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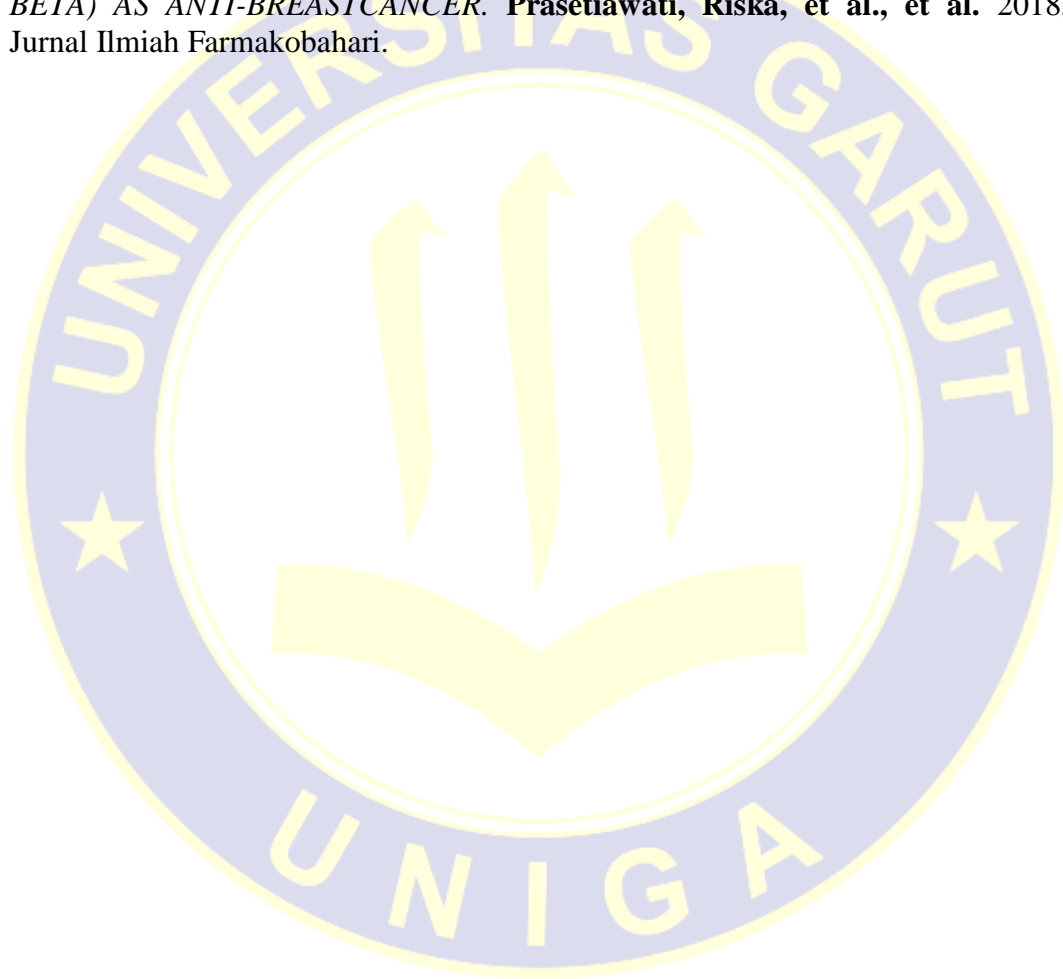
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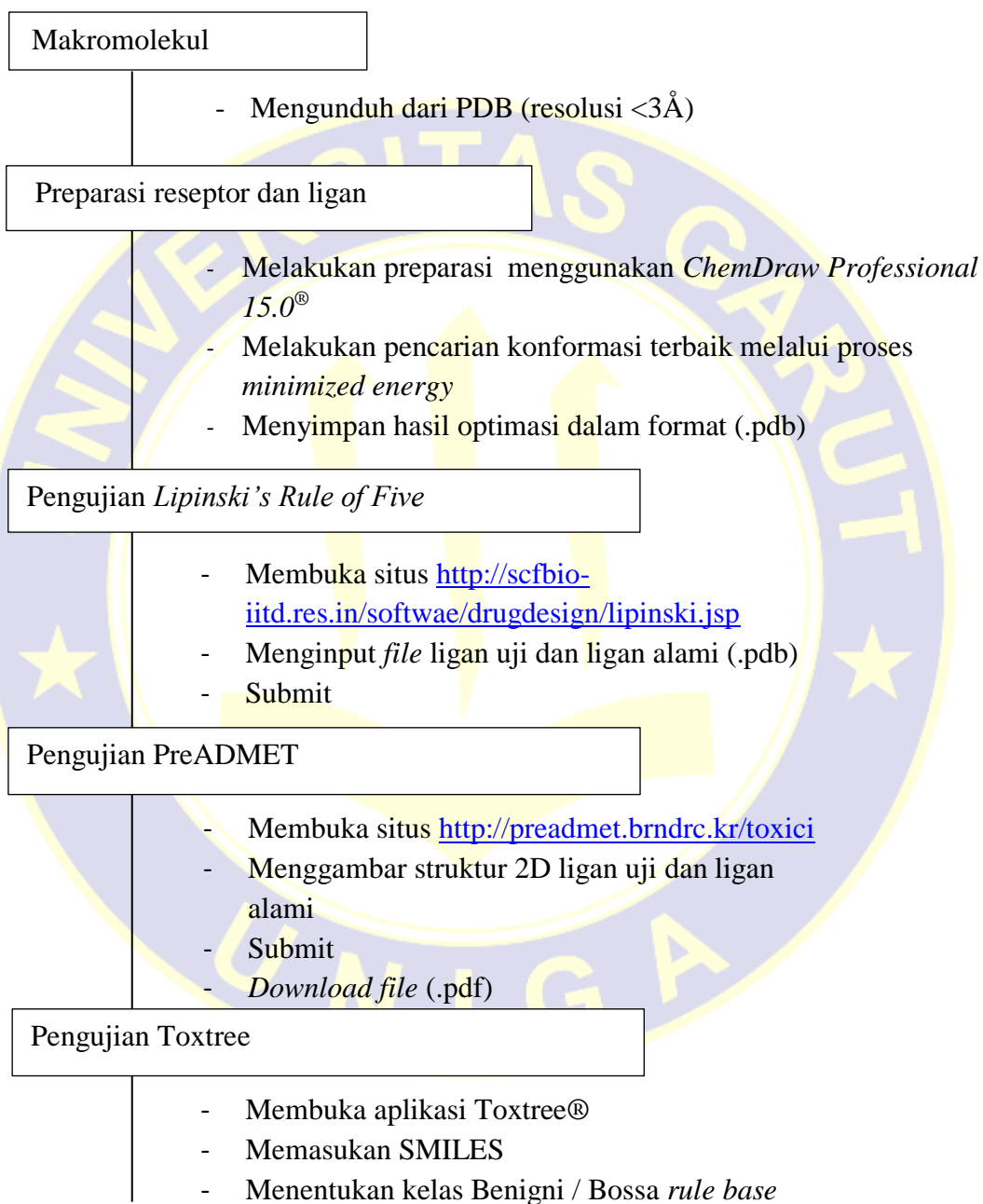


