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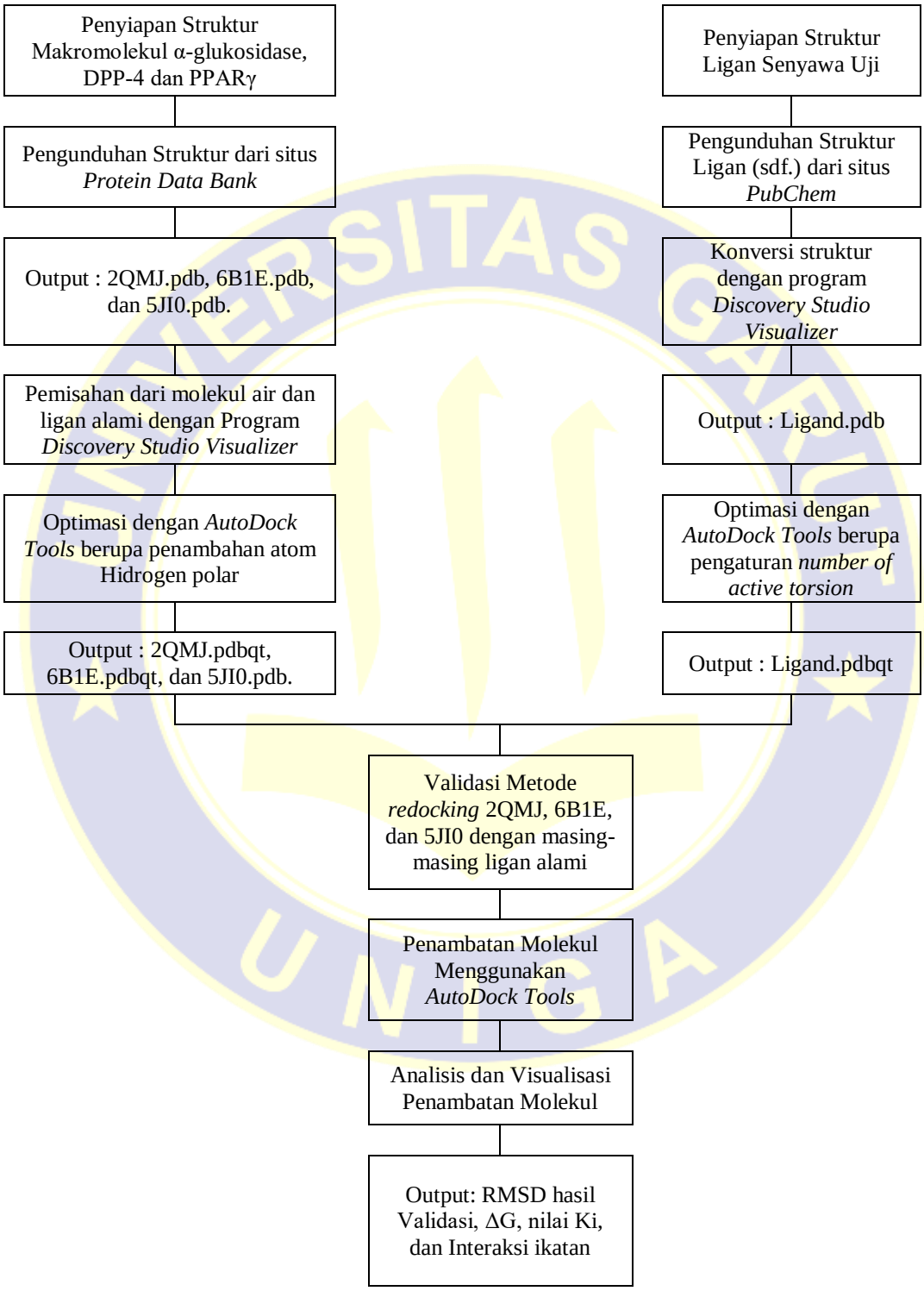
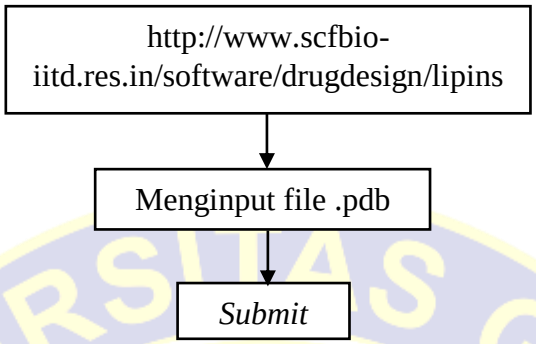
LAMPIRAN 1

ALUR PENELITIAN

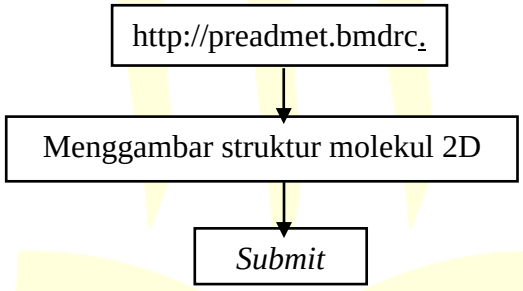


Gambar IV.1 Alur penelitian penambatan molekul

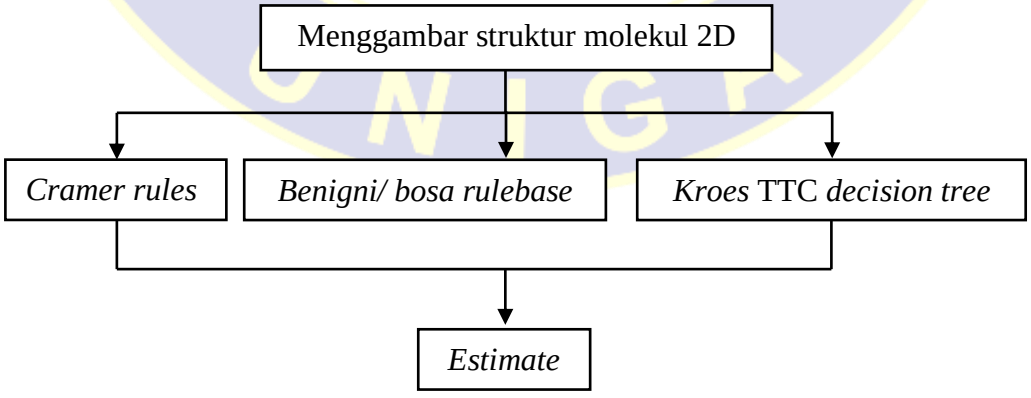
LAMPIRAN 1
(LANJUTAN)



