 | ALA751, LYS753, ILE752, VAL734, VAL797, THR798, THR862, ASP863, LEU785, ARG784, PHE864, MET774, SER783, ALA771, GLU770, ILE767, LEU796 |
| 10 | 2-butanone | -3.05 | 5.77 | LEU755, GLY865, ILE767, GLU770, LEU796, PHE864, LYS753, ASP863 |
| 11 | 2-butenal | -.3.12 | 5.19 | LEU755, LEU796, GLU770, LEU785, MET774, PHE864, ASP863, GLY865, LYS753 |

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

**Tabel VII. 4**

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 12 | 2-cyclohexenone | -4.25 | 764.47 | THR862, ASP863, PHE864, MET774, LEU796, LEU785, ARG784, THR798, SER783 |
| 13 | 3,4-isopropylidene | -7.27 | 4.70 | THR798, CYS805, LEU726, LEU852, SER728, GLY727, GLY729, ARG849, VAL734, ASN850, ALA751, THR862, LYS753, ASP863 |
| 14 | 6-isopropenyl | -6.23 | 27.33 | MET774, PHE864, ARG784, LEU796, LEU785, THR798, VAL797, ALA751, ILE752, VAL734, LYS753, ASP863, THR862, SER783 |
| 15 | 9-octadecenoic acid | -7.19 | 5.39 | ASP863, THR798, THR862, LYS753, VAL734, ALA751, LEU726, LEU852, GLN799, LEU800, GLY804, MET801, SER783, PHE864, ALA771, MET774, LEU796, GLU770, LEU785 |

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

**Tabel VII. 4**

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 16 | Benzofuran | -4.94 | 237.75 | GLU770, ALA771, MET774, LEU785, LEU796, ARG784, PHE864, THR798, SER783, THR862, ASP863 |
| 17 | Cadinene | -7.68 | 2.36 | GLU770, LEU796, ASP863, ILE752, VAL797, THR798, ALA751, LYS753, VAL734, MET774, SER783, ARG784, LEU785, PHE864 |
| 18 | Calarene | -7.35 | 4.07 | ALA771, GLU770, MET774, ASP863, LEU796, LEU785, LYS753, VAL797, THR798, PHE864, ARG784, SER783, THR862 |
| 19 | Caryophyllene oxide | -7.18 | 5.47 | GLU770, LEU796, PHE864, MET774, LEU785, ARG784, SER783, LEU786, VAL797, ALA751, THR798, THR862, ASP863, VAL734, LYS753 |

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

**Tabel VII. 4**

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 20 | Cyclohexane | -4.12 | 956.76 | ILE767, GLU770, ASP863, LEU796, PHE864 |
| 21 | Cyclohexene | -4.01 | 1.15 | ASP863, PHE864, GLU770, MET774, LEU796, LEU785, ALA771, ILE767 |
| 22 | Gamma-gurjunene | -8.25 | 889.96 | LYS753, LEU796, ASP863, GLU770, ALA771, LEU785, MET774, ARG784, SER783, THR798, PHE864, ILE752, VAL797, ALA751, VAL734 |
| 23 | Hexadecane | -6.48 | 17.71 | GLY729, VAL734, ASP863, LYS753, THR862, ALA751, VAL797, THR798, ILE767, LEU785, SER783, PHE864, LEU796, GLU770, ALA771, ARG784, MET774 |

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

**Tabel VII. 4**

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 24 | Isopropenyl | -7.64 | 2.52 | SER783, ARG784, THR798, VAL797, ALA751, ILE752, VAL734, LYS753, THR862, ASP863, MET774, LEU796, GLU770, PHE864, ALA771, LEU785 |
| 25 | Ledene | -7.55 | 2.93 | ALA771, LEU785, PHE864, GLU770, MET774, LEU796, ASP863, LYS753, THR862, THR798, SER783, ARG784 |
| 26 | Longifolenaldehyde | -8.46 | 625.51 | PHE864, LEU796, LEU785, ALA771, GLU770, MET774, SER783, LYS753, THR798, THR862, ASP863 |
| 27 | Longiverbenone | -8.58 | 517.11 | PHE864, VAL797, LEU796, THR798, MET774, GLU770, LEU785, ARG784, SER783, THR862, ASP863, LYS753 |