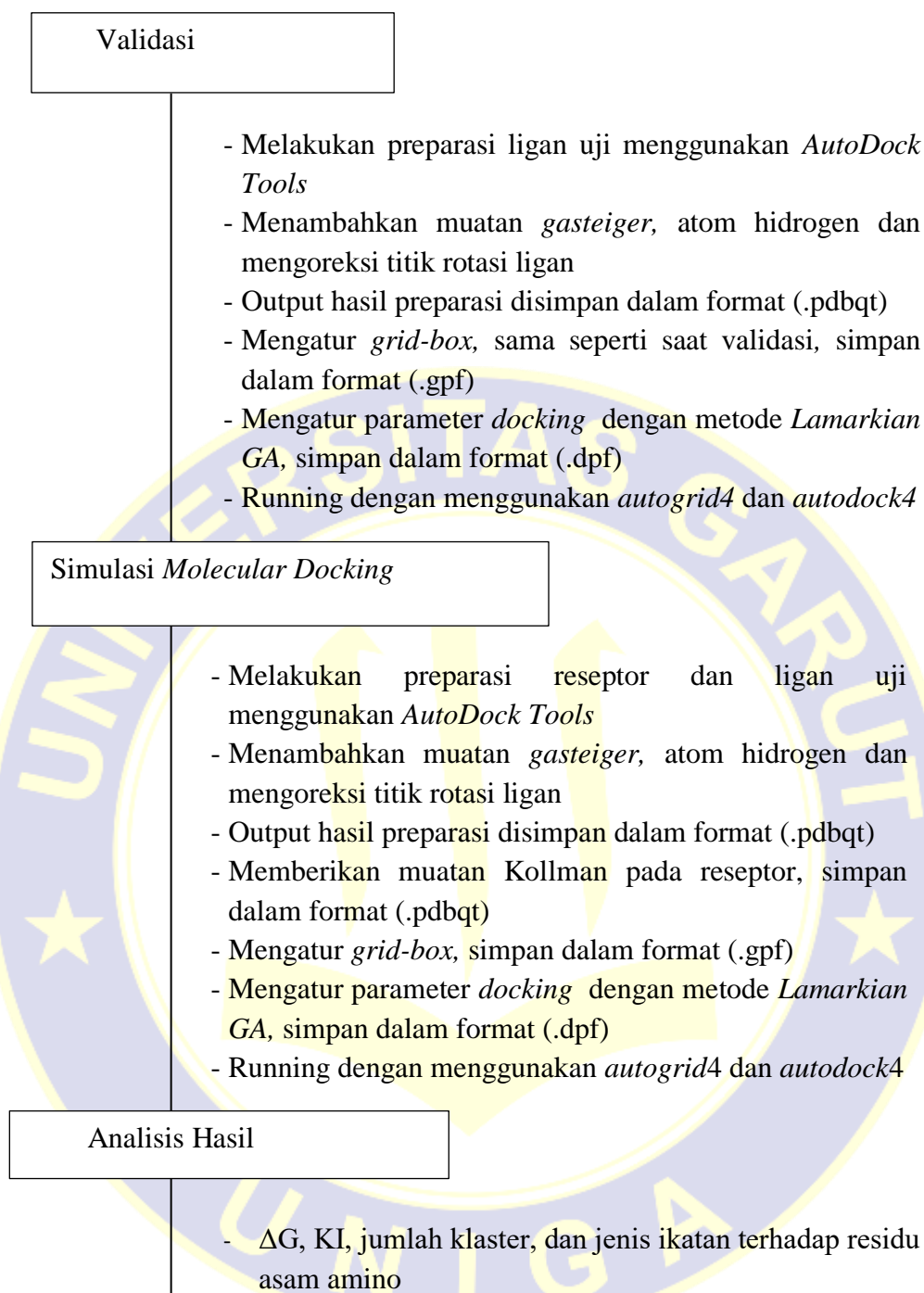
LAMPIRAN 1
TANAMAN KUMIS KUCING



Gambar VII.1 Tanaman Kumis Kucing (*Orthosiphon stamineus* Benth)

LAMPIRAN 2

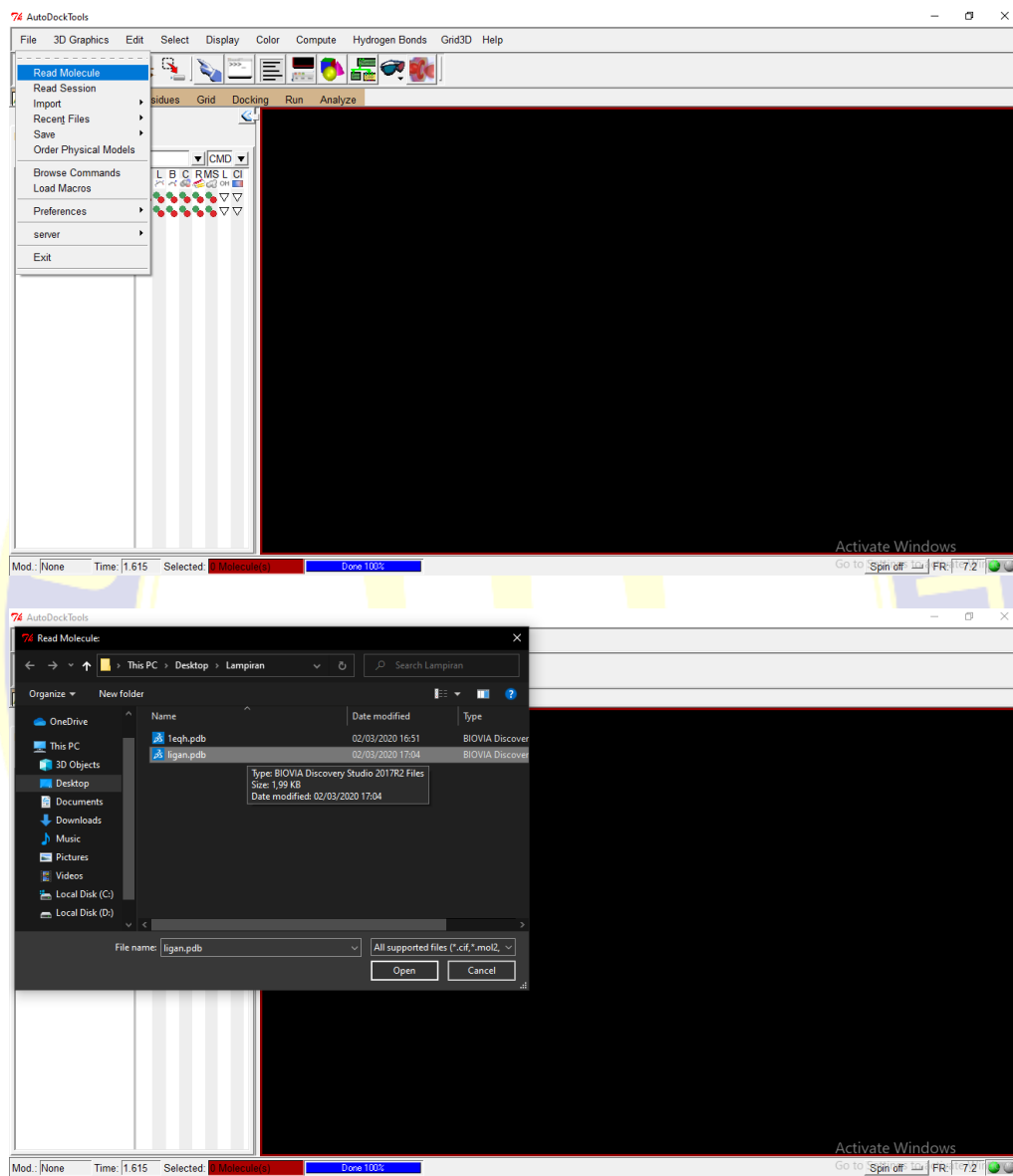