Gambar IV.2 Analisis *Lipinski Rule of Five*



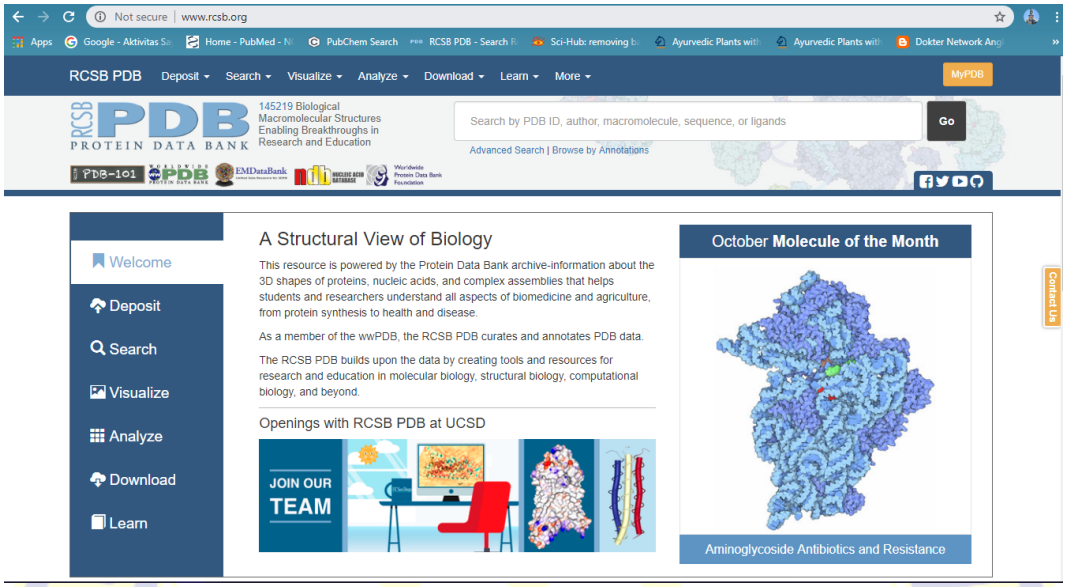
Gambar IV.3 Analisis Pre-ADME



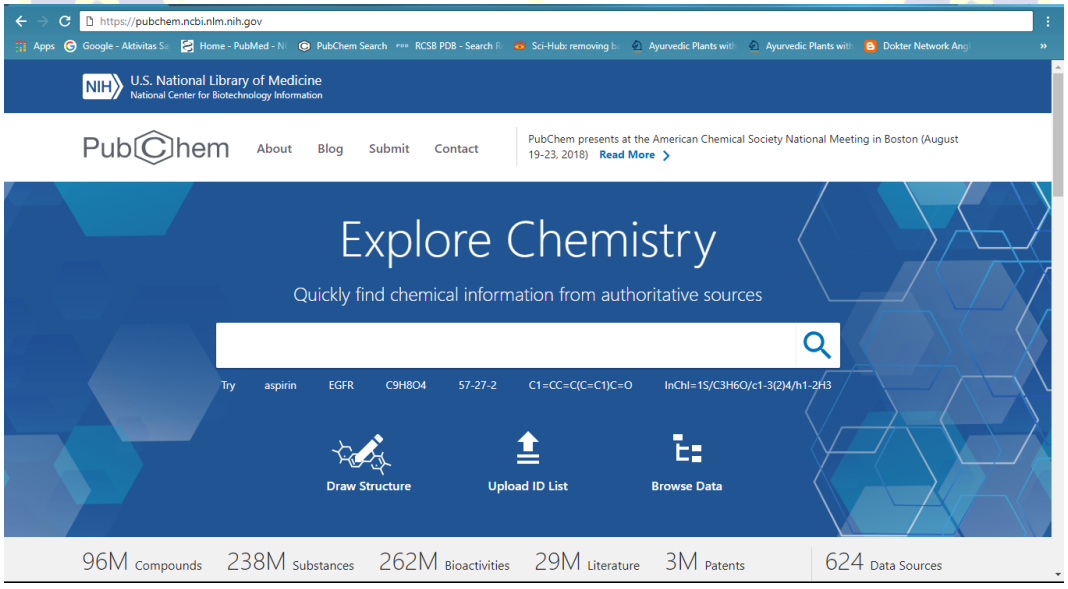
Gambar IV.4 Analisis Toksisitas

LAMPIRAN 2

SITUS

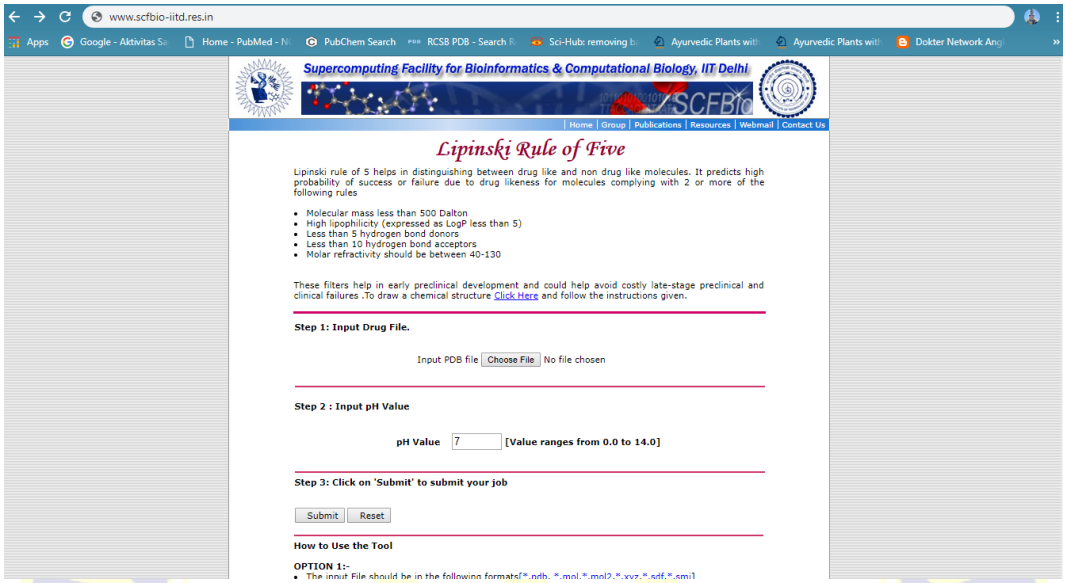


Gambar IV.5 Tampilan situs *Protein Data Bank*

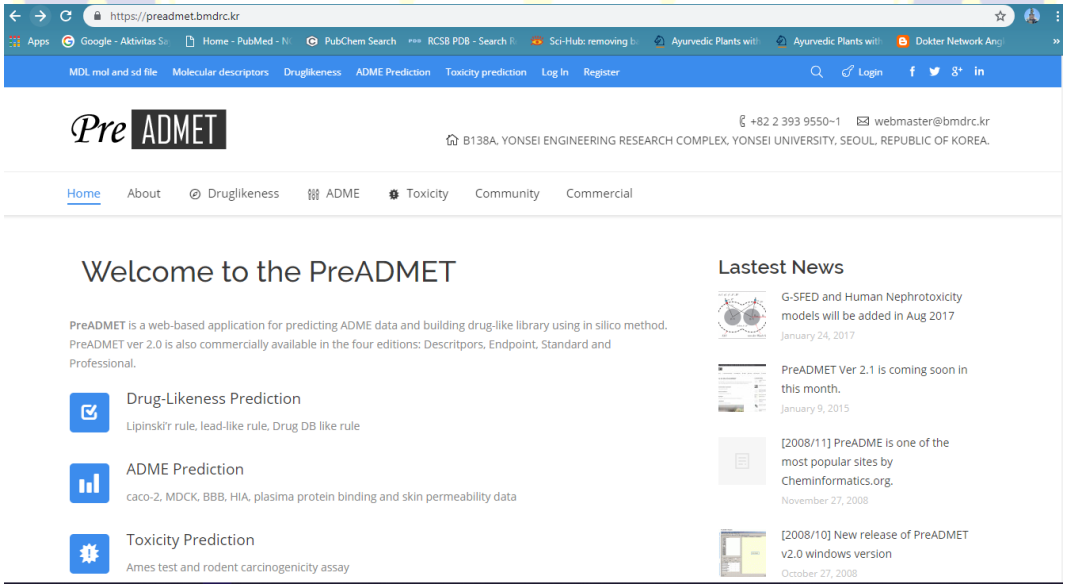


Gambar IV.6 Tampilan situs *Pubchem*

LAMPIRAN 2
(LANJUTAN)



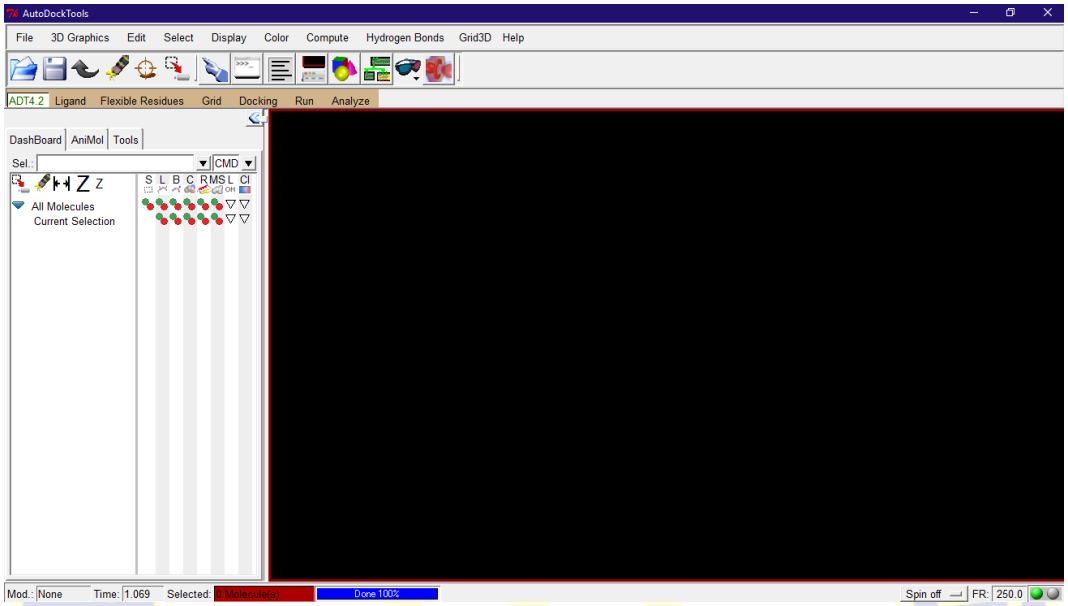
Gambar IV.7 Tampilan situs *Lipinski Rule of Five*



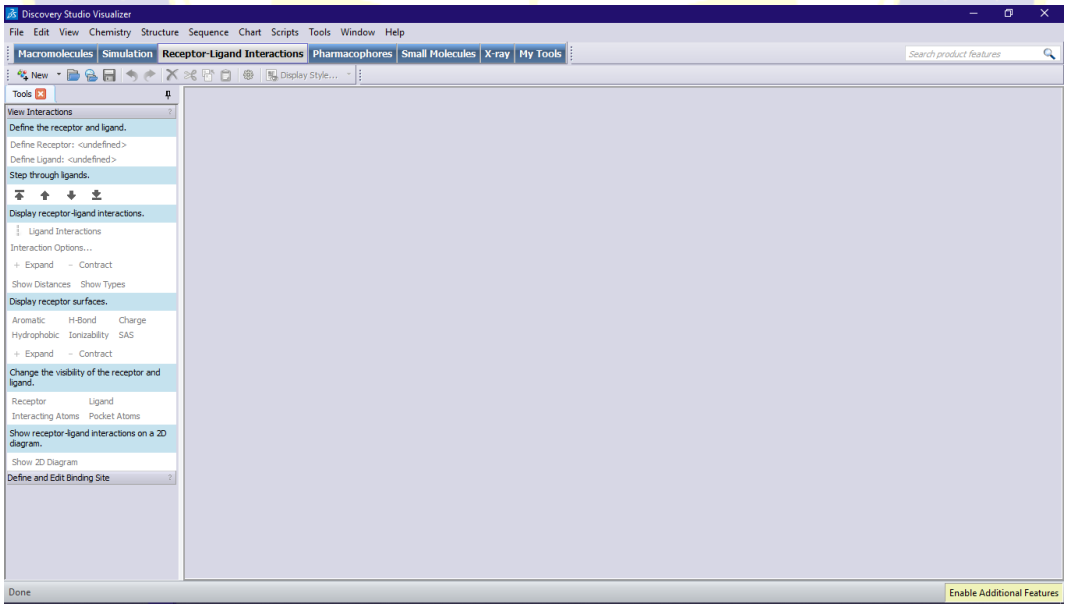
Gambar IV.8 Tampilan situs Pre-ADME

LAMPIRAN 3

SOFTWARE

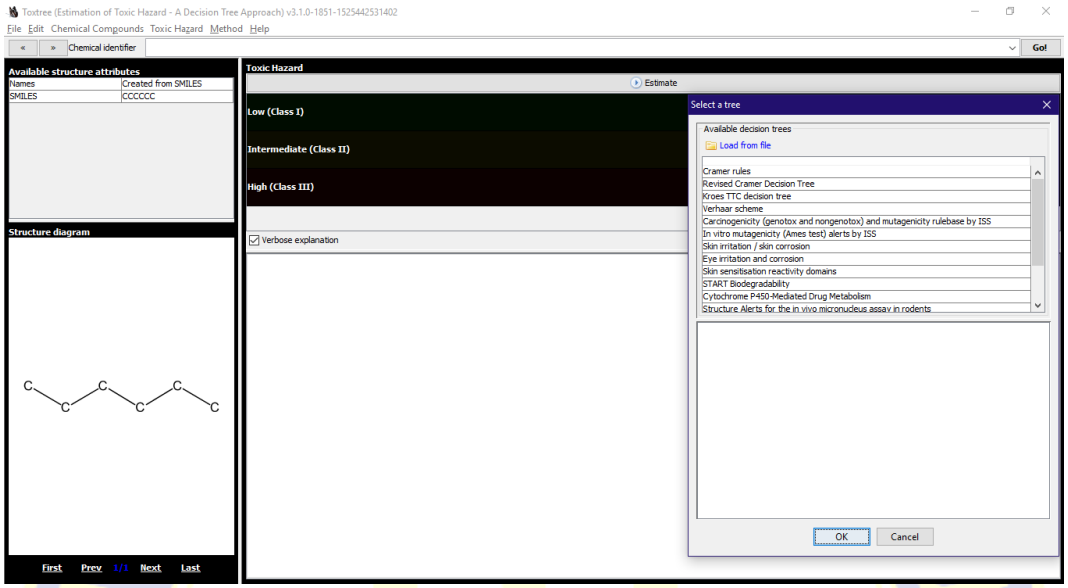


Gambar IV.9 Tampilan aplikasi *AutoDock Tools*®

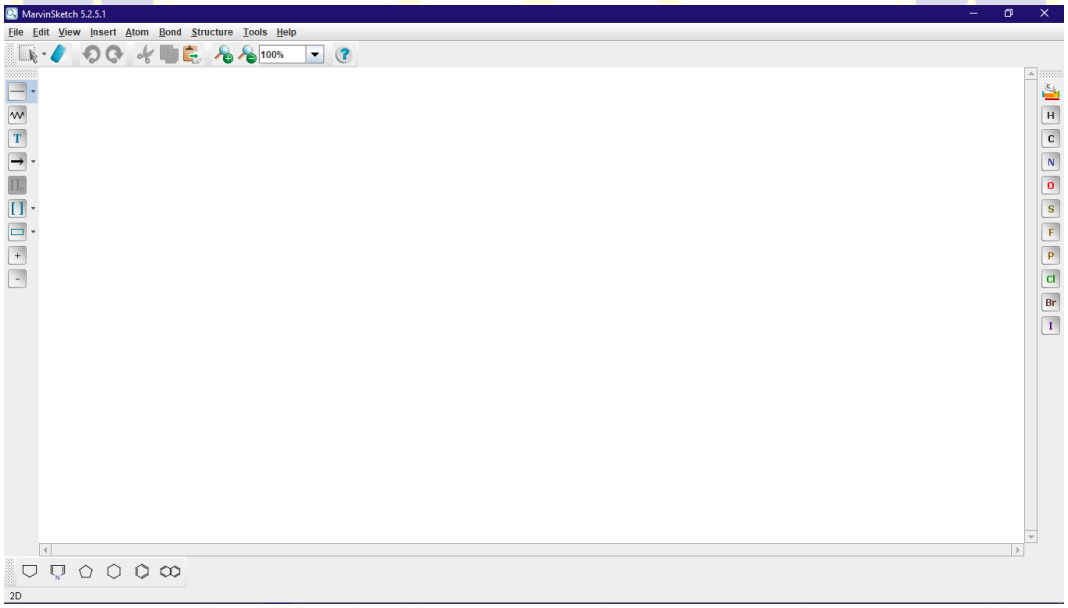


Gambar IV.10 Tampilan aplikasi *Discovery Studio Visualizer*®

LAMPIRAN 3
(LANJUTAN)



Gambar IV.11 Tampilan aplikasi *Toxtree*®

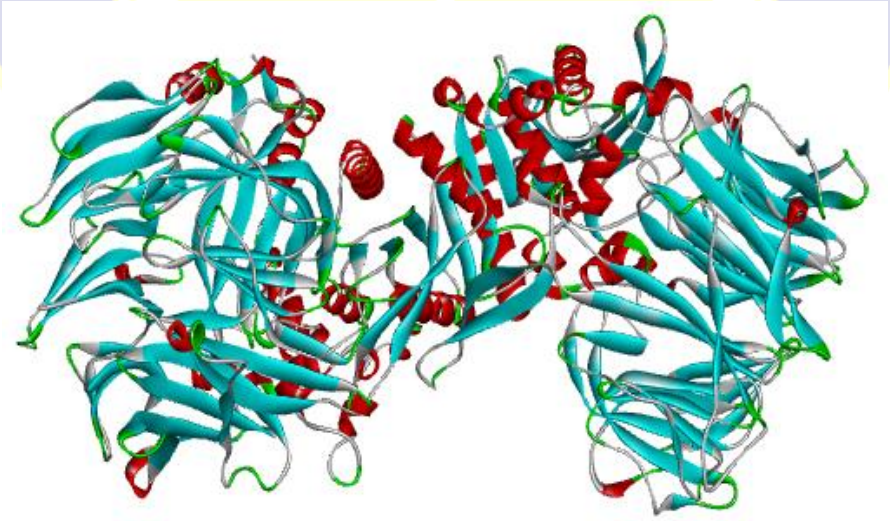


Gambar IV.12 Tampilan aplikasi *Marvin Sketch*®

LAMPIRAN 4

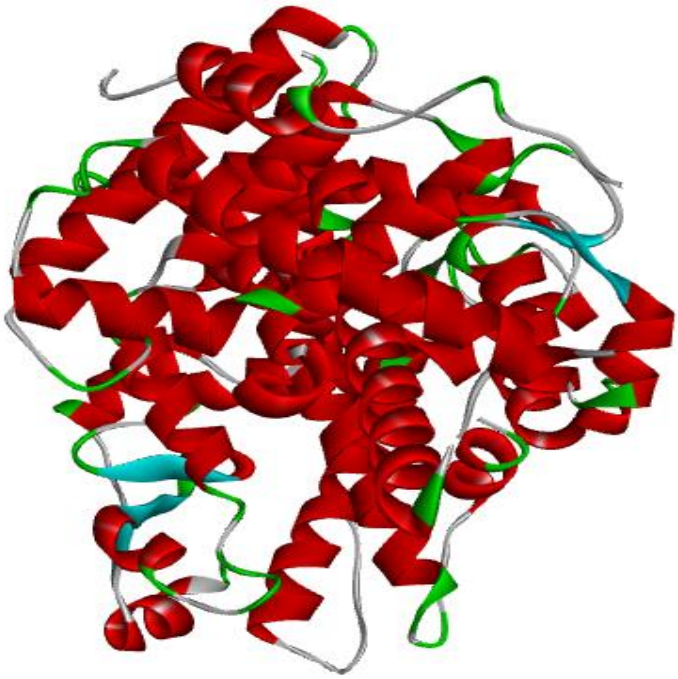
STRUKTUR 3D MAKROMOLEKUL PROTEIN

Gambar V.1 Reseptor α-Glukosidase dengan PDB ID 2QMJ



Gambar V.2 Reseptor DPP-4 dengan PDB ID 6B1E

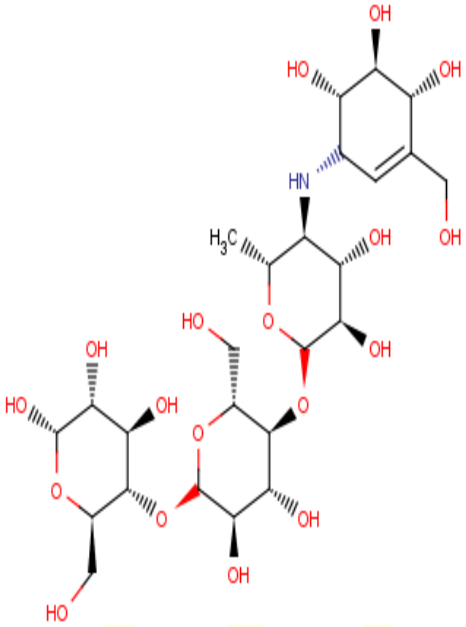
LAMPIRAN 4
(LANJUTAN)



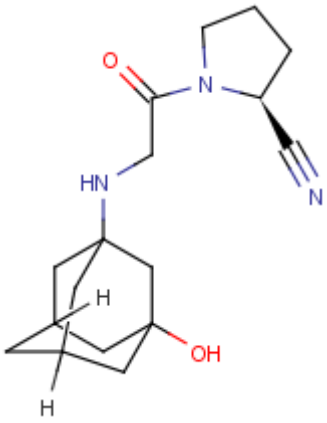
Gambar V.3 Reseptor PPARγ dengan PDB ID 5JI0

LAMPIRAN 5

STRUKTUR 2D LIGAN ALAMI

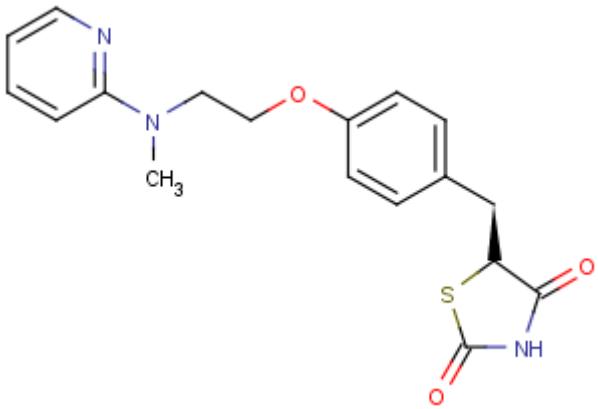


Gambar V.4 α-Glukosidase (Acarbose)



Gambar V.5 DPP-4 (Vildagliptin)

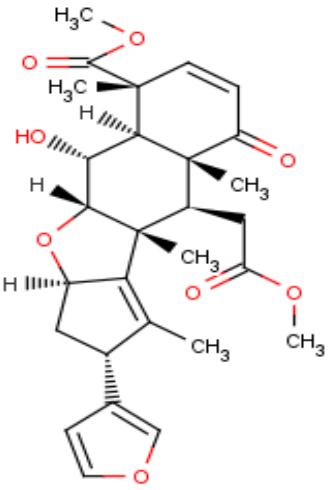
LAMPIRAN 5
(LANJUTAN)



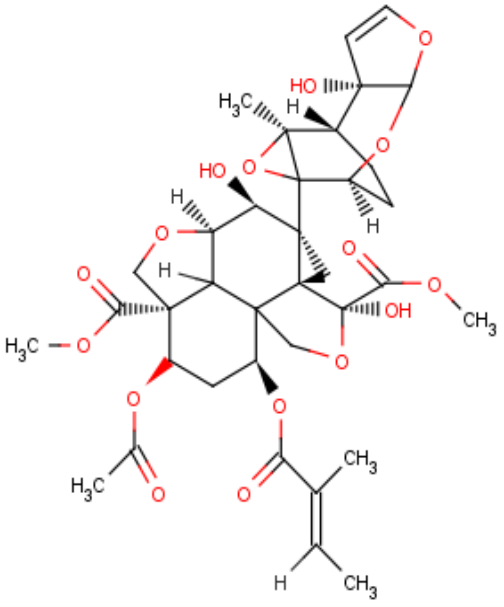
Gambar V.6 PPARγ (Rosiglitazone)

LAMPIRAN 6

STRUKTUR 2D SENYAWA UJI

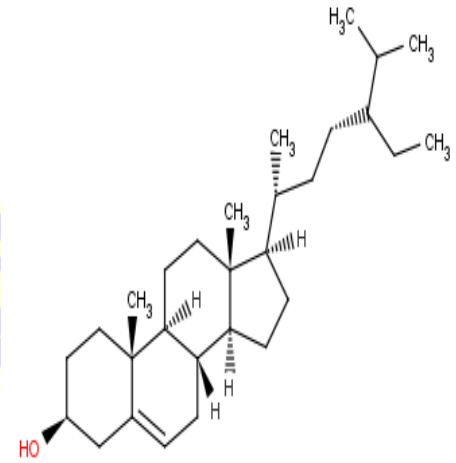


Gambar V.7 6-Deacetylnimbin

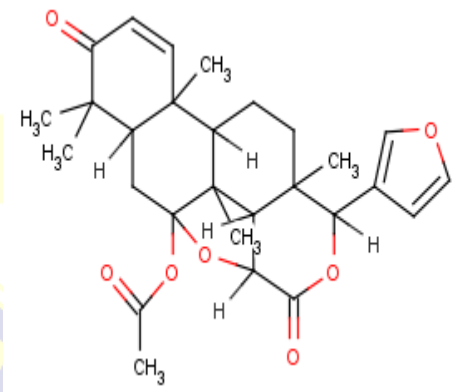


Gambar V.8 Azadirachtin

LAMPIRAN 6
(LANJUTAN)

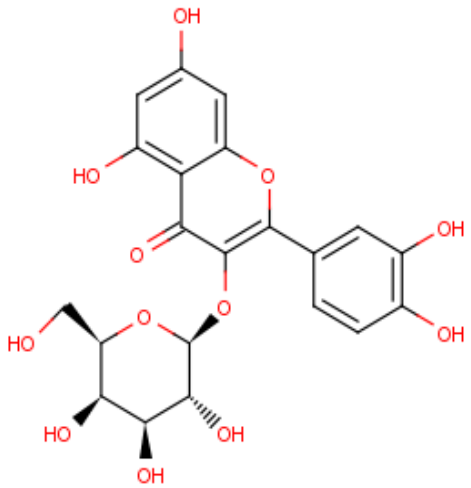


Gambar V.9 Beta Sitosterol

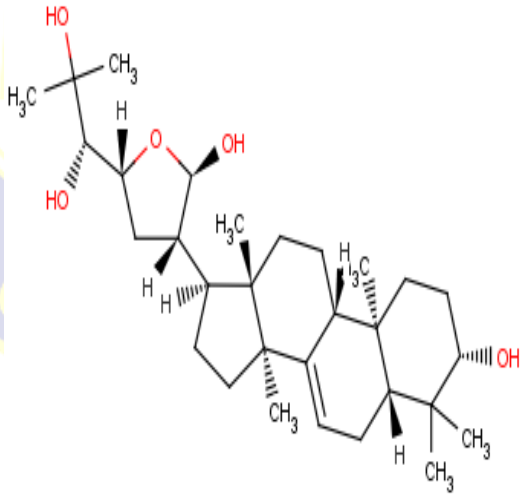


Gambar V.10 Gedunin

LAMPIRAN 6
(LANJUTAN)

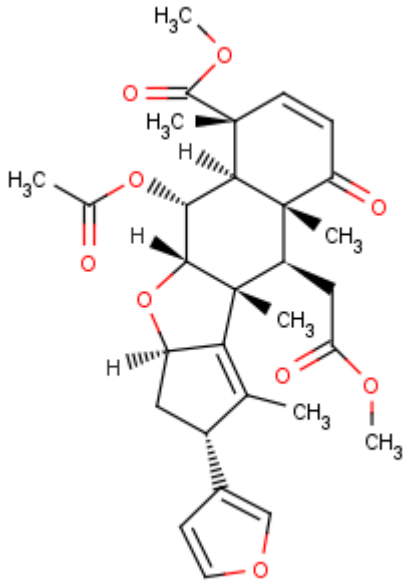


Gambar V.11 Hyperoside

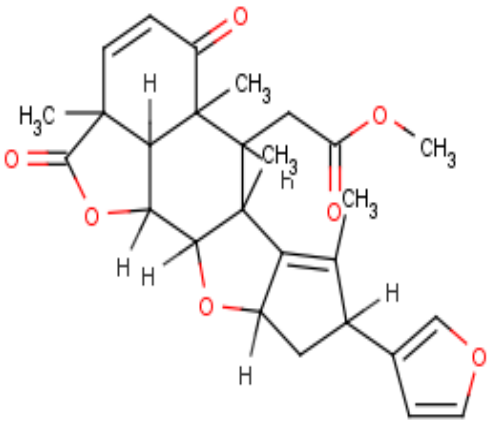


Gambar V.12 Meliantriol

LAMPIRAN 6
(LANJUTAN)

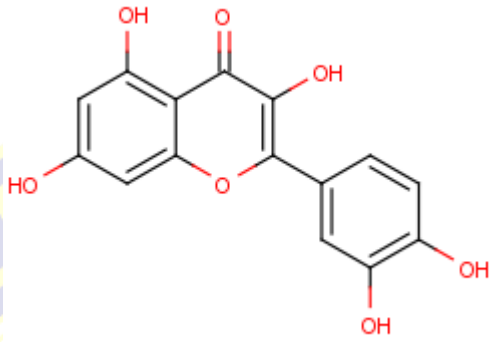


Gambar V.13 Nimbin

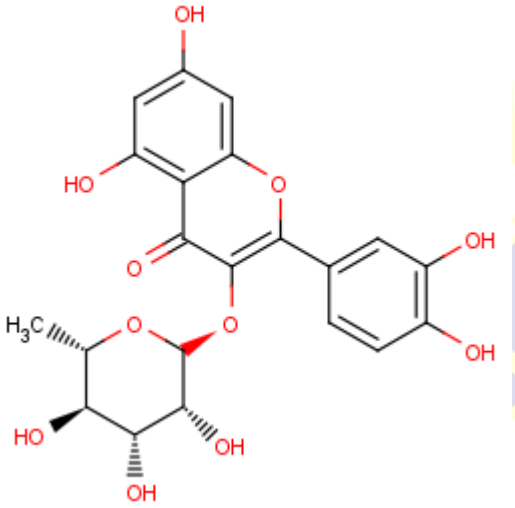


Gambar V.14 Nimbolida

LAMPIRAN 6
(LANJUTAN)

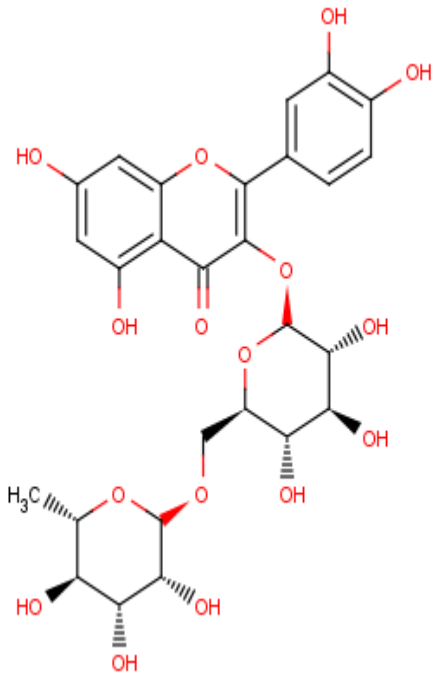


Gambar V.15 Quercetin

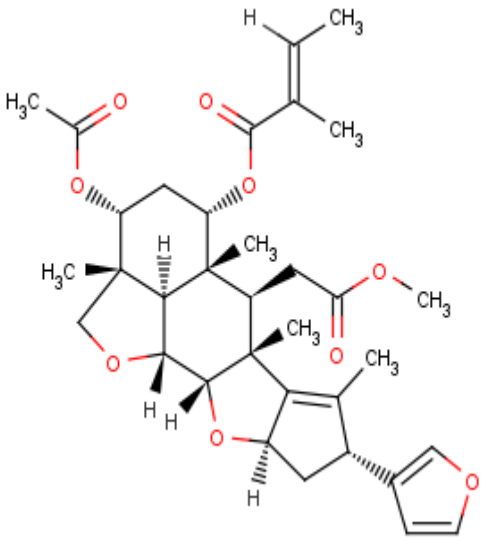


Gambar V.16 Quercitrin

LAMPIRAN 6
(LANJUTAN)



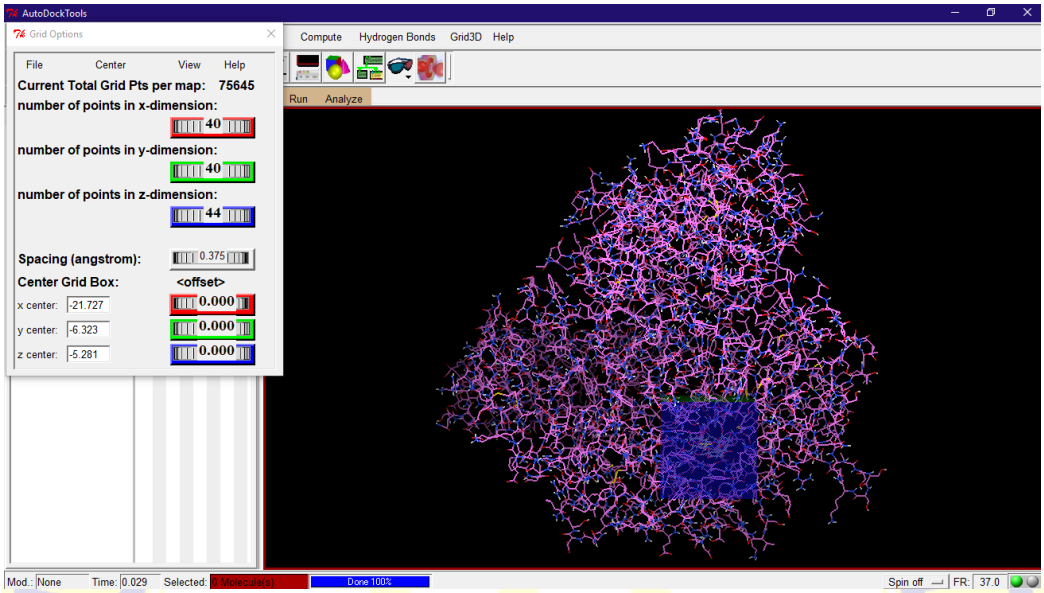
Gambar V.17 Rutin



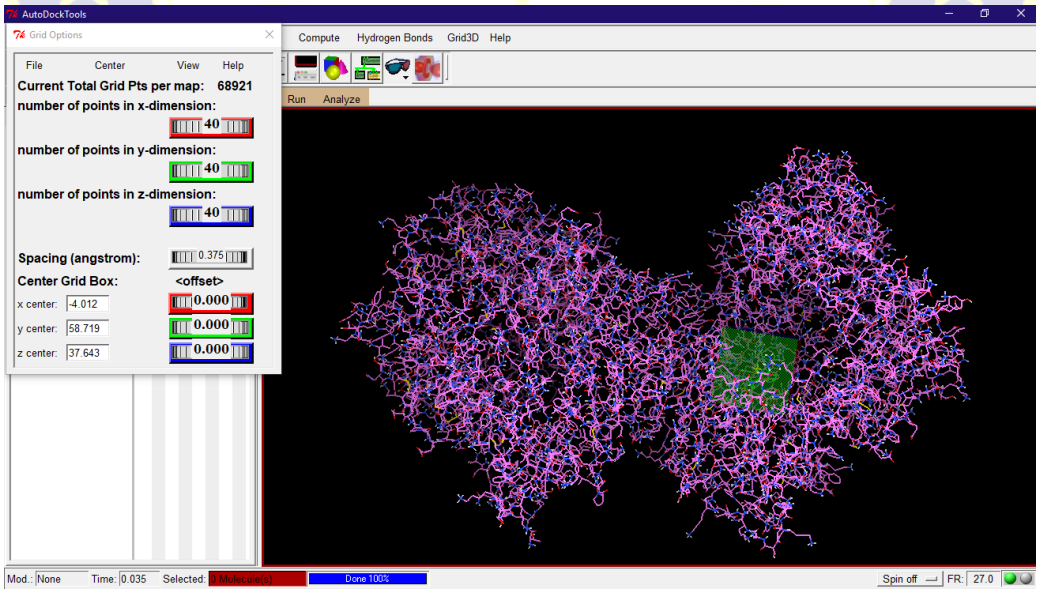
Gambar V.18 Salannin

LAMPIRAN 7

PARAMETER *GRIDBOX*

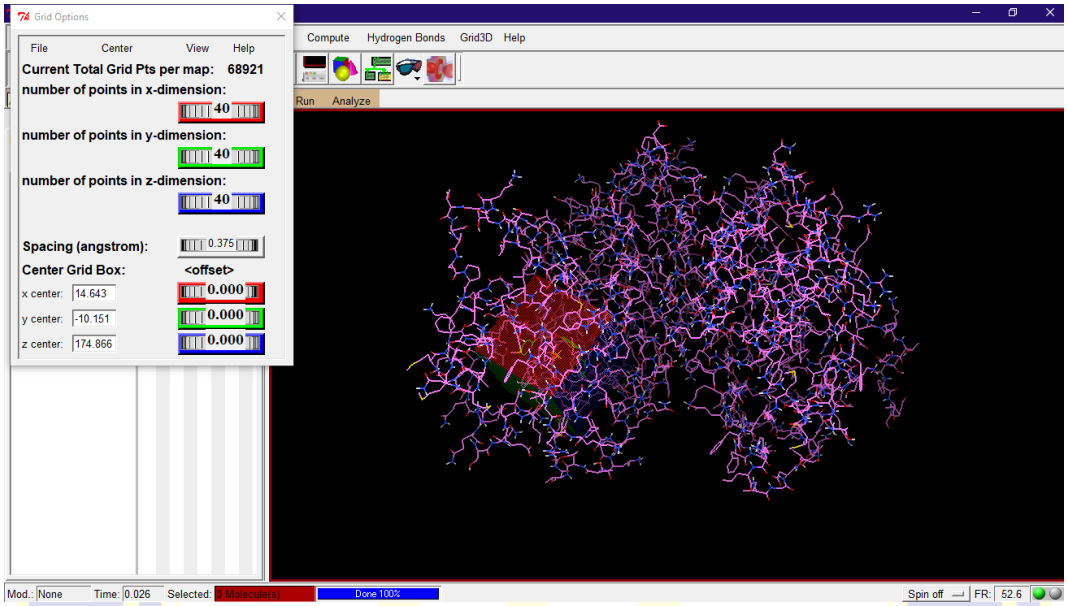


Gambar V.19 Tampilan parameter *gridbox* reseptor α-Glukosidase



Gambar V.20 Tampilan parameter *gridbox* reseptor DPP-4

LAMPIRAN 7
(LANJUTAN)



Gambar V.21 Tampilan parameter *gridbox* reseptor PPARγ

LAMPIRAN 8

HASIL VALIDASI METODE

```
    CLUSTERING HISTOGRAM
    ____________________

_____________________________________________________________________________
     |           |     |           |     |
Clus | Lowest    | Run | Mean      | Num | Histogram
-ter | Binding   |     | Binding   | in  |
Rank | Energy    |     | Energy    | Clus|    5    10   15   20   25   30   35
_____|___________|_____|___________|_____|___:____|___:____|___:____|___:____|___:__
   1 |     -7.75 |  56 |     -7.75 | 100 |#########################################################################################################
_____|___________|_____|___________|_____|_____________________________________


Number of multi-member conformational clusters found = 1, out of 100 runs.

    RMSD TABLE
    __________

_____________________________________________________________________
     |      |     |           |         |                |
Rank | Sub- | Run | Binding   | Cluster | Reference      | Grep
     | Rank |     | Energy    | RMSD    | RMSD           | Pattern
_____|______|_____|___________|_________|________________|________
   1     1    56       -7.75      0.00      0.71          RANKING
   1     2    22       -7.75      0.01      0.71          RANKING
   1     3    30       -7.75      0.01      0.71          RANKING
   1     4     2       -7.75      0.00      0.71          RANKING
   1     5    11       -7.75      0.00      0.71          RANKING
   1     6    98       -7.75      0.00      0.71          RANKING
   1     7     6       -7.75      0.01      0.71          RANKING
   1     8    80       -7.75      0.00      0.72          RANKING
   1     9    64       -7.75      0.00      0.71          RANKING
   1    10    59       -7.75      0.01      0.71          RANKING
   1    11    67       -7.75      0.01      0.71          RANKING
   1    12    31       -7.75      0.02      0.70          RANKING
   1    13   100       -7.75      0.01      0.71          RANKING
   1    14    12       -7.75      0.01      0.71          RANKING
   1    15    96       -7.75      0.01      0.71          RANKING
   1    16    97       -7.75      0.02      0.71          RANKING
   1    17    86       -7.75      0.01      0.71          RANKING
```

Gambar V.22 Hasil validasi metode *redocking* α-Glukosidase 2QMJ

LAMPIRAN 8
(LANJUTAN)

```
    CLUSTERING HISTOGRAM
    ____________________

_____________________________________________________________________
    |           |     |           |     |
Clus| Lowest    | Run | Mean      | Num | Histogram
-ter| Binding   |     | Binding   | in  |
Rank| Energy    |     | Energy    | Clus|    5    10   15   20   25   30   35
____|___________|_____|___________|_____|___:____|____:____|____:____|____:___
   1|     -8.27 |  38 |     -8.27 | 100 |##########################################################################################################
____|___________|_____|___________|_____|_____________________________


Number of multi-member conformational clusters found = 1, out of 100 runs.

    RMSD TABLE
    __________


_____________________________________________________________________
    |      |     |           |         |                |
Rank| Sub- | Run | Binding   | Cluster | Reference      | Grep
    | Rank |     | Energy    | RMSD    | RMSD           | Pattern
____|______|_____|___________|_________|________________|_________
   1      1    38       -8.27      0.00      1.86          RANKING
   1      2    21       -8.27      0.02      1.86          RANKING
   1      3    69       -8.27      0.01      1.86          RANKING
   1      4    13       -8.27      0.00      1.86          RANKING
   1      5    98       -8.27      0.01      1.85          RANKING
   1      6    22       -8.27      0.01      1.86          RANKING
   1      7    73       -8.27      0.01      1.86          RANKING
   1      8    80       -8.27      0.00      1.86          RANKING
   1      9    11       -8.27      0.00      1.86          RANKING
   1     10    42       -8.27      0.01      1.86          RANKING
   1     11    32       -8.27      0.00      1.86          RANKING
   1     12     9       -8.27      0.01      1.86          RANKING
   1     13    74       -8.27      0.01      1.86          RANKING
   1     14    16       -8.27      0.01      1.86          RANKING
   1     15     4       -8.27      0.01      1.86          RANKING
   1     16    66       -8.27      0.01      1.86          RANKING
   1     17    60       -8.27      0.02      1.85          RANKING
```

Gambar V.23 Hasil validasi metode *redocking* DPP-4 6B1E

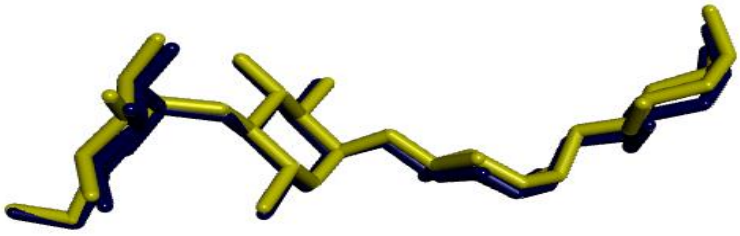
LAMPIRAN 8
(LANJUTAN)

```
    CLUSTERING HISTOGRAM
    ____________________

_____________________________________________________________________
    |           |     |           |     |
Clus | Lowest    | Run | Mean      | Num | Histogram
-ter | Binding   |     | Binding   | in  |
Rank | Energy    |     | Energy    | Clus|    5    10   15   20   25   30   35
_____|___________|_____|___________|_____|____:____|____:____|____:____|____:___
   1 |    -10.05 |  32 |    -10.05 | 100 |##########################################################################################################
_____|___________|_____|___________|_____|_____________________________________


Number of multi-member conformational clusters found = 1, out of 100 runs.

    RMSD TABLE
    __________

_____________________________________________________________________
    |      |      |           |         |                 |
Rank | Sub- | Run  | Binding   | Cluster | Reference       | Grep
     | Rank |      | Energy    | RMSD    | RMSD            | Pattern
_____|______|______|___________|_________|_________________|_________
   1      1     32      -10.05      0.00      0.75          RANKING
   1      2      8      -10.05      0.00      0.75          RANKING
   1      3      7      -10.05      0.00      0.75          RANKING
   1      4     50      -10.05      0.00      0.75          RANKING
   1      5     59      -10.05      0.00      0.75          RANKING
   1      6     84      -10.05      0.01      0.75          RANKING
   1      7     69      -10.05      0.01      0.75          RANKING
   1      8     91      -10.05      0.00      0.75          RANKING
   1      9     36      -10.05      0.01      0.74          RANKING
   1     10      9      -10.05      0.01      0.75          RANKING
   1     11     89      -10.05      0.00      0.75          RANKING
   1     12     73      -10.05      0.01      0.75          RANKING
   1     13     17      -10.05      0.01      0.75          RANKING
   1     14     41      -10.05      0.01      0.75          RANKING
   1     15     98      -10.05      0.01      0.75          RANKING
   1     16     24      -10.05      0.01      0.75          RANKING
   1     17     78      -10.05      0.01      0.75          RANKING
```

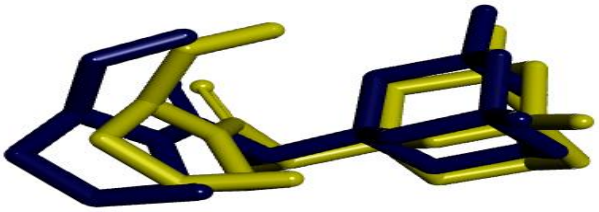
Gambar V.24 Hasil validasi metode *redocking* PPARγ 5JI0

LAMPIRAN 9

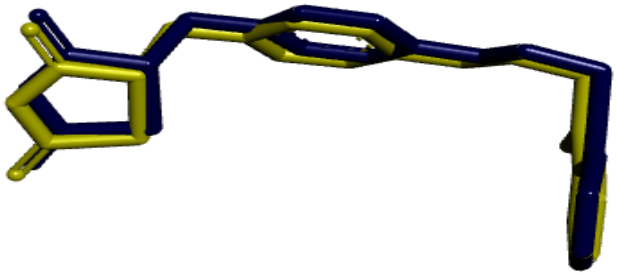
VISUALISASI *REDOCKING*



Gambar V.25 Hasil visualisasi tumpang tindih ligan alami dari reseptor α-Glukosidase dari hasil kristalografi sinar-X (Biru) dengan ligan hasil *redocking* (kuning)



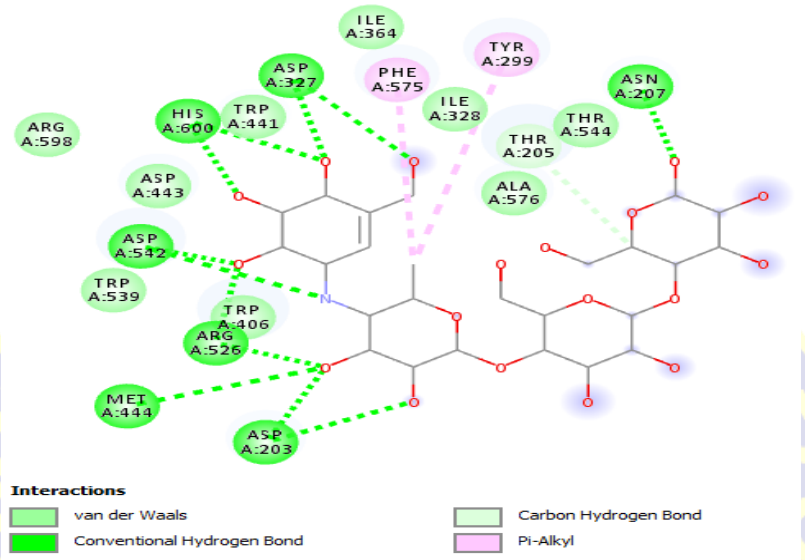
Gambar V.26 Hasil visualisasi tumpang tindih ligan alami dari reseptor DPP-4 dari hasil kristalografi sinar-X (biru) dengan ligan hasil *redocking* (kuning)



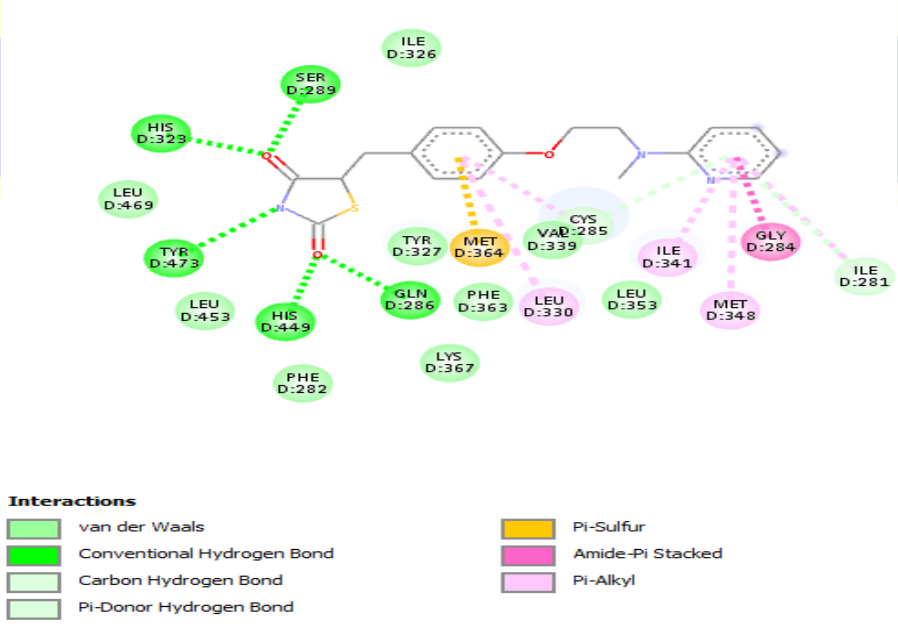
Gambar V.27 Hasil visualisasi tumpang tindih ligan alami dari reseptor PPARγ dari hasil kristalografi sinar-X (biru) dengan ligan hasil *redocking* (kuning)

LAMPIRAN 10

VISUALISASI INTERAKSI IKATAN KIMIA

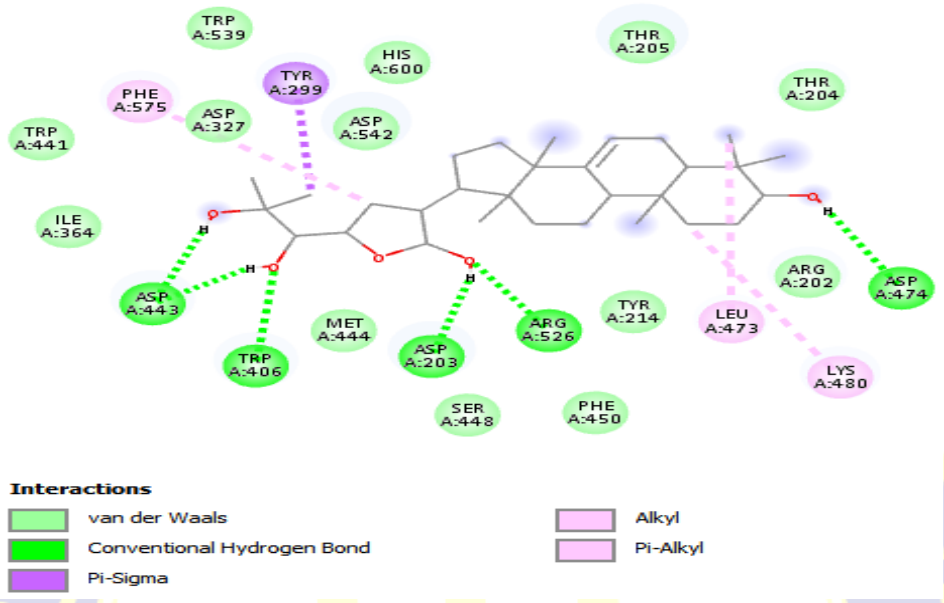


Gambar V.28 Interaksi ikatan kimia ligan alami pada reseptor α-Glukosidase

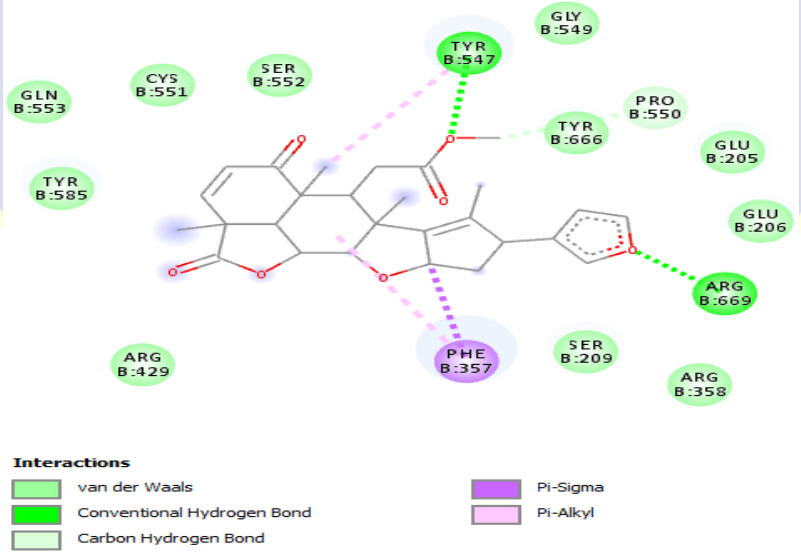


Gambar V.29 Interaksi ikatan kimia ligan alami pada reseptor PPARγ

LAMPIRAN 10
(LANJUTAN)

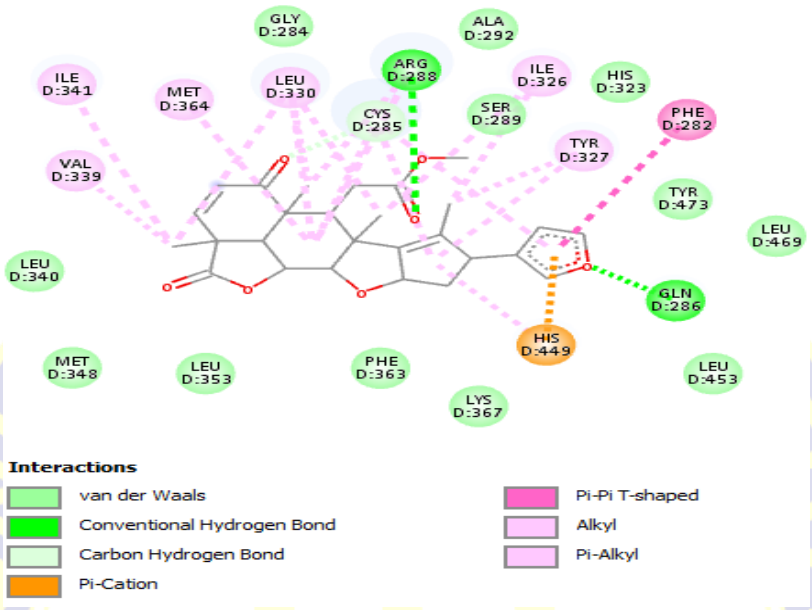


Gambar V.30 Interaksi ikatan kimia ligan uji terbaik Meliantriol pada reseptor α-Glukosidase



Gambar V.31 Interaksi ikatan kimia ligan uji terbaik Nimbolida pada reseptor DPP-4

LAMPIRAN 10
(LANJUTAN)



Gambar V.32 Interaksi ikatan kimia ligan uji terbaik Nimbolida pada reseptor PPARγ