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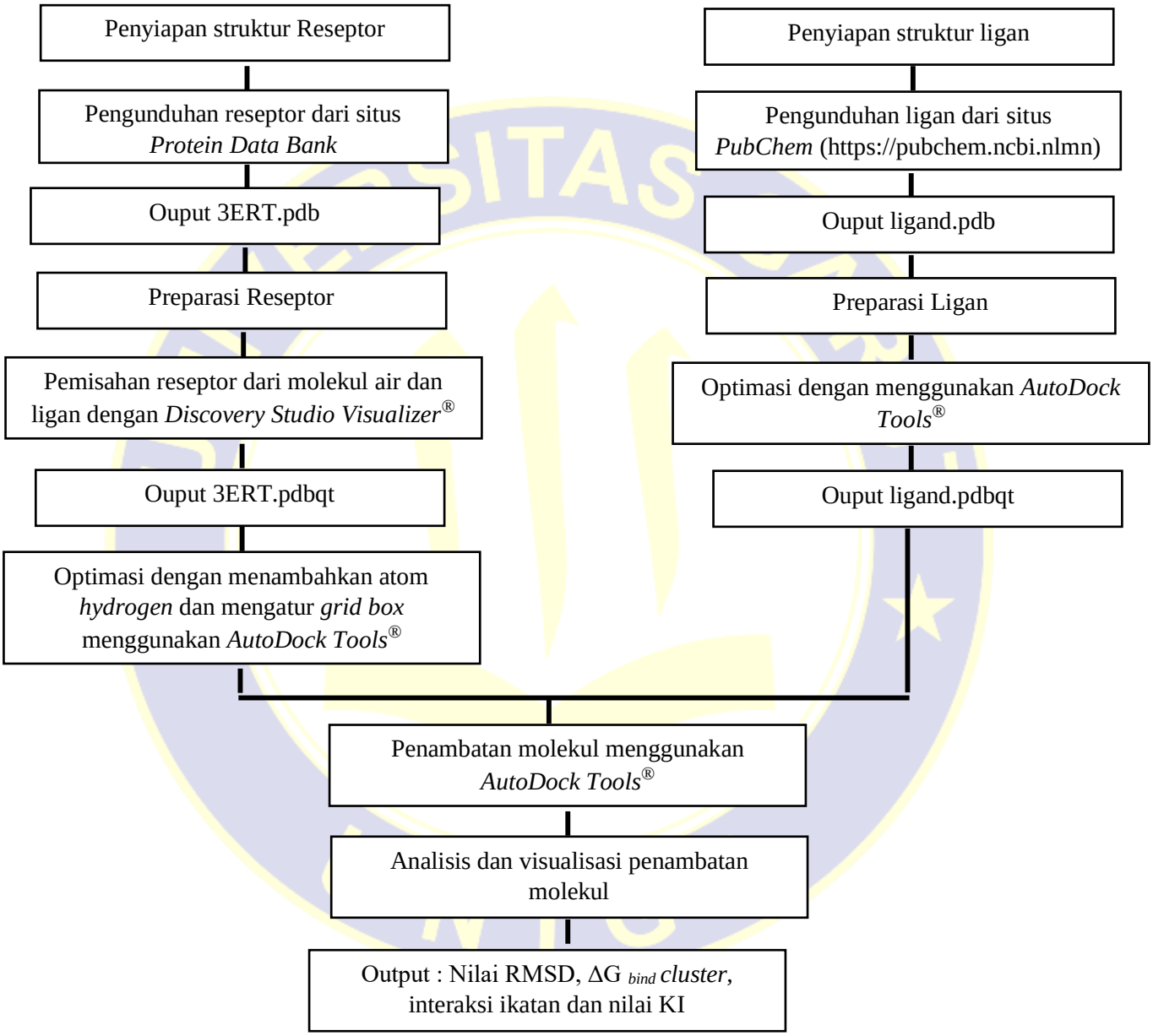
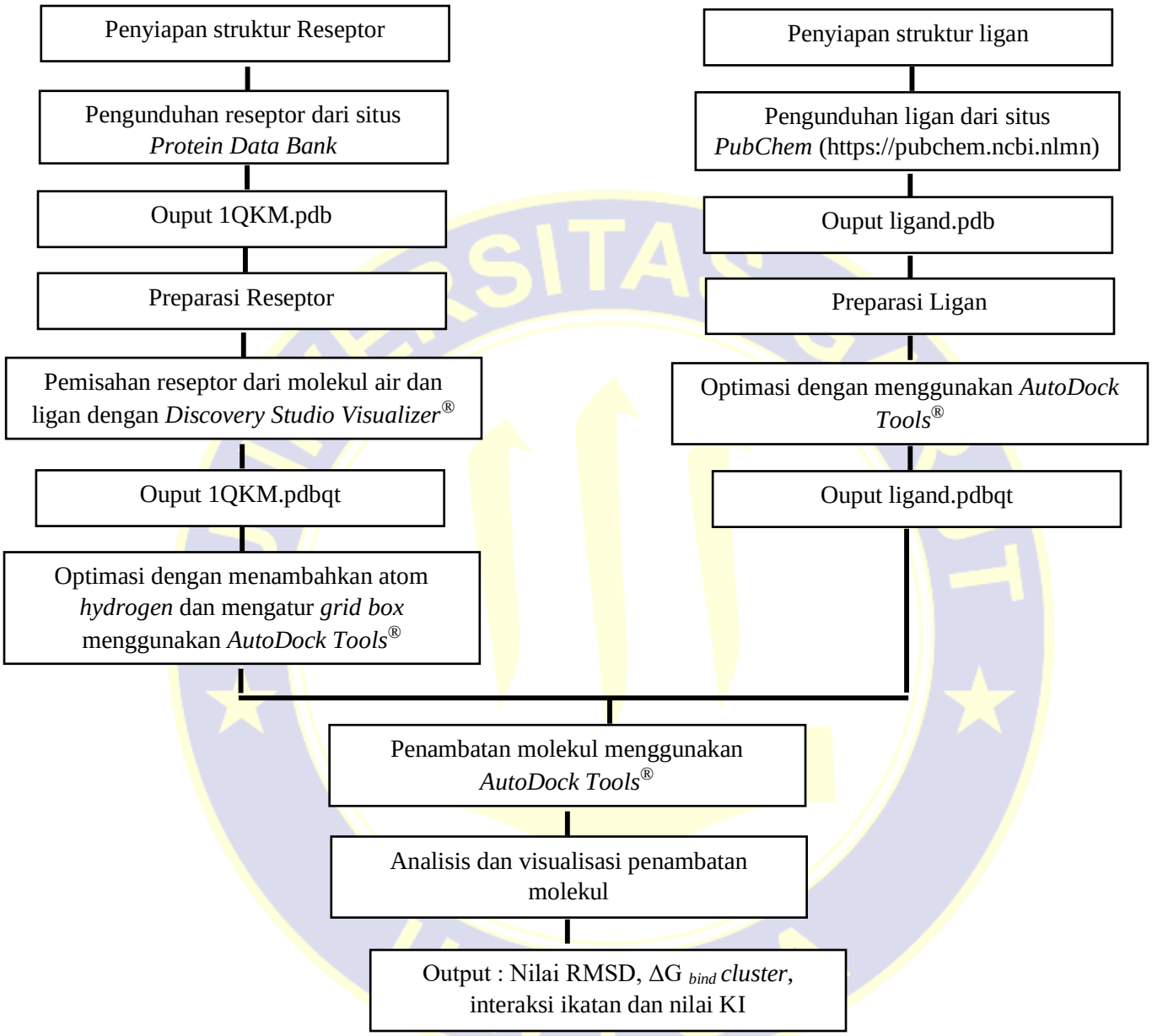
## LAMPIRAN 1