ALUR PENELITIAN SIMULASI *MOLECULAR DOCKING*



Gambar VII.2 Alur Penelitian

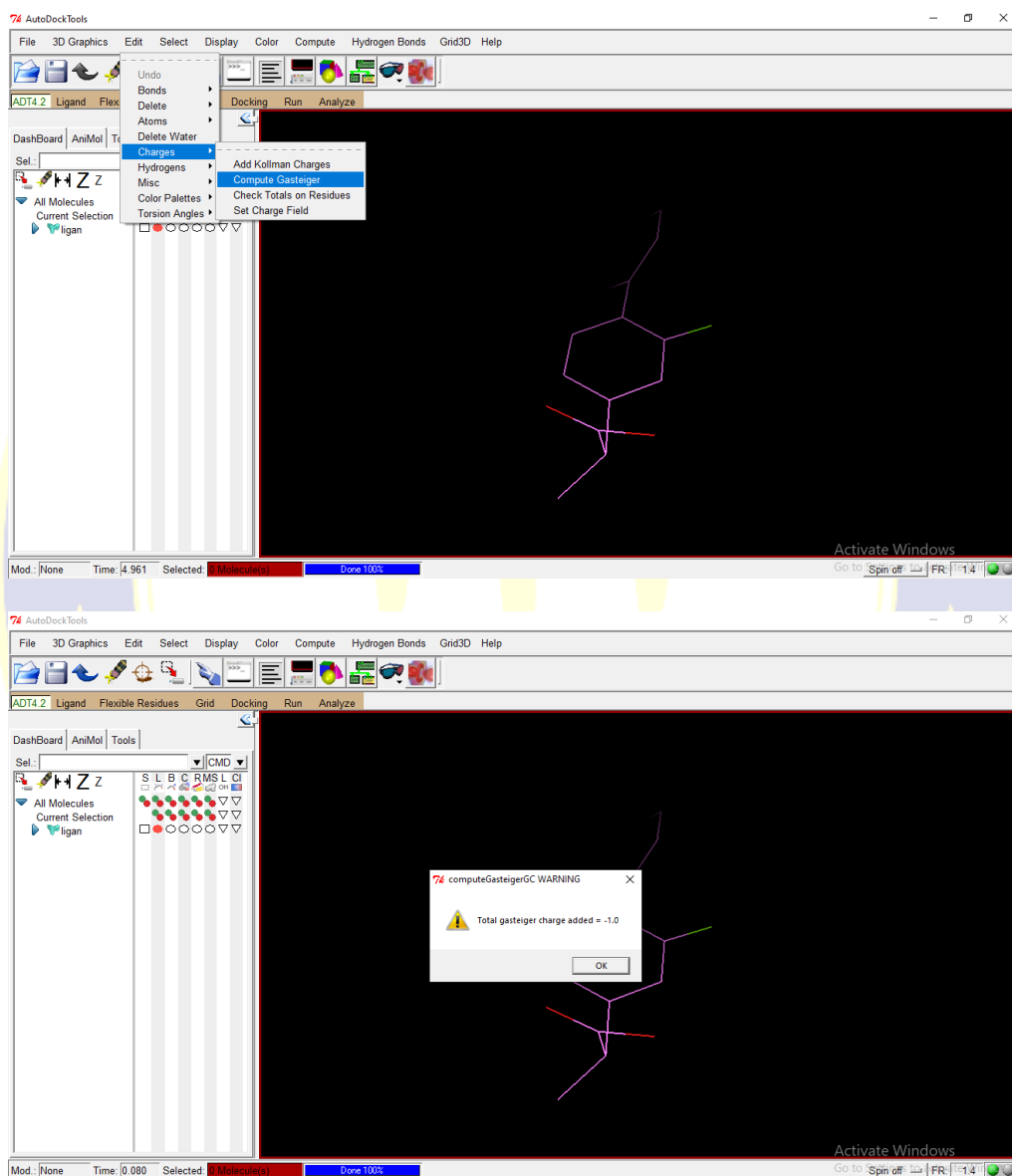
LAMPIRAN 3

LANGKAH – LANGKAH PREPARASI LIGAN DENGAN APLIKASI *AutoDock Tools*