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

**Tabel VII. 4**

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 28 | Naphthalene | -5.95 | 43.56 | ARG784, THR798, SER783, THR862, PHE864, ASP863, LEU785, MET774, LEU796, GLU770, ALA771 |
| 29 | Nootkatane | -8.27 | 864.24 | ALA771, GLU770, PHE864, MET774, LEU796, LEU785, ARG784, THR798, SER783, THR862, ALA751, VAL734, LEU852, LYS753, ASP863 |
| 30 | Nootkatone | -8.27 | 867.12 | ALA771, GLU770, PHE864, MET774, LEU796, LEU785, ARG784, THR798, SER783, THR862, ALA751, VAL734, LEU852, LYS753, ASP863 |
| 31 | Sesquirosefuran | -8.09 | 1.17 | LEU785, GLU770, ILE767, ALA771, ILE752, LEU796, LYS753, VAL734, ALA751, THR798, VAL797, PHE864, MET774, THR862, SER783, ARG784, ASP863 |

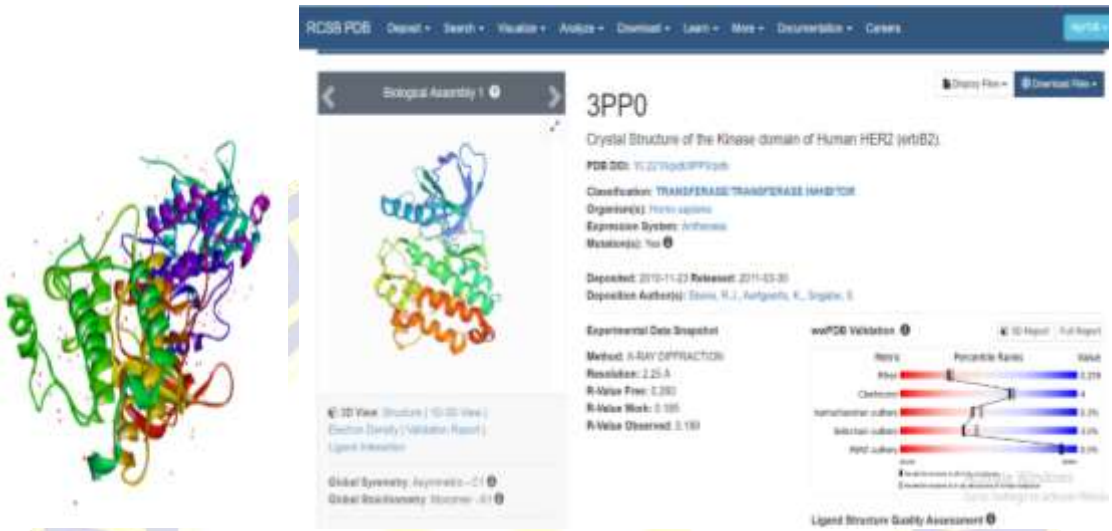
**LAMPIRAN 6**
**(LANJUTAN)**

**Tabel VII. 4**

| No | Nama Senyawa | (ΔG) (kkal/mol) | KI (nM) | Residu Asam Amino |
|---|---|---|---|---|
| 32 | Spathulenol | -6.83 | 9.87 | GLU770, ALA771, MET774, PHE864, ARG784, SER783, THR798, LEU785, THR862, ASP863, LEU796, LYS753 |
| 33 | Tetralone | -6.27 | 25.40 | ALA771, GLU770, LEU796, PHE864, ASP863, MET774, LYS753, THR862, SER783, THR798, ARG784, LEU785 |
| 34 | Zierone | -7.83 | 1.84 | ASP863, LEU755, THR862, ILE752, ALA751, LYS753, VAL797, THR798, ARG784, LEU785, SER783, PHE864, LEU796, MET774, GLU770 |