## ALUR PENELITIAN *MOLECULAR DOCKING*




**Gambar VII. 1** Alur penelitian penambatan molekul reseptor 3ERT

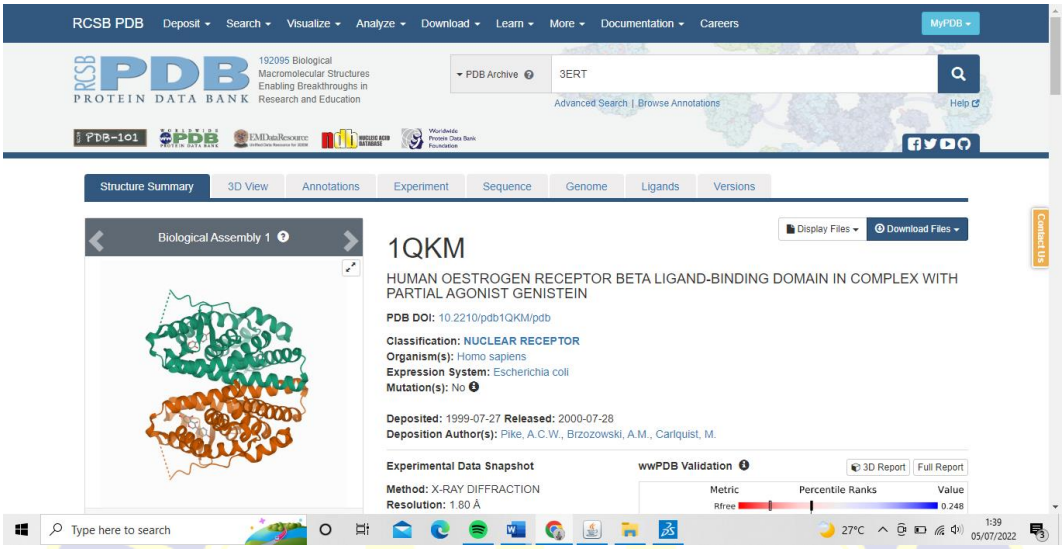
**LAMPIRAN 1**
**(LANJUTAN)**




**Gambar VII. 2** Alur penelitian penambatan molekul reseptor 1QKM

**LAMPIRAN 2**

# SITUS PDB (PROTEIN DATA BANK)




**Gambar VII. 3** Situs online PDB (*Protein Data Bank*)

# LAMPIRAN 3

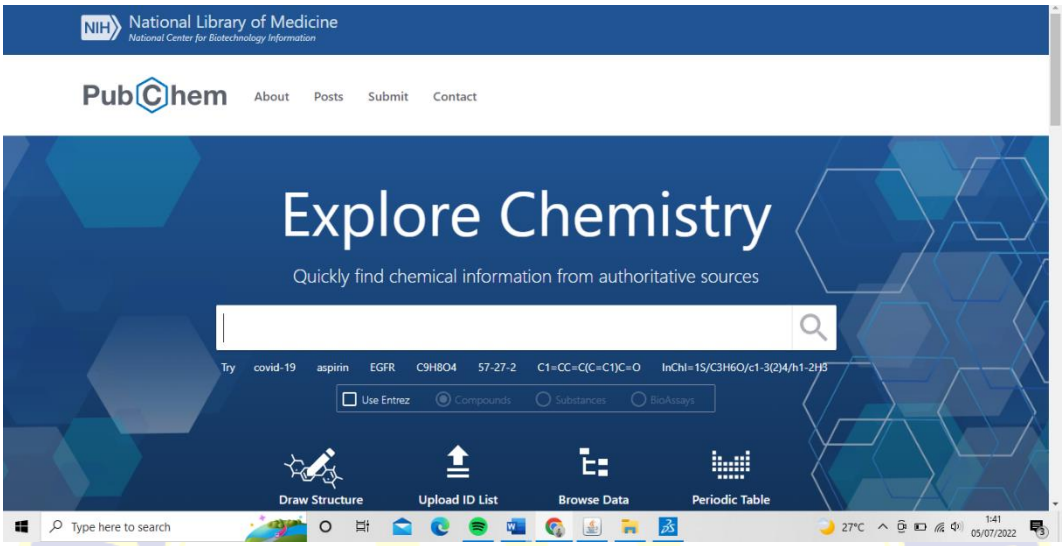
## SITUS *PassOnline-Way2drug*



**Gambar VII. 4** Situs *PassOnline-Way2drug*

# LAMPIRAN 4

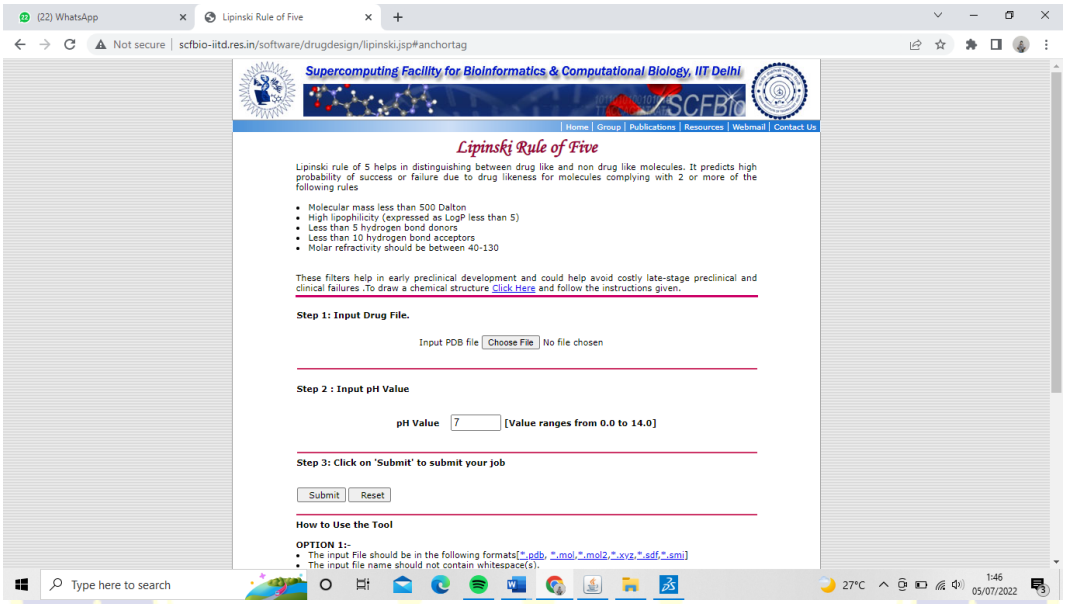
## SITUS *PubChem*




**Gambar VII**. 5 Situs *PubChem*

# LAMPIRAN 5

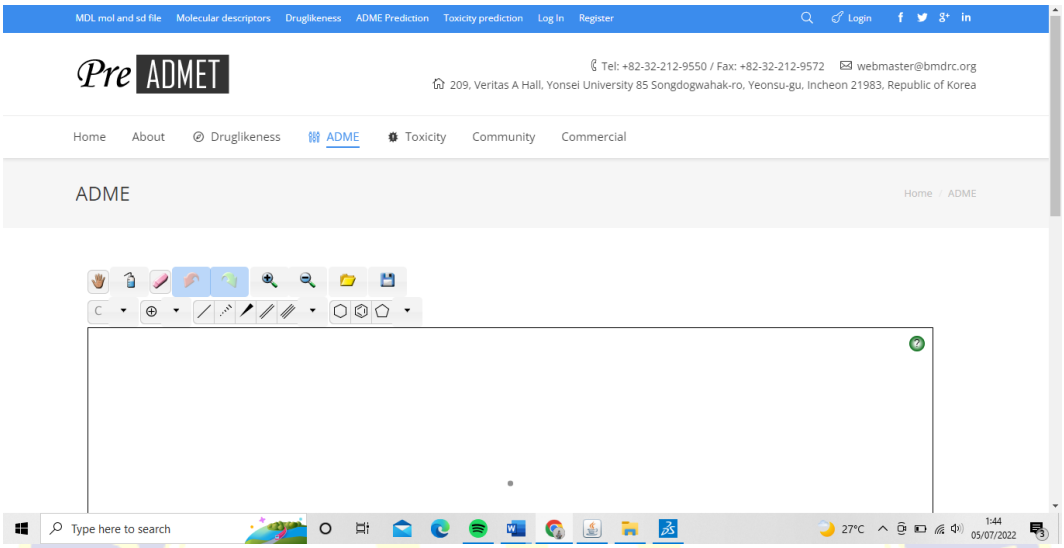
## SITUS *Lipinski Rule of Five*




**Gambar VII. 6** Situs *Lipinski Rule of Five*

# LAMPIRAN 6

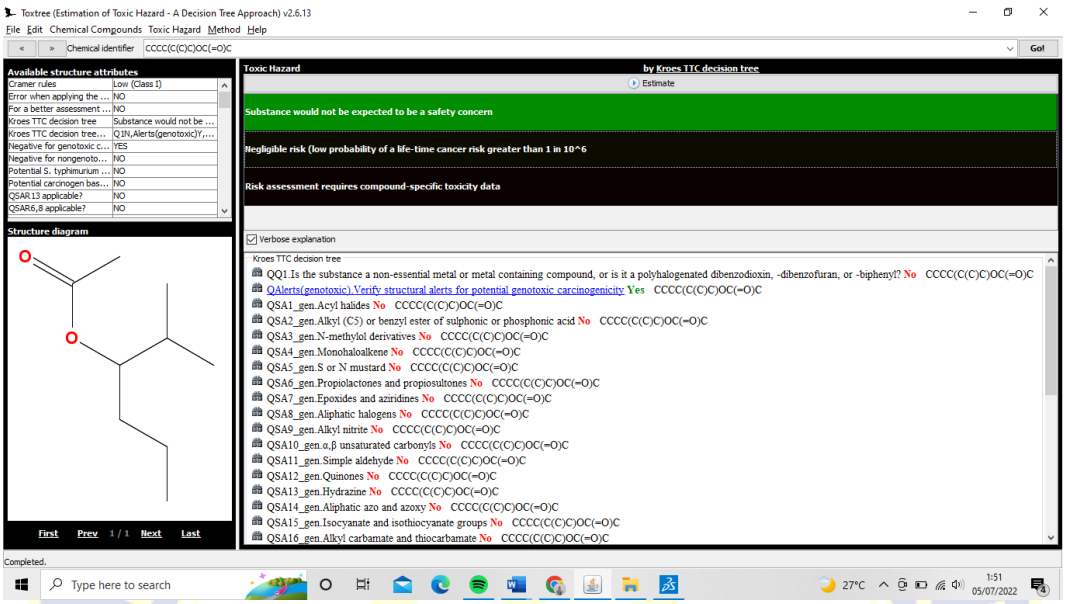
## SITUS *Pre-ADMET*




**Gambar VII. 7** Situs *Pre-ADMET*

# LAMPIRAN 7

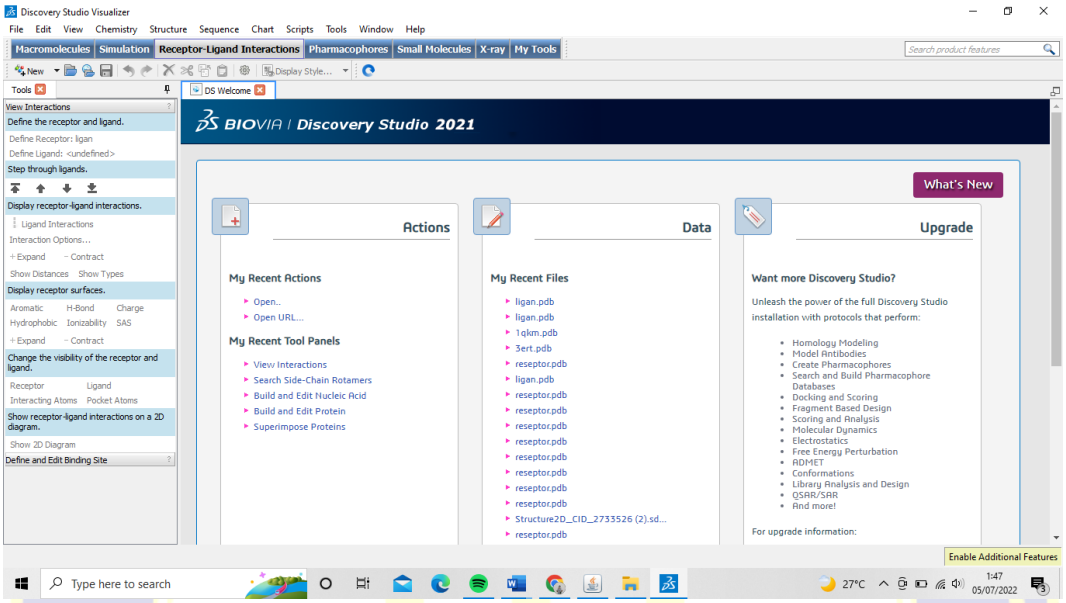
## PERANGKAT LUNAK *TOXTREE*




**Gambar VII. 8** Perangkat lunak *toxtree*

# LAMPIRAN 8

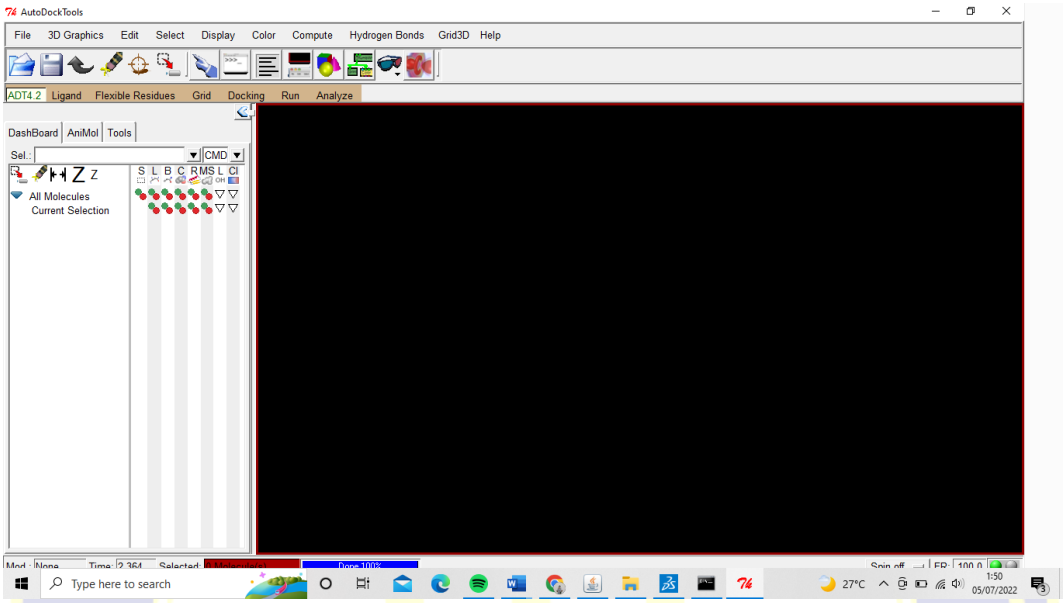