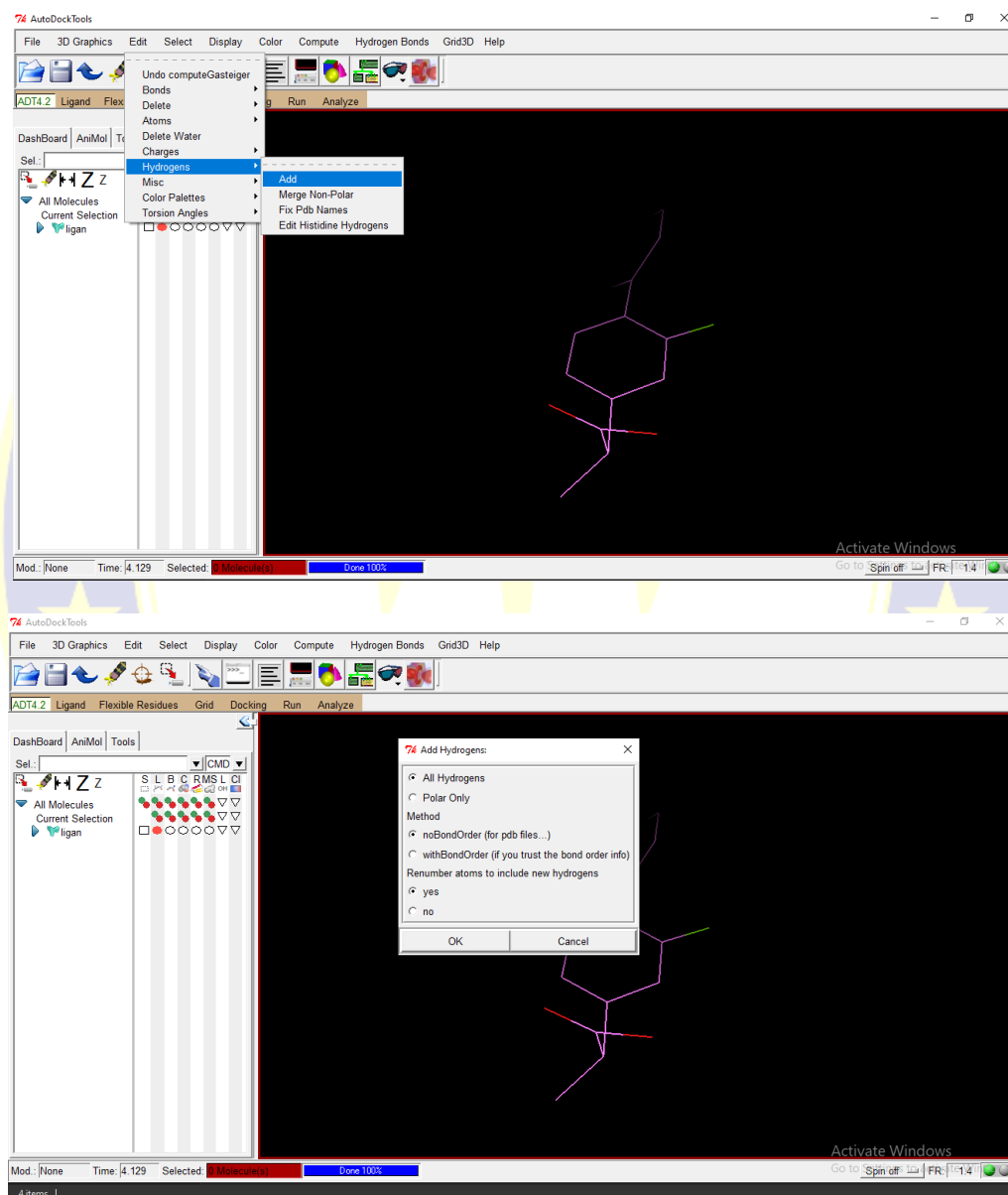
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LANGKAH – LANGKAH PREPARASI LIGAN DENGAN APLIKASI *AutoDock Tools*



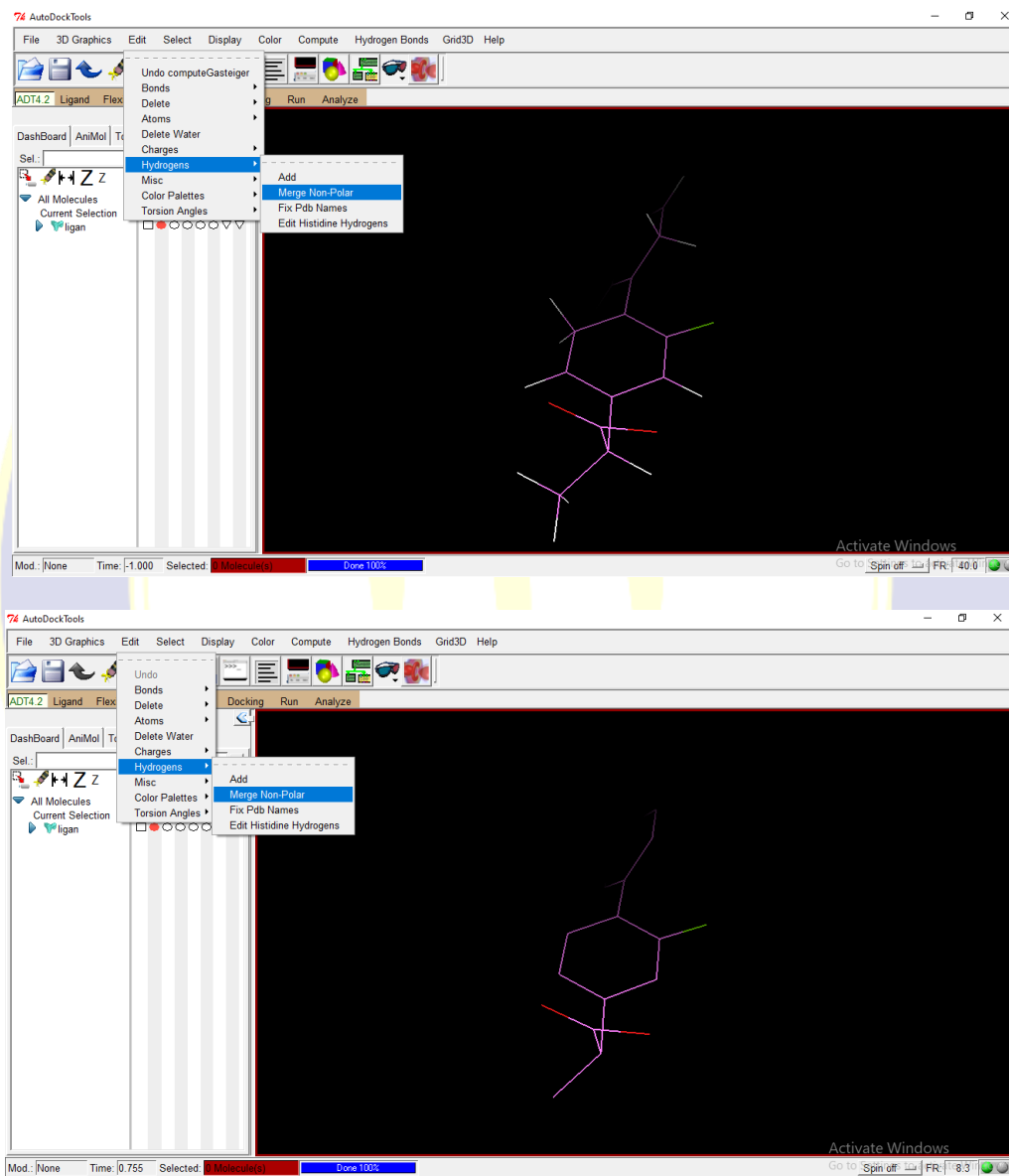
LAMPIRAN 3 (LANJUTAN)

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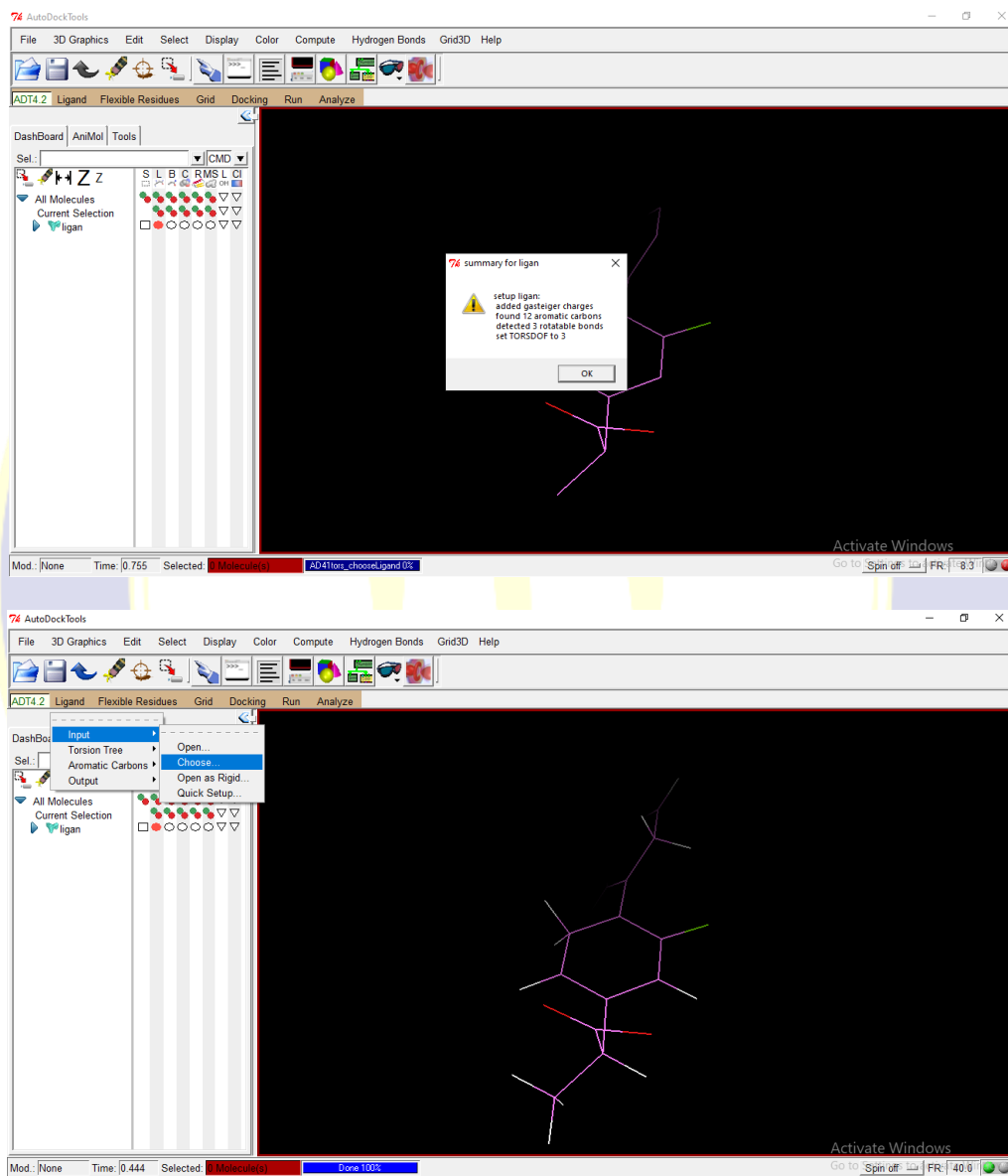
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LANGKAH – LANGKAH PREPARASI LIGAN DENGAN APLIKASI *AutoDock Tools*



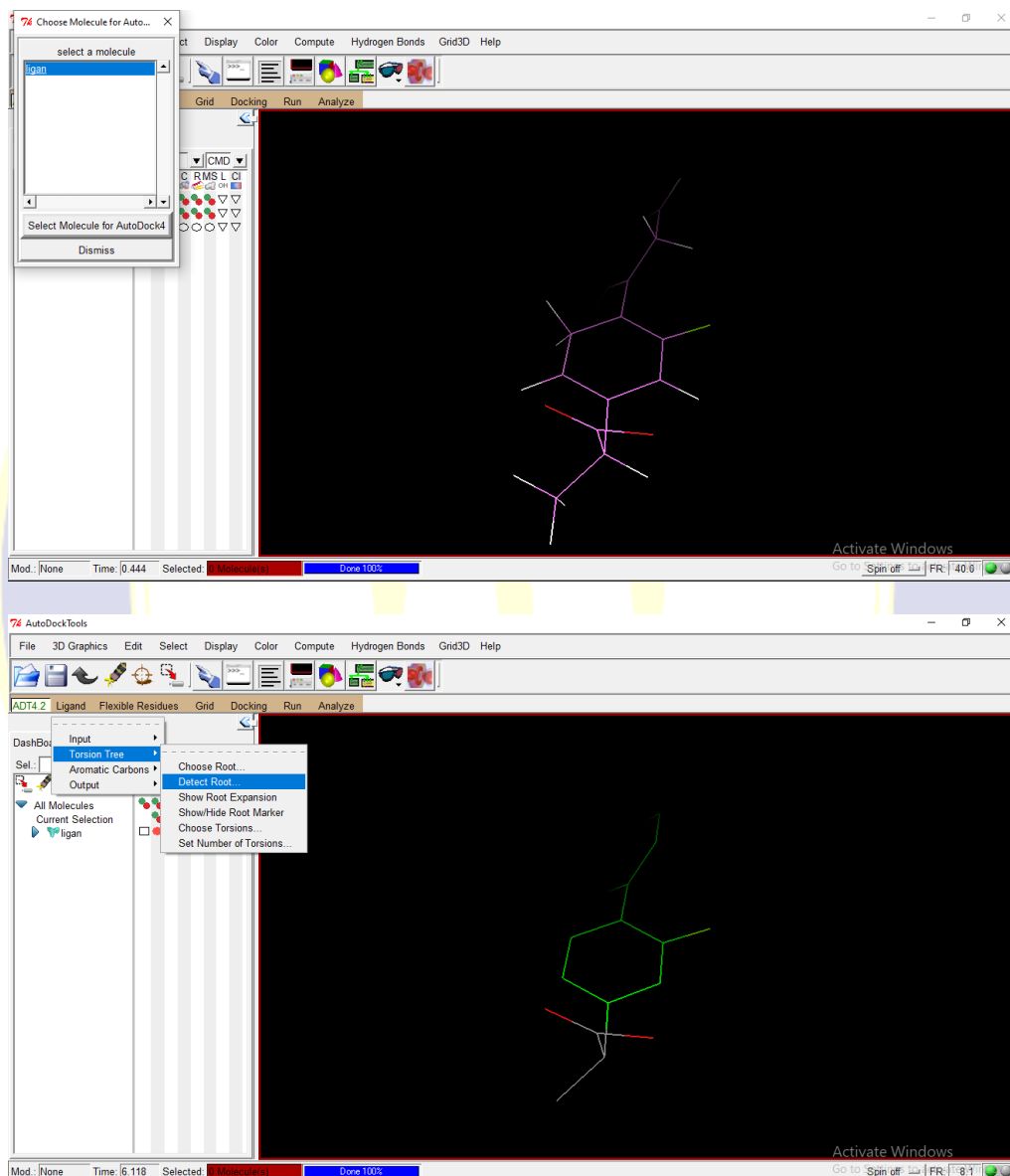
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LANGKAH – LANGKAH PREPARASI LIGAN DENGAN APLIKASI *AutoDock Tools*



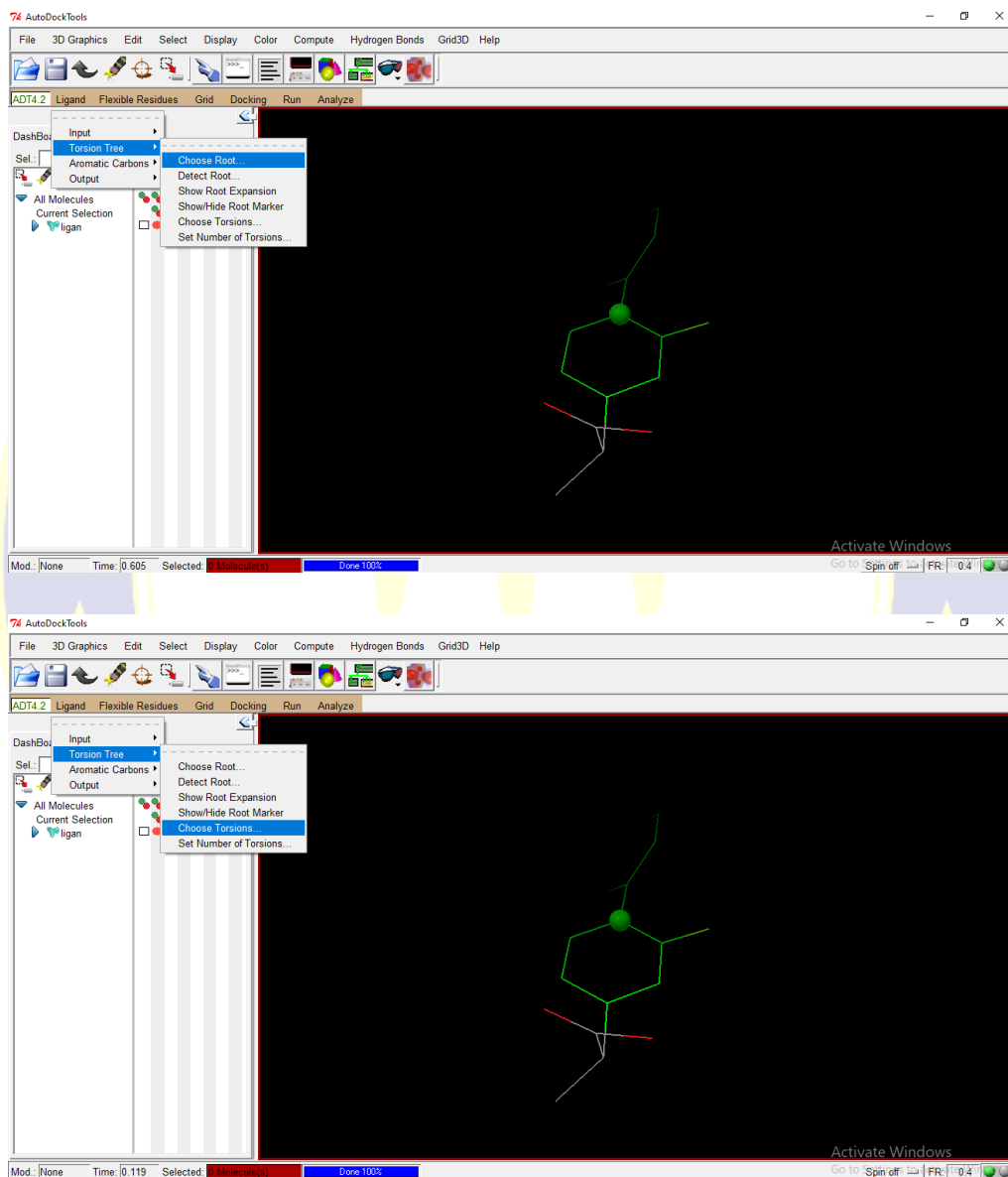
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LANGKAH – LANGKAH PREPARASI LIGAN DENGAN APLIKASI *AutoDock Tools*



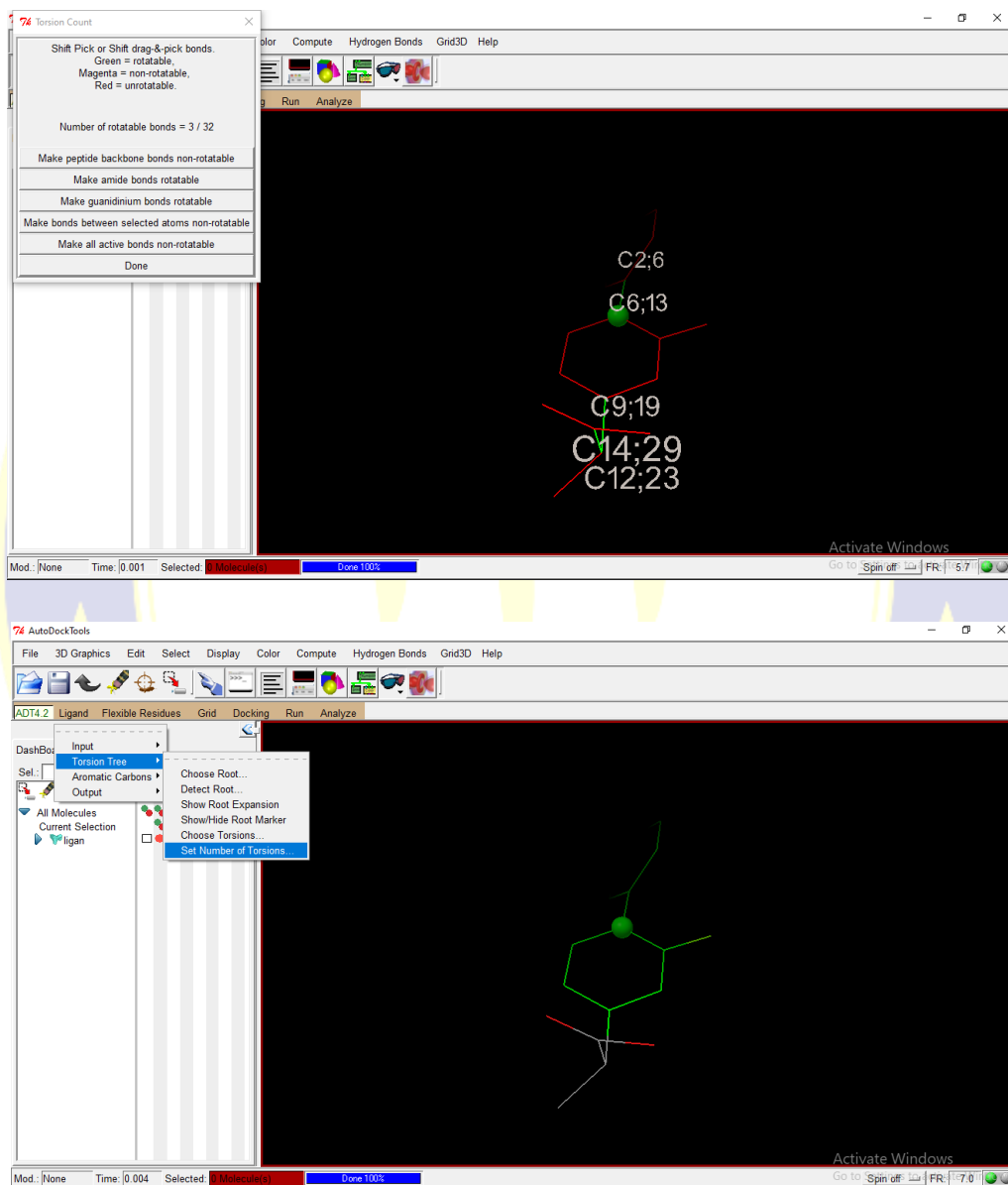
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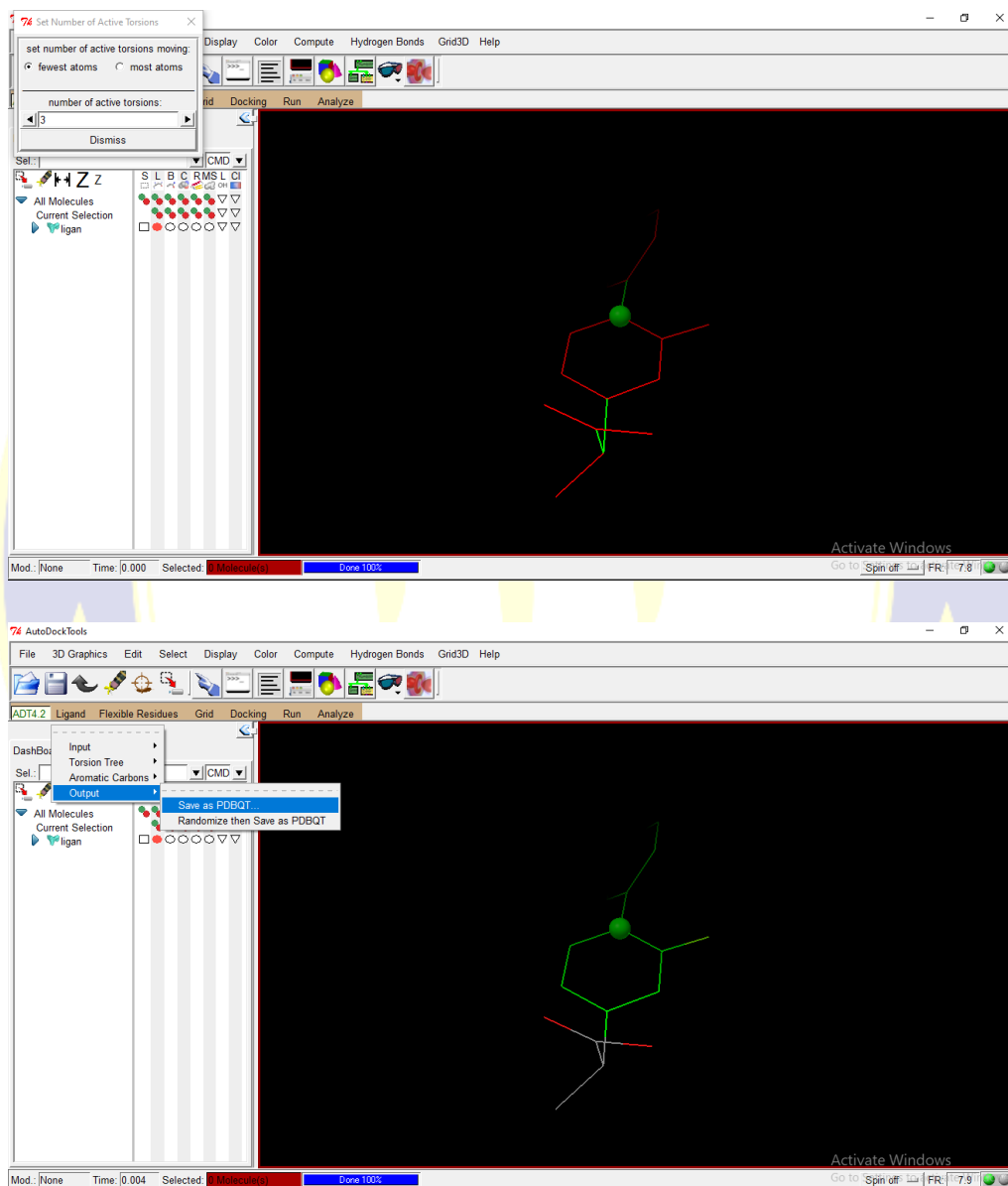
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