# LAMPIRAN 7

# DOKUMENTASI




**Gambar VII. 12** Struktur 3D makromolekul ID 3PP0

**LAMPIRAN 7**
**(LANJUTAN)**

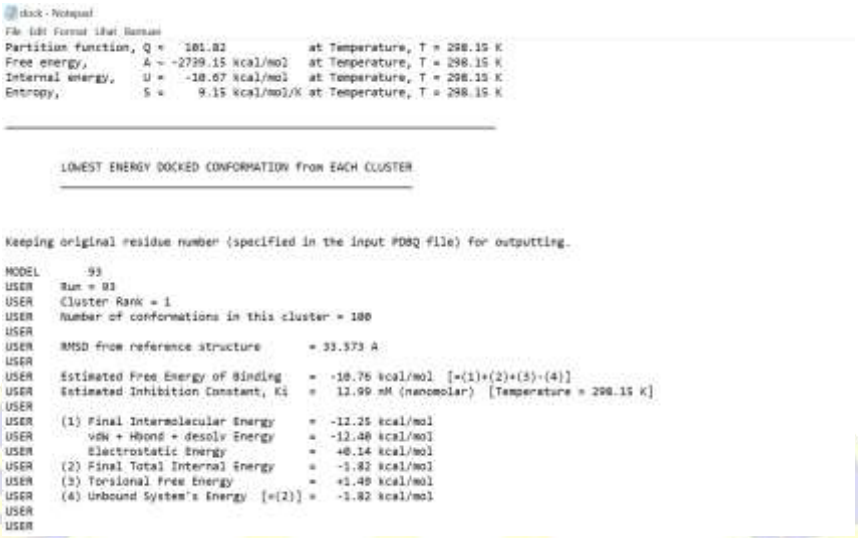

**Gambar VII. 13** Grid-Box pada Reseptor ID 3PP0

**LAMPIRAN 7**
**(LANJUTAN)**

```
LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
_____________________________________________________


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL     35
USER    Run = 35
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 48
USER
USER    RMSD from reference structure       = 0.642 A
USER
USER    Estimated Free Energy of Binding    =  -10.62 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   16.34 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -13.61 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -13.56 kcal/mol
USER        Electrostatic Energy            =   -0.04 kcal/mol
USER    (2) Final Total Internal Energy     =   -1.71 kcal/mol
USER    (3) Torsional Free Energy           =   +2.90 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -1.71 kcal/mol
USER
USER
USER
USER    DPF = dock.dpf
USER    NEWDPF move     ligand.pdbqt
USER    NEWDPF about    17.039001 16.548700 26.600599
USER    NEWDPF trans0   17.294184 16.638910 26.480320
USER    NEWDPF axisangle0       0.935453 0.348295 -0.060159 -4.115121
USER    NEWDPF quaternion0      0.033586 0.012505 -0.002160 -0.999355
USER    NEWDPF dihe0    162.45 95.05 29.97 -127.54 42.75 12.34 -5.08 1.65 -7.59 12.60
```