## PERANGKAT LUNAK *DISCOVERY STUDIO VISUALIZER*




**Gambar VII. 9** Perangkat lunak *discovery studio visualizer*

# LAMPIRAN 9

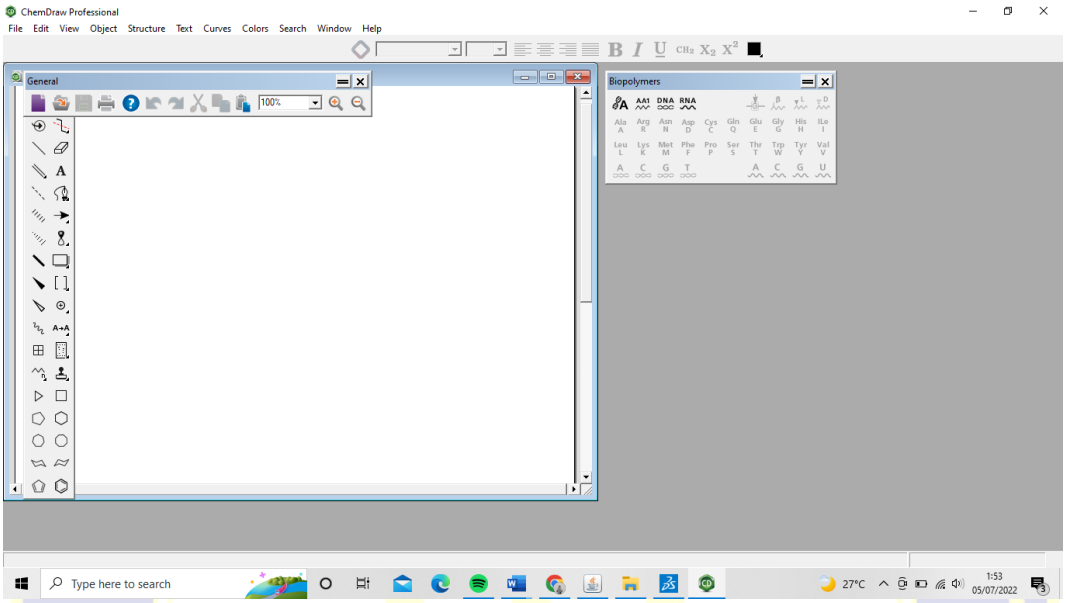
## PERANGKAT LUNAK *AUTODOCK TOOLS*




**Gambar VII. 10** Perangkat lunak *autodock tools*

# LAMPIRAN 10

## PERANGKAT LUNAK *CHEM DRAW*

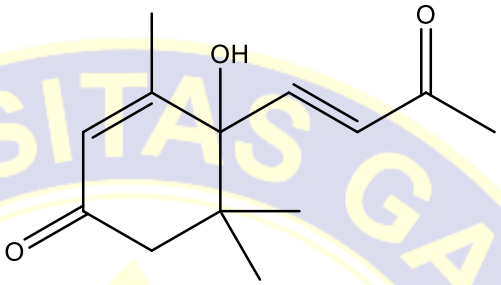
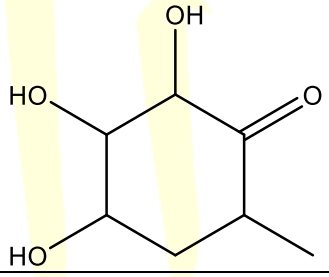
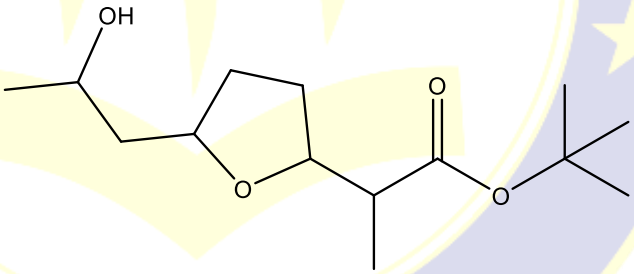
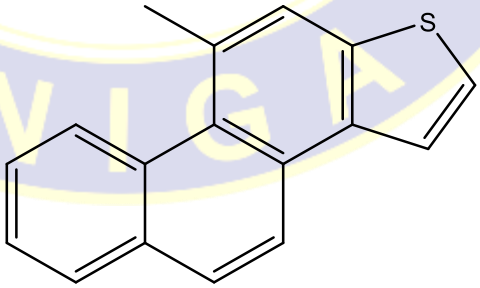



**Gambar VII. 11** Perangkat lunak *chemdraw*

## LAMPIRAN 11

## SENYAWA BELIMBING WULUH (*Averrhoa bilimbi L.*)

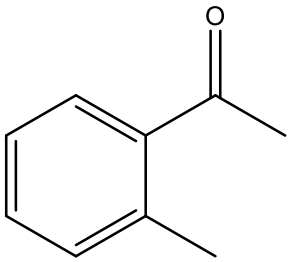
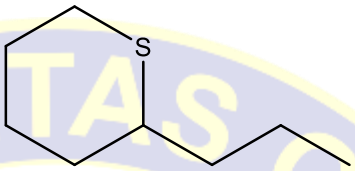
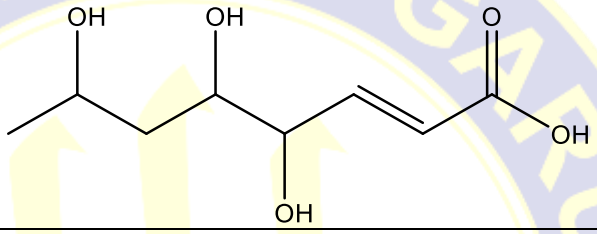
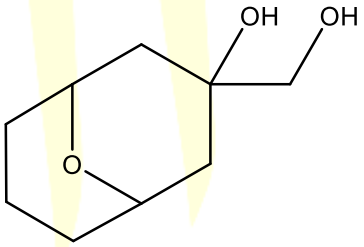
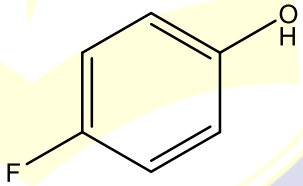
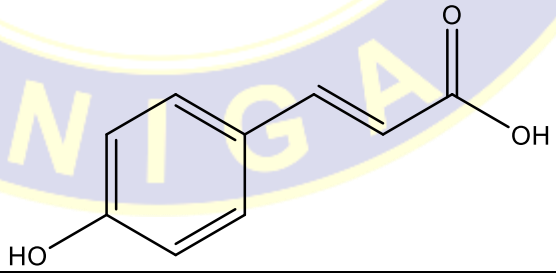
**Tabel VII. 1**
Struktur 2D Senyawa Aktif Belimbing Wuluh

| No | Senyawa | Struktur 2D |
|---|---|---|
| 1. | *(s)-dehydrovomifoliol* |  |
| 2. | *1-Heneicosyl formate* |  |
| 3. | *2,3,4-Trihydroxy-6-methylcyclohexanone* |  |
| 4. | *2-[5-(2-Hydroxy-propyl)-tetrahydrofuran-2-yl]-propionic acid, t-butyl ester* |  |
| 5. | *2-Furancarboxylic acid, tert-butyldimethylsilyl ester* |  |

## LAMPIRAN 11
## (LANJUTAN)

**Tabel VII.1**

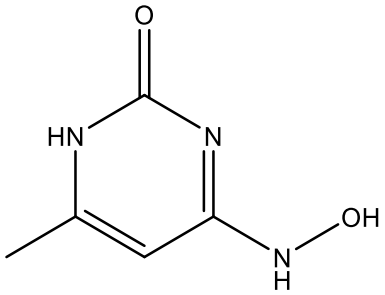
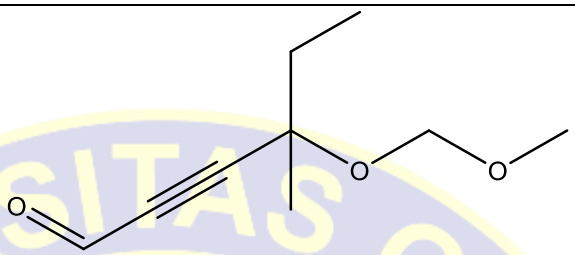
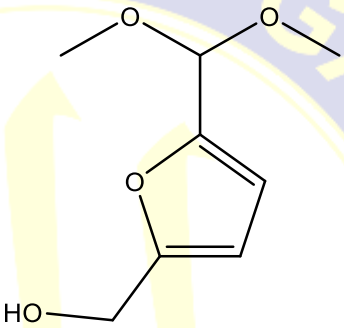
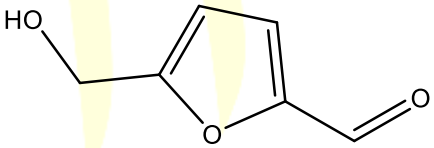
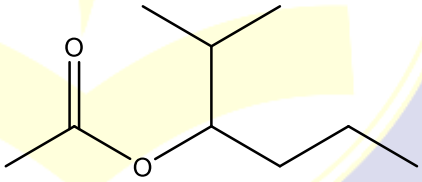
Lanjutan

| No | Senyawa | Struktur 2D |
|---|---|---|
| 6 | *2-Methylacetophenone* |  |
| 7 | *2-n-Propylthiane* |  |
| 8. | *2-Octenoic acid, 4,5,7-trhydroxy* |  |
| 9. | *3-(hydroxymethyl)-9-Oxabicyclo [3.3.1] nonan-3-ol* |  |
| 10. | *4-fluorophenol* |  |
| 11. | *4-hydroxycinnamic acid* |  |

**LAMPIRAN 11**
**(LANJUTAN)**

**Tabel VII.1**
Lanjutan

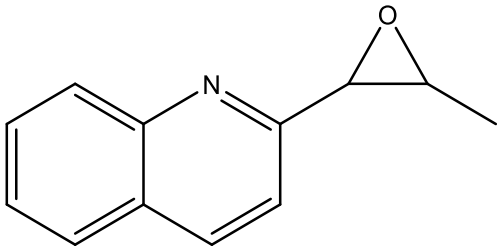
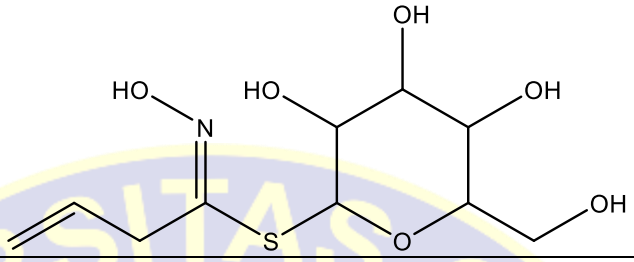
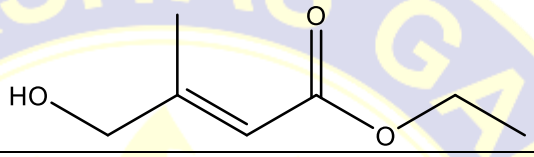
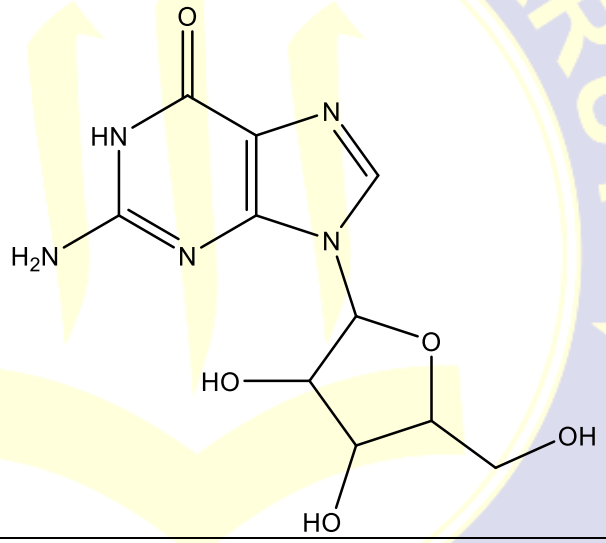
| No | Senyawa | Struktur 2D |
|---|---|---|

| | | |
|---|---|---|
| 12. | *4-Hydroxylamino-6-methylpyrimidin-2(1H)-one* |  |
| 13. | *4-Methoxymethoxy-4-methyl-hex-2-ynal* |  |
| 14. | *5-(hydroxymethyl)-2-(dimethoxymethyl) Furan* |  |
| 15. | *5-Hydroxymethylfurfural* |  |
| 16. | *Acetic acid, 2-methylhex-3-yl ester* |  |

**LAMPIRAN 11**
**(LANJUTAN)**

**Tabel VII.1**
Lanjutan

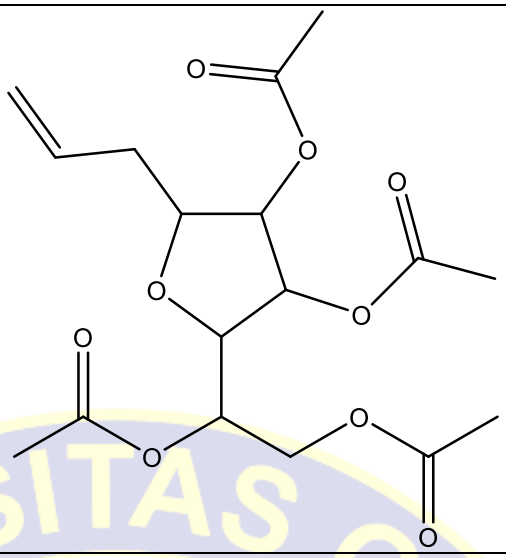
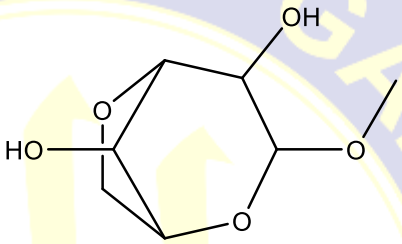
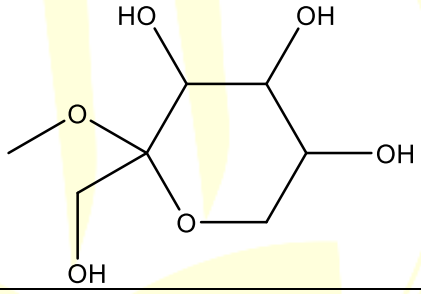
| No | Senyawa | Struktur 2D |
|---|---|---|

| | | |
|---|---|---|
| 17. | *Chimanine D* |  |
| 18. | *Desulphosinigrin* |  |
| 19. | *Ethyl 4-hydroxy-3-methylbut-2-enoate* |  |
| 20. | *Guanosine* |  |

**LAMPIRAN 11**
**(LANJUTAN)**

**Tabel VII.1**
Lanjutan

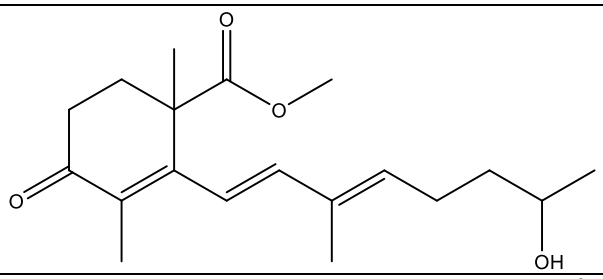
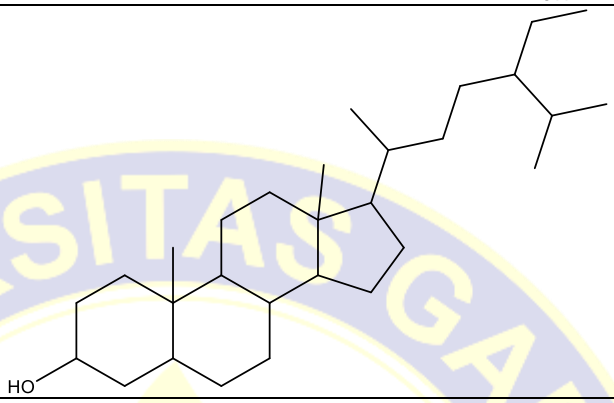
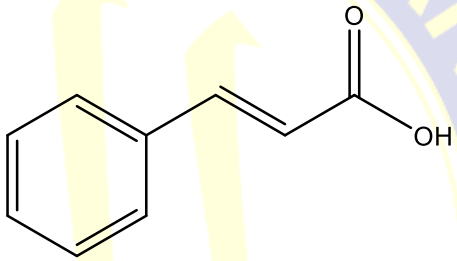
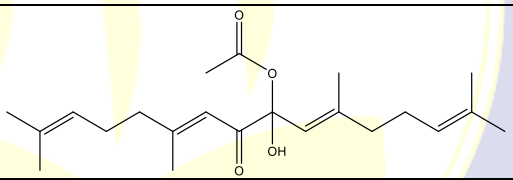
| No | Senyawa | Struktur 2D |
|---|---|---|

| | | |
|---|---|---|
| 21. | *Mannofuranoside, 1-allyl-2,3-5,6-tetra-O-acetyl* |  |
| 22. | *Methyl 3,6-anhydro-a-D-galactopyranoside* |  |
| 23. | *Methyl fructopyranoside* |  |

**LAMPIRAN 11**
**(LANJUTAN)**

**Tabel VII.1**
Lanjutan

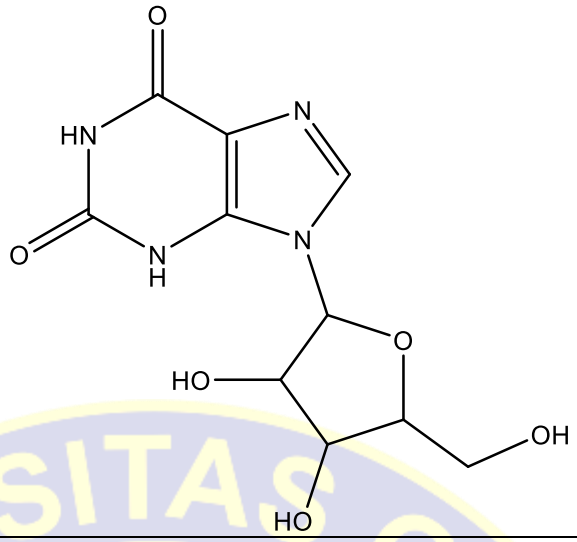
| No | Senyawa | Struktur 2D |
|---|---|---|

| | | |
|---|---|---|
| 24. | *Methyl trisporate C* |  |
| 25. | *Stigmastanol* |  |
| 26. | *Trans cinnamic acid* |  |
| 27. | *Trans geranylgeraniol* |  |

**LAMPIRAN 11**
**(LANJUTAN)**

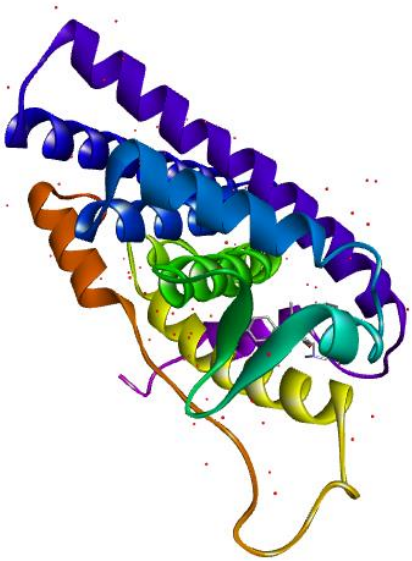
**Tabel VII.1**
Lanjutan

| No | Senyawa | Struktur 2D |
|---|---|---|

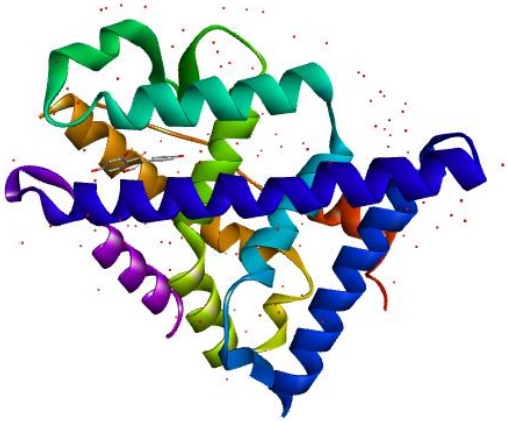
| | | |
|---|---|---|
| 28. | *Xanthosine* |  |

**LAMPIRAN 12**

**RESEPTOR Erα dan Erβ**



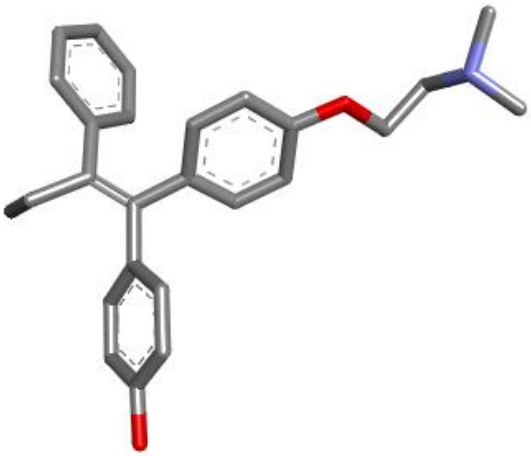
**Gambar VII. 12** Struktur 3D reseptor Erα (3ERT)



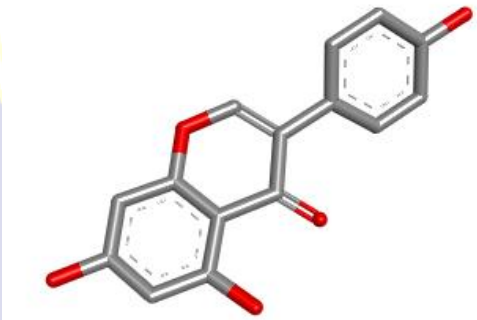
**Gambar VII. 13** Struktur 3D reseptor Erβ (1QKM)

**LAMPIRAN 13**

**LIGAN ALAMI**



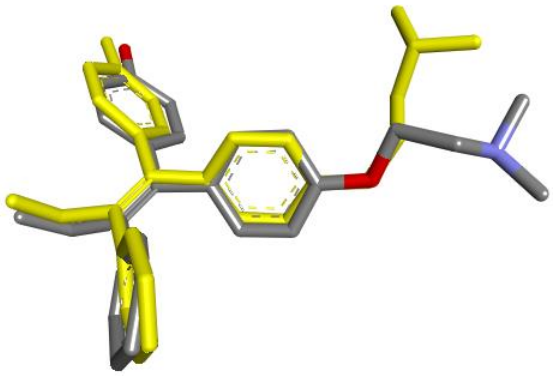
**Gambar VII. 14** Struktur (*4-hydroxytamoxifen*) dari reseptor Erα



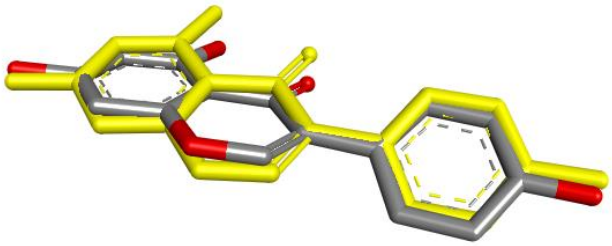
**Gambar VII. 15** Struktur (*Genistein*) dari reseptor Erβ

# LAMPIRAN 14

## HASIL VALIDASI



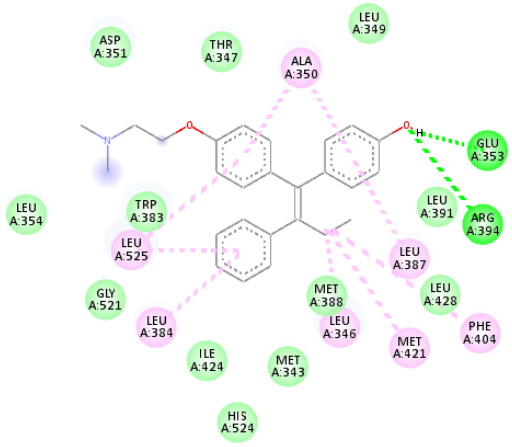
**Gambar VII. 16** Visualisasi tumpang tindih ligan alami dengan ligan hasil *redocking* dari reseptor estrogen alfa (Erα)



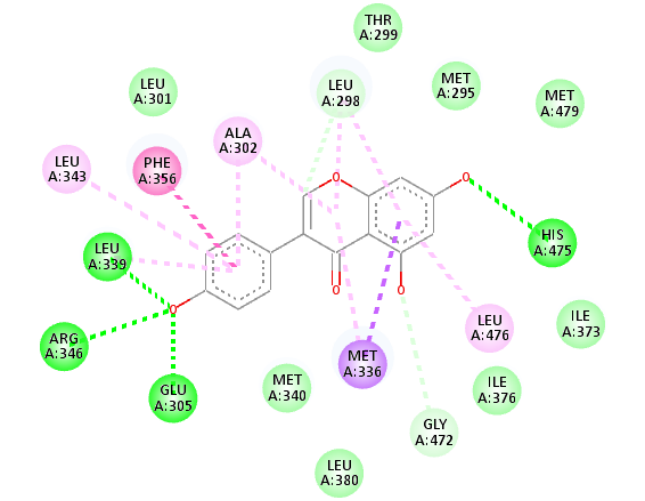
**Gambar VII. 17** Visualisasi tumpang tindih ligan alami dengan ligan hasil *redocking* dari reseptor estrogen beta (Erβ)

**LAMPIRAN 14**

**(LANJUTAN)**




**Gambar VII. 18** Visualisasi interaksi residu asam amino ligan alami dengan reseptor estrogen alfa (Erα)




**Gambar VII. 19** Visualisasi interaksi residu asam amino ligan alami dengan reseptor estrogen beta (Erβ)

**LAMPIRAN 14**
**(LANJUTAN)**

**Tabel VII. 2**
Hasil Validasi ERα dan ERβ

| Reseptor | Grid Box | | RMSD | ΔG (Energi Bebas) | Konstanta Inhibisi (KI) |
|---|---|---|---|---|---|
| | Center | Size | | | |
| *Estrogen Reseptor Alpha* (ERα) kode 3ERT | X: 30.282<br>Y: -1.913<br>Z: 24.207 | X: 28<br>Y: 22<br>Z: 26 | 1.125 Å | -11.41 | 4.36 |
| *Estrogen Reseptor Alpha* (Erβ) kode 1QKM | X: 22.438<br>Y: 8.003<br>Z:113.539 | X: 30<br>Y: 22<br>Z: 30 | 0.452 Å | -12.11 | 1.33 |

## LAMPIRAN 15

## HASIL *MOLECULAR DOCKING*

**Tabel VII. 3**
Hasil *Docking* Senyawa Aktif dari Belimbing Wuluh (*Averrhoa bilimbi* L.) terhadap Reseptor Estrogen Alfa (ERα) Kode 3ERT

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan | |
|---|---|---|---|---|---|
| | | | | Hidrofobik | Hidrogen |
| 1. | *(s)-dehydrovomifoliol* | -6.82 | 9.95 | - | ARG394 |
| 2 | *1-Heneicosyl formate* | -5.57 | 82.27 | TRP383, ALA350, LEU525, LEU346, LEU349, MET421, MET388, ILE424, LEU391, LEU387 | - |
| 3 | *2,3,4-Trihydroxy-6-methylcyclohexanone* | -5.64 | 73.55 | - | LEU346, GLU353, ARG394 |
| 4 | *2-[5-(2-Hydroxy-propyl)-tetrahydrofuran-2-yl]-propionic acid, t-butyl ester* | -6.65 | 13.30 | MET343, LEU525 | ARG494, GLU353 |
| 5 | *2-Furancarboxylic acid, tert-butyldimethylsilyl ester* | -8.22 | 936.69 | MET343, LEU346, ALA350, MET421, LEU525 | HIS524 |
| 6 | *2-Methylacetophenone* | -5.01 | 212.97 | MET388, LEU387, LEU391 | ARG394 |
| 7 | *2-n-Propylthiane* | -4.77 | 320.30 | MET388, LEU428, ALA350, LEU346, LEU349, LEU391, LEU387 | - |

## LAMPIRAN 15
## (LANJUTAN)

**Tabel VII.3**

Lanjutan

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan | |
|---|---|---|---|---|---|
| | | | | Hidrofobik | Hidrogen |
| 8 | *2-Octenoic acid, 4,5,7-trhydroxy* | -4.10 | 994.92 | - | GLU353, ARG394 |
| 9 | *3-(hydroxymethyl)-9-Oxabicyclo [3.3.1] nonan-3-ol* | -5.59 | 79.69 | ALA350, LEU346, LEU387 | GLU353 |
| 10 | *4-fluorophenol* | -4.39 | 609.46 | LEU387, LEU391 | GLU353 |
| 11 | *4-hydroxycinnamic acid* | -4.44 | 556.82 | ALA350, LEU387, LEU346, LEU349 | GLU353, THR347 |
| 12 | *4-Hydroxylamino-6-methylpyrimidin-2(1H)-one* | -4.67 | 375.72 | LEU387, MET388, ALA350, LEU391, LEU384 | LEU346, GLU353, ARG394 |
| 13 | *4-Methoxymethoxy-4-methyl-hex-2-ynal* | -3.73 | 1.85 | GLU353, LEU346, LEU349, ALA350, | ARG394 |
| 14 | *5-(hydroxymethyl)-2-(dimethoxymethyl) Furan* | -4.18 | 869.03 | LEU349, LEU387, LEU346, ALA350 | ARG394, GLU353 |
| 15 | *5-Hydroxymethylfurfural* | -3.59 | 2.35 | LEU387, ALA350, LEU391, LEU346 | GLU353 |
| 16 | *Acetic acid, 2-methylhex-3-yl ester* | -4.31 | 690.31 | MET388, LEU384, LEU391, LEU387, LEU346, ALA345 | ARG349 |

**LAMPIRAN 15**
**(LANJUTAN)**

**Tabel VII.3**
Lanjutan

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan |
|---|---|---|---|---|

| | | | | Hidrofobik | Hidrogen |
|---|---|---|---|---|---|
| 17 | *Chimanine D* | -5.71 | 65.51 | LEU391, MET388, ILE424, MET421, LEU387 | - |
| 18 | *Desulphosinigrin* | -5.33 | 124.93 | LEU346, LEU387, ALA350 | ARG394, THR347, GLU353 |
| 19 | *Ethyl 4-hydroxy-3-methylbut-2-enoate* | -4.36 | 638.48 | ALA350, LEU346 | GLU353 |
| 20 | *Guanosine* | -7.05 | 6.79 | ALA350, LEU387, LEU384, MET388 | GLU353, LEU346, MET343, THR347 |
| 21 | *Mannofuranoside, 1-allyl-2,3-5,6-tetra-O-acetyl* | -6.12 | 32.67 | GLY521, ALA350, LEU346, LEU349 | - |
| 22 | *Methyl 3,6-anhydro-a-D-galactopyranoside* | -4.94 | 239.87 | LEU346 | GLU535, ARG394, LEU346 |
| 23 | *Methyl fructopyranoside* | -4.51 | 495.35 | GLU353 | ARG394, LEU346, GLU353 |
| 24 | *Methyl trisporate C* | -8.27 | 864.71 | GLU353, TRP383, ALA350, LEU346 | ARG394, ASP351 |
| 25 | *Stigmastanol* | -10.58 | 17.67 | LEU391, LEU346, LEU387, LEU384, ALA350, LEU525 | - |
| 26 | *Trans cinnamic acid* | -4.21 | 817.08 | MET388, MET421, LEU391 | GLU353, ARG394 |

**LAMPIRAN 15**
**(LANJUTAN)**

**Tabel VII.3**
Lanjutan

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan | |
|---|---|---|---|---|---|
| | | | | Hidrofobik | Hidrogen |
| 27 | *Trans geranylgeraniol* | -7.59 | 2.72 | LEU387, LEU346, | ARG394, GLU353 |

| | | | | | |
|---|---|---|---|---|---|
| | | | | LEU354, TRP383, ALA350, LEU525, LEU384 | |
| 28 | *Xanthosine* | -6.17 | 29.94 | LEU391, ALA350, MET388 | GLU353, PHE404, LEU346 |

# LAMPIRAN 16

## HASIL *MOLECULAR DOCKING*

**Tabel VII. 4**
Hasil *Docking* Senyawa Aktif dari Belimbing Wuluh (*Averrhoa bilimbi* L.) terhadap Reseptor Estrogen Beta (ERβ) Kode 1QKM

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan | |
|---|---|---|---|---|---|
| | | | | Hidrofobik | Hidrogen |
| 1. | *(s)-dehydrovomifoliol* | -7.37 | 3.96 | ALA302, PHE356, LEU339, LEU301 | LEU298, MET340 |
| 2 | *1-Heneicosyl formate* | -7.47 | 3.33 | LEU343, MET340, PHE356 | - |
| 3 | *2,3,4-Trihydroxy-6-methylcyclohexanone* | -5.91 | 46.26 | - | LEU298, GLU305, ARG346 |
| 4 | *2-[5-(2-Hydroxy-propyl)-tetrahydrofuran-2-yl]-propionic acid, t-butyl ester* | -7.88 | 1.68 | LEU476, LEU298, PHE356, LEU343, ALA302, MET336, MET340, LEU339 | HIS475, GLY472 |
| 5 | *2-Furancarboxylic acid, tert-butyldimethylsilyl ester* | -9.73 | 73.83 | MET336, HIS475, ALA302, LEU339, LEU476, MET340, LEU298 | - |
| 6 | *2-Methylacetophenone* | -5.57 | 81.95 | LEU298, LEU476 | HIS475 |

**(LAMPIRAN) 16**
**(LANJUTAN)**

**Tabel VII.4**
Lanjutan

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan | |
|---|---|---|---|---|---|
| | | | | Hidrofobik | Hidrogen |
| 7 | *2-n-Propylthiane* | -5.32 | 126.27 | LEU343, LEU339, MET340, PHE356, LEU301, LEU298, ALA302 | - |
| 8 | *2-Octenoic acid, 4,5,7-trhydroxy* | -4.07 | 1.04 | - | ALA302, LEU298, GLU305, ARG346 |
| 9 | *3-(hydroxymethyl)-9-Oxabicyclo [3.3.1] nonan-3-ol* | -6.08 | 34.75 | LEU298, PHE356, MET336, ALA302 | GLU305, ARG346 |
| 10 | *4-fluorophenol* | -4.60 | 427.80 | PHE356, MET340, LEU343, LEU339 | GLU305, ARG346 |
| 11. | *4-hydroxycinnamic acid* | -5.30 | 130.96 | LEU476, ALA302, LEU298 | LEU298, HIS475, GLY472 |
| 12. | *4-Hydroxylamino-6-methylpyrimidin-2(1H)-one* | -4.96 | 232.27 | MET336, LEU339, LEU343, MET340 | GLU305, PHE356 |
| 13. | *4-Methoxymethoxy-4-methyl-hex-2-ynal* | -4.51 | 495.87 | LEU380, MET340, PHE356, MET336, ILE376, PHE377 | HIS475 |
| 14. | *5-(hydroxymethyl)-2-(dimethoxymethyl) Furan* | -4.72 | 344.79 | PHE356, LEU339, LEU301, ALA302 | ARG346, GLU305 |

**LAMPIRAN) 16**
**(LANJUTAN)**

**Tabel VII.4**

Lanjutan

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan | |
|---|---|---|---|---|---|
| | | | | Hidrofobik | Hidrogen |
| 15. | *5-Hydroxymethylfurfural* | -3.93 | 1.32 | MET340, MET336, PHE356, LEU343 | GLU305, ARG346 |
| 16. | *Acetic acid, 2-methylhex-3-yl ester* | -5.00 | 217.72 | VAL487, PHE356, ILE376, MET336, LEU380, LEU298, MET340, LEU476, ALA302 | HIS475 |
| 17. | *Chimanine D* | -6.84 | 9.69 | PHE356, LEU343, ALA302, LEU298, VAL487, LEU476, LEU339, TRP335, MET336 | - |
| 18. | *Desulphosinigrin* | -5.81 | 55.10 | MET336, | MET336, LEU298, GLU305 |
| 19. | *Ethyl 4-hydroxy-3-methylbut-2-enoate* | -4.69 | 366.94 | LEU339 | ARG346, GLU305 |
| 20. | *Guanosine* | -7.59 | 2.74 | ALA302, MET336, PHE356, MET340, LEU339 | GLY472, HIS475, LEU298, GLU305 |

**LAMPIRAN) 16**
**(LANJUTAN)**

**Tabel VII.4**
Lanjutan

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan |
|---|---|---|---|---|

| | | | | Hidrofobik | Hidrogen |
|---|---|---|---|---|---|
| 21. | *Mannofuranoside, 1-allyl-2,3-5,6-tetra-O-acetyl* | -8.30 | 821.82 | LEU298, LEU343, MET340, LEU339, PHE356 | HIS475 |
| 22. | *Methyl 3,6-anhydro-a-D-galactopyranoside* | -5.21 | 150.72 | - | LEU298, ARG346, GLU305 |
| 23. | *Methyl fructopyranoside* | -3.72 | 1.87 | - | LEU298, MET336, GLU305 |
| 24. | *Methyl trisporate C* | -11.03 | 8.28 | ILE376, MET340, MET336, LEU339, TRP335, ALA302 | HIS475, ARG346, GLU305 |
| 25. | *Stigmastanol* | -10.80 | 12.21 | HIS475, MET295, LEU476, LEU298, ILE376, MET340, LEU343, PHE356, LEU301, LEU339 | GLU305, ARG346 |
| 26. | *Trans cinnamic acid* | -5.08 | 190.15 | LEU476, LEU298, MET336, ALA302 | GLY472, HIS475 |

**LAMPIRAN) 16**
**(LANJUTAN)**

**Tabel VII.4**
Lanjutan

| No. | Senyawa | ΔG (kkal/mol) | KI (nM) | Residu asam amino yang beriakatan | |
|---|---|---|---|---|---|
| | | | | Hidrofobik | Hidrogen |

| | | | | | |
|---|---|---|---|---|---|
| 27. | *Trans geranylgeraniol* | -9.36 | 138.64 | GLU305 LEU476, ALA302, ILE376, MET336, PHE356, MET340, LEU339, LEU343 | LEU298 |
| 28. | *Xanthosine* | -12.11 | 1.33 | LEU298, ALA302, MET340, MET336, PHE356, LEU339 | HIS475, LEU298, ALA302, GLU305 |

**LAMPIRAN 17**

**HASIL PENGUJIAN PREADMET**

**Tabel VII. 5**
Hasil Pengujian Pre-ADMET

| No. | Senyawa | Absorpsi | | Distribusi |
|---|---|---|---|---|
| | | **$Caco_2$ ($nm.Sec^{-1}$)** | **HIA (%)** | **PPB (%)** |
| 1 | *(s)-dehydrovomifoliol,* | 23.2095 | 94.391464 | 87.450942 |
| 2 | *1-Heneicosyl formate* | 29.4161 | 100 | 100 |
| 3 | *2,3,4-Trihydroxy-6-methylcyclohexanone* | 14.5638 | 62.269322 | 59.145813 |
| 4 | *2-[5-(2-Hydroxy-propyl)-tetrahydrofuran-2-yl]-propionic acid, t-butyl ester* | 56.6429 | 93.1465720 | 84.162398 |
| 5 | *2-Furancarboxylic acid, tert-butyldimethylsilyl ester* | 45.6568 | 100 | 100 |
| 6 | *2-Methylacetophenone* | 46.068 | 100 | 12.147080 |
| 7 | *2-n-Propylthiane* | 24.6256 | 100 | 100 |
| 8 | *2-Octenoic acid, 4,5,7-trhydroxy* | 18.8975 | 44.245409 | 19.280506 |
| 9 | *3-(hydroxymethyl)-9-Oxabicyclo [3.3.1] nonan-3-ol* | 10.723 | 85.386008 | 21.849481 |
| 10 | *4-fluorophenol* | 23.3068 | 100 | 90.993698 |
| 11 | *4-hydroxycinnamic acid* | 21.1093 | 92.095876 | 63.055072 |
| 12 | *4-Hydroxylamino-6-methylpyrimidin-2(1H)-one* | 19.7799 | 67.888890 | 11.073953 |
| 13 | *4-Methoxymethoxy-4-methyl-hex-2-ynal* | 4.38965 | 97.797528 | 29.076706 |
| 14 | *5-(hydroxymethyl)-2-(dimethoxymethyl) Furan* | 36.8875 | 90.081475 | 78.387735 |
| 15 | *5-Hydroxymethylfurfural* | 6.41666 | 88.682048 | 49.465993 |
| 16 | *Acetic acid, 2-methylhex-3-yl ester* | 54.0067 | 100 | 100 |
| 17 | *Chimanine D* | 57.6147 | 100 | 85.761905 |
| 18 | *Desulphosinigrin* | 0.375984 | 31.323035 | 23.626939 |
| 19 | *Ethyl 4-hydroxy-3-methylbut-2-enoate* | 19.4914 | 89.780046 | 91.378979 |
| 20 | *Guanosine* | 9.42339 | 25.895030 | 8.044443 |
| 21 | *Mannofuranoside, 1-allyl-2,3-5,6-tetra-O-acetyl* | 13.1418 | 77.310454 | 45.726354 |

**LAMPIRAN 17**
**LANJUTAN**

**VII.5**
Lanjutan

| No. | Senyawa | Absorpsi | | Distribusi |
|---|---|---|---|---|
| | | **$Caco_2$ ($nm.Sec^{-1}$)** | **HIA (%)** | **PPB (%)** |
| 22 | *Methyl 3,6-anhydro-a-D-galactopyranoside* | 6.60318 | 72.712474 | 33.421886 |
| 23 | *Methyl fructopyranoside* | 3.45388 | 35.574635 | 5.522551 |
| 24 | *Methyl trisporate C* | 22.8813 | 96.003816 | 85.929266 |
| 25 | *Stigmastanol* | 52.4418 | 100 | 100 |
| 26 | *Trans cinnamic acid* | 21.0342 | 97.845200 | 60.852531 |
| 27 | *Trans geranylgeraniol* | 33.7556 | 96.037673 | 99.005260 |
| 28 | *Xanthosine* | 13.6448 | 24.716318 | 12.768312 |

***Keterangan:*** *in vitro CaCo-2 cell permeability (nm. $Sec^{-1}$): >70 higher permeability, 4-70 medium permeability, <4 low permeability; % human intestinal absorption (%HIA): 700-100% well absorbed, 20-70% moderately absorbed, 0-20% poorly absorbed; %plasma protein binding: >90% strongly bound, <90% weakly bound.*

## LAMPIRAN 18

## HASIL PENGUJIAN TOKSISITAS

**Tabel VII. 6**
Hasil Pengujian Toksisitas

| No | Senyawa | Crame rules | Kores TCC | Benigne/bosarulebase |
|---|---|---|---|---|
| 1 | *(s)-dehydrovomifoliol* | 3 | 2 | 1,9 |
| 2 | *1-Heneicosyl formate* | 1 | 1 | 8,9 |
| 3 | *2,3,4-Trihydroxy-6-methylcyclohexanone* | 2 | 1 | 8,9 |
| 4 | *2-[5-(2-Hydroxy-propyl)-tetrahydrofuran-2-yl]-propionic acid, t-butyl ester* | 3 | 1 | 8,9 |
| 5 | *2-Furancarboxylic acid, tert-butyldimethylsilyl ester* | 3 | 2 | 1,9 |
| 6 | *2-Methylacetophenone* | 1 | 1 | 8,9 |
| 7 | *2-n-Propylthiane* | 3 | 1 | 8,9 |
| 8 | *2-Octenoic acid, 4,5,7-trhydroxy* | 2 | 1 | 8,9 |
| 9 | *3-(hydroxymethyl)-9-Oxabicyclo [3.3.1] nonan-3-ol* | 3 | 1 | 8,9 |
| 10 | *4-fluorophenol* | 3 | 1 | 2,8 |
| 11 | *4-hydroxycinnamic acid* | 1 | 1 | 8,9 |
| 12 | *4-Hydroxylamino-6-methylpyrimidin-2(1H)-one* | 3 | 1 | 8,9 |
| 9 | *3-(hydroxymethyl)-9-Oxabicyclo [3.3.1] nonan-3-ol* | 3 | 1 | 8,9 |
| 10 | *4-fluorophenol* | 3 | 1 | 2,8 |
| 9 | *3-(hydroxymethyl)-9-Oxabicyclo [3.3.1] nonan-3-ol* | 3 | 1 | 8,9 |
| 10 | *4-fluorophenol* | 3 | 1 | 2,8 |
| 11 | *4-hydroxycinnamic acid* | 1 | 1 | 8,9 |
| 12 | *4-Hydroxylamino-6-methylpyrimidin-2(1H)-one* | 3 | 1 | 8,9 |
| 13 | *4-Methoxymethoxy-4-methyl-hex-2-ynal* | 3 | 2 | 1,9 |
| 14 | *5-(hydroxymethyl)-2-(dimethoxymethyl) Furan* | 3 | 1 | 8,9 |
| 15 | *5-Hydroxymethylfurfural* | 3 | 2 | 8,9 |

**LAMPIRAN 18**
**(LANJUTAN)**

**Tabel VII.6**
Lanjutan

| No | Senyawa | Crame rules | Kores TCC | Benigne/bosarulebase |
|---|---|---|---|---|
| 16 | *Acetic acid, 2-methylhex-3-yl ester* | 1 | 1 | 2,8 |
| 17 | *Chimanine D* | 3 | 2 | 1,9 |
| 18 | *Desulphosinigrin* | 3 | 1 | 8,9 |
| 19 | *Ethyl 4-hydroxy-3-methylbut-2-enoate* | 1 | 1 | 8,9 |
| 20 | *Guanosine* | 1 | 1 | 8,9 |
| 21 | *Mannofuranoside, 1-allyl-2,3-5,6-tetra-O-acetyl* | 3 | 1 | 8,9 |
| 22 | *Methyl 3,6-anhydro-a-D-galactopyranoside* | 3 | 1 | 8,9 |
| 23 | *Methyl fructopyranoside* | 3 | 1 | 8,9 |
| 24 | *Methyl trisporate C* | 2 | 2 | 1,9 |
| 25 | *Stigmastanol* | 3 | 1 | 8,9 |
| 26 | *Trans cinnamic acid* | 1 | 1 | 8,9 |
| 27 | *Trans geranylgeraniol* | 3 | 1 | 8,9 |
| 28 | *Xanthosine* | 1 | 1 | 8,9 |

***Keterangan:*** *Cramer ruler class 1: low, class 2 : intermediet, class 3 : high. Benigni/bosa rulebase 1 (structural alert for genotoxic carcinogenicity) 2 (Structural alert for nongenotoxic carcinogenicity), 8 (negative for genotoxic carcinogenity), 9 (negative for non-genotoxic carcinogencity). 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 ))*

## LAMPIRAN 19

## HASIL PENGUJIAN *LIPINSKI'S RULE OF FIVE*

**Tabel VII. 7**
Hasil Pengujian *Lipinski's Rule of Five*

| No | Senyawa | BM | LOG P | Ikatan hidrogen | | Keterangan |
|---|---|---|---|---|---|---|
| | | | | Donor | Akseptor | |
| 1 | *(s)-dehydrovomifoliol* | 222 | 2.7568 | 0 | 3 | Memenuhi syarat |
| 2 | *1-Heneicosyl formate* | 340 | 6.2857 | 0 | 2 | Tidak memenuhi syarat |
| 3 | *2,3,4-Trihydroxy-6-methylcyclohexanone* | 160 | 0.9428 | 3 | 4 | Memenuhi syarat |
| 4 | *2-[5-(2-Hydroxy-propyl)-tetrahydrofuran-2-yl]-propionic acid, t-butyl ester* | 258 | 3.4593 | 1 | 4 | Memenuhi syarat |
| 5 | *2-Furancarboxylic acid, tert-butyldimethylsilyl ester* | 248 | 1.9753 | 0 | 0 | Memenuhi syarat |
| 6 | *2-Methylacetophenone* | 134 | 1.8768 | 0 | 1 | Memenuhi syarat |
| 7 | *2-n-Propylthiane* | 144 | 2.4584 | 0 | 0 | Memenuhi syarat |
| 8 | *2-Octenoic acid, 4,5,7-trhydroxy* | 190 | 0.4847 | 3 | 5 | Memenuhi syarat |
| 9 | *3-(hydroxymethyl)-9-Oxabicyclo [3.3.1] nonan-3-ol* | 172 | 1.3590 | 2 | 3 | Memenuhi syarat |
| 10 | *4-fluorophenol* | 112 | 0.9431 | 1 | 1 | Memenuhi syarat |
| 11 | *4-hydroxycinnamic acid* | 164 | 0.1526 | 2 | 3 | Memenuhi syarat |
| 12 | *4-Hydroxylamino-6-methylpyrimidin-2(1H)-one* | 141 | -1.9379 | 3 | 2 | Memenuhi syarat |
| 13 | *4-Methoxymethoxy-4-methyl-hex-2-ynal* | 170 | 2.2282 | 0 | 3 | Memenuhi syarat |
| 14 | *5-(hydroxymethyl)-2-(dimethoxymethyl) Furan* | 172 | 1.3966 | 1 | 4 | Memenuhi syarat |
| 15 | *5-Hydroxymethylfurfural* | 126 | 0.7557 | 1 | 3 | Memenuhi syarat |
| 16 | *Acetic acid, 2-methylhex-3-yl ester* | 158 | 2.5610 | 0 | 2 | Memenuhi syarat |
| 17 | *Chimanine D* | 185 | 1.8391 | 0 | 1 | Memenuhi syarat |
| 18 | *Desulphosinigrin* | 279 | 0.8094 | 5 | 6 | Memenuhi syarat |
| 19 | *Ethyl 4-hydroxy-3-methylbut-2-enoate* | 144 | 1.2456 | 1 | 3 | Memenuhi syarat |
| 20 | *Guanosine* | 283 | -1.5298 | 6 | 6 | Tidak memenuhi syarat |
| 21 | *Mannofuranoside, 1-allyl-2,3-5,6-tetra-O-acetyl* | 372 | 3.1490 | 0 | 9 | Memenuhi syarat |

## LAMPIRAN 19
## (LANJUTAN)

**Tabel VII.7**
Lanjutan

| No | Senyawa | BM | LOG P | Ikatan hidrogen | | Keterangan |
|---|---|---|---|---|---|---|
| | | | | Donor | Akseptor | |
| 22 | *Methyl 3,6-anhydro-a-D-galactopyranoside* | 176 | 0.3662 | 2 | 5 | Memenuhi syarat |
| 23 | *Methyl fructopyranoside* | 194 | 0.7597 | 4 | 6 | Memenuhi syarat |
| 24 | *Methyl trisporate C* | 320 | 4.1393 | 1 | 4 | Memenuhi syarat |
| 25 | *Stigmastanol* | 416 | 7.9601 | 1 | 1 | Tidak memenuhi syarat |
| 26 | *Trans cinnamic acid* | 148 | 0.7444 | 1 | 2 | Memenuhi syarat |
| 27 | *Trans geranylgeraniol* | 290 | 5.0780 | 1 | 1 | Memenuhi syarat |
| 28 | *Xanthosine* | 284 | -0.9848 | 5 | 6 | Memenuhi syarat |

**LAMPIRAN 20**

# HASIL VALIDASI *DOCKING* 3ERT PADA RESEPTOR ERα

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

MODEL        31
USER    Run = 31
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 99
USER
USER    RMSD from reference structure       = 1.125 A
USER
USER    Estimated Free Energy of Binding    =  -11.41 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    4.36 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -13.79 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -12.71 kcal/mol
USER        Electrostatic Energy            =   -1.08 kcal/mol
USER    (2) Final Total Internal Energy     =   -2.13 kcal/mol
USER    (3) Torsional Free Energy           =   +2.39 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -2.13 kcal/mol
USER
```

# LAMPIRAN 21

## HASIL *DOCKING* SENYAWA PEMBANDING TAMOKSIFEN TERHADAP RESEPTOR ERα

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

MODEL       59
USER    Run = 59
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 100
USER
USER    RMSD from reference structure       = 37.822 A
USER
USER    Estimated Free Energy of Binding    =  -10.51 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   19.67 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -12.90 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -11.78 kcal/mol
USER        Electrostatic Energy            =   -1.12 kcal/mol
USER    (2) Final Total Internal Energy     =   -2.28 kcal/mol
USER    (3) Torsional Free Energy           =   +2.39 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -2.28 kcal/mol
USER
```

# LAMPIRAN 22

## HASIL *DOCKING* SENYAWA UJI TRANS-GERANYLGERANIOL TERHADAP RESEPTOR ERα

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

MODEL       59
USER    Run = 59
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 32
USER
USER    RMSD from reference structure       = 34.888 A
USER
USER    Estimated Free Energy of Binding    =   -7.59 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    2.72 uM (micromolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -10.87 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -10.55 kcal/mol
USER        Electrostatic Energy            =   -0.33 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.97 kcal/mol
USER    (3) Torsional Free Energy           =   +3.28 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.97 kcal/mol
USER
```

# LAMPIRAN 23

## HASIL VALIDASI *DOCKING* 1QKM PADA RESEPTOR ERβ

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

MODEL       36
USER    Run = 36
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 100
USER
USER    RMSD from reference structure       = 0.452 A
USER
USER    Estimated Free Energy of Binding    =  -10.08 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =   40.90 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -10.38 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -10.34 kcal/mol
USER        Electrostatic Energy            =   -0.04 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.31 kcal/mol
USER    (3) Torsional Free Energy           =   +0.30 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.31 kcal/mol
USER
```

# LAMPIRAN 24

## HASIL *DOCKING* SENYAWA PEMBANDING GENISTEIN TERHADAP RESEPTOR ERβ

```
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 = 100
USER
USER    RMSD from reference structure       = 114.880 A
USER
USER    Estimated Free Energy of Binding    =   -9.44 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =  120.15 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -10.63 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -10.19 kcal/mol
USER        Electrostatic Energy            =   -0.45 kcal/mol
USER    (2) Final Total Internal Energy     =   -0.88 kcal/mol
USER    (3) Torsional Free Energy           =   +1.19 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -0.88 kcal/mol
USER
```

# LAMPIRAN 25

## HASIL *DOCKING* SENYAWA UJI METHYL TRISPORATE C TERHADAP RESEPTOR ERβ

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

MODEL       95
USER    Run = 95
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 76
USER
USER    RMSD from reference structure       = 115.279 A
USER
USER    Estimated Free Energy of Binding    =  -11.03 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    8.28 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -13.41 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -13.02 kcal/mol
USER        Electrostatic Energy            =   -0.39 kcal/mol
USER    (2) Final Total Internal Energy     =   -1.18 kcal/mol
USER    (3) Torsional Free Energy           =   +2.39 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -1.18 kcal/mol
USER
```

# LAMPIRAN 26

## HASIL *DOCKING* SENYAWA UJI XANTHOSINE TERHADAP RESEPTOR ERβ

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

MODEL       72
USER    Run = 72
USER    Cluster Rank = 1
USER    Number of conformations in this cluster = 13
USER
USER    RMSD from reference structure       = 114.169 A
USER
USER    Estimated Free Energy of Binding    =  -12.11 kcal/mol  [=(1)+(2)+(3)-(4)]
USER    Estimated Inhibition Constant, Ki   =    1.33 nM (nanomolar)  [Temperature = 298.15 K]
USER
USER    (1) Final Intermolecular Energy     =  -13.60 kcal/mol
USER        vdW + Hbond + desolv Energy     =  -13.60 kcal/mol
USER        Electrostatic Energy            =   +0.00 kcal/mol
USER    (2) Final Total Internal Energy     =   -2.11 kcal/mol
USER    (3) Torsional Free Energy           =   +1.49 kcal/mol
USER    (4) Unbound System's Energy  [=(2)] =   -2.11 kcal/mol
USER
```

# DAFTAR RIWAYAT HIDUP

## I. IDENTITAS DIRI

**Nama** : Abdussyukur

**Tempat, Tanggal Lahir** : Jakarta, 28 Juni 2000

**Jenis Kelamin** : Laki-Laki

**Agama** : Islam

**Kewarganegaraan** : Indonesia

**Status** : Mahasiswa

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## II. RIWAYAT HIDUP

| Jenjang Pendidikan | Nama Sekolah/Perguruan Tinggi | Tahun Masuk | Tahun Lulus |
|---|---|---|---|
| SD/MI | SDN 02 Kramat Jati | 2006 | 2012 |
| SMP/MTs | MTs Al-Ihsan | 2012 | 2015 |
| SMA/MA/SMK | MAN 6 Jakarta | 2015 | 2018 |
| Perguruan Tinggi | Universitas Garut | 2018 | 2022 |

## III. PENGALAMAN ORGANISASI

1. Member of External Departement BEM KEMA FMIPA UNIGA
2. Member of Media and Relation Division Association of Indonesia Mathematic and Science Student (ILMMIPA) (2020-2021 - Riau, Indonesia)

3. Leadership Skill in Priangan Pharmaceutical Leadership Forum (PPLF) Association of Indonesia Pharmacy Student (ISMAFARSI) Priangan (2021 - Tasikmalaya, West Java, Indonesia)