**Gambar VII. 14** Hasil Validasi Reseptor HER-2 ID 3PP0 pada AutoDock Tools®

**LAMPIRAN 7**
**(LANJUTAN)**



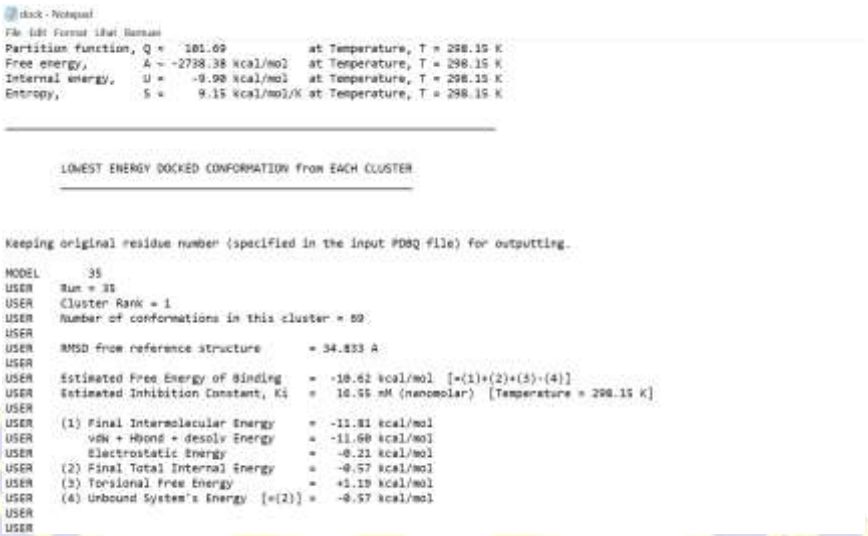
dock - Notepad

File Edit Format View Help

```
Partition function, Q =   101.82            at Temperature, T = 298.15 K
Free energy,        A = -2739.15 kcal/mol   at Temperature, T = 298.15 K
Internal energy,    U =   -10.67 kcal/mol   at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K


        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER


Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL     93
USER    Run = 93
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 100
USER
USER    RMSD from reference structure       = 33.573 A
USER
USER    Estimated Free Energy of Binding    =  -10.76 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   12.99 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -12.25 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -12.40 kcal/mol
USER        Electrostatic Energy            =   +0.14 kcal/mol
USER    (2) Final Total Internal Energy     =   -1.82 kcal/mol
USER    (3) Torsional Free Energy           =   +1.48 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -1.82 kcal/mol
USER
USER
```

**Gambar VII. 15** Hasil *docking* senyawa pembanding terhadap reseptor 3PP0

**LAMPIRAN 7**
**(LANJUTAN)**



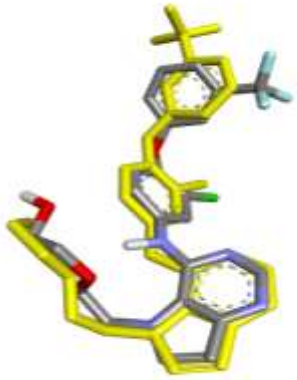
dock - Notepad

File Edit Format View Help

```
Partition function, Q =   101.69           at Temperature, T = 298.15 K
Free energy,        A = -2738.38 kcal/mol  at Temperature, T = 298.15 K
Internal energy,    U =    -0.90 kcal/mol  at Temperature, T = 298.15 K
Entropy,            S =     9.15 kcal/mol/K at Temperature, T = 298.15 K

_____________________________________________________________________________

        LOWEST ENERGY DOCKED CONFORMATION from EACH CLUSTER
        ___________________________________________________

Keeping original residue number (specified in the input PDBQ file) for outputting.

MODEL       35
USER    Run = 35
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 80
USER
USER    RMSD from reference structure       = 34.833 A
USER
USER    Estimated Free Energy of Binding    =  -10.62 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   16.55 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -11.81 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -11.60 kcal/mol
USER        Electrostatic Energy            =   -0.21 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.57 kcal/mol
USER    (3) Torsional Free Energy           =   +1.19 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.57 kcal/mol
USER
USER
```

**Gambar VII. 16** Hasil *docking* senyawa 2,2,6,7-tetramethyl terhadap reseptor 3PP0

**LAMPIRAN 7**
**(LANJUTAN)**



**Gambar VII. 17** Visualisasi tumpang tindih ligan alami dengan ligan hasil re*docking* dari reseptor HER-2

# DAFTAR RIWAYAT HIDUP

## I. IDENTITAS DIRI


Nama : Triana Ramadhanty
Tempat, Tanggal Lahir : Garut, 3 Januari 2000
Jenis Kelamin : Perempuan
Agama : Islam
Kewarganegaraan : Indonesia
Status : Mahasiswa
Alamat : Kp. Panyosogan, Cibatu-Garut
Telepon : 089613713359
Email : ramadhantytriana1@gmail.com
Instagram : trianarmdhy


## II. RIWAYAT HIDUP

| Jenjang Pendidikan | Nama Sekolah/Perguruan Tinggi | Tahun Masuk | Tahun Lulus |
|---|---|---|---|
| SD/MI | SDN KERESEK VI & SDN WANAKERTA 1 | 2006 | 2012 |
| SMP/MTS | SMP NEGERI 1 CIBATU | 2012 | 2015 |
| SMA/MA/SMK | SMA NEGERI 3 GARUT | 2015 | 2018 |
| Perguruan Tinggi | Universitas Garut | 2018 | 2022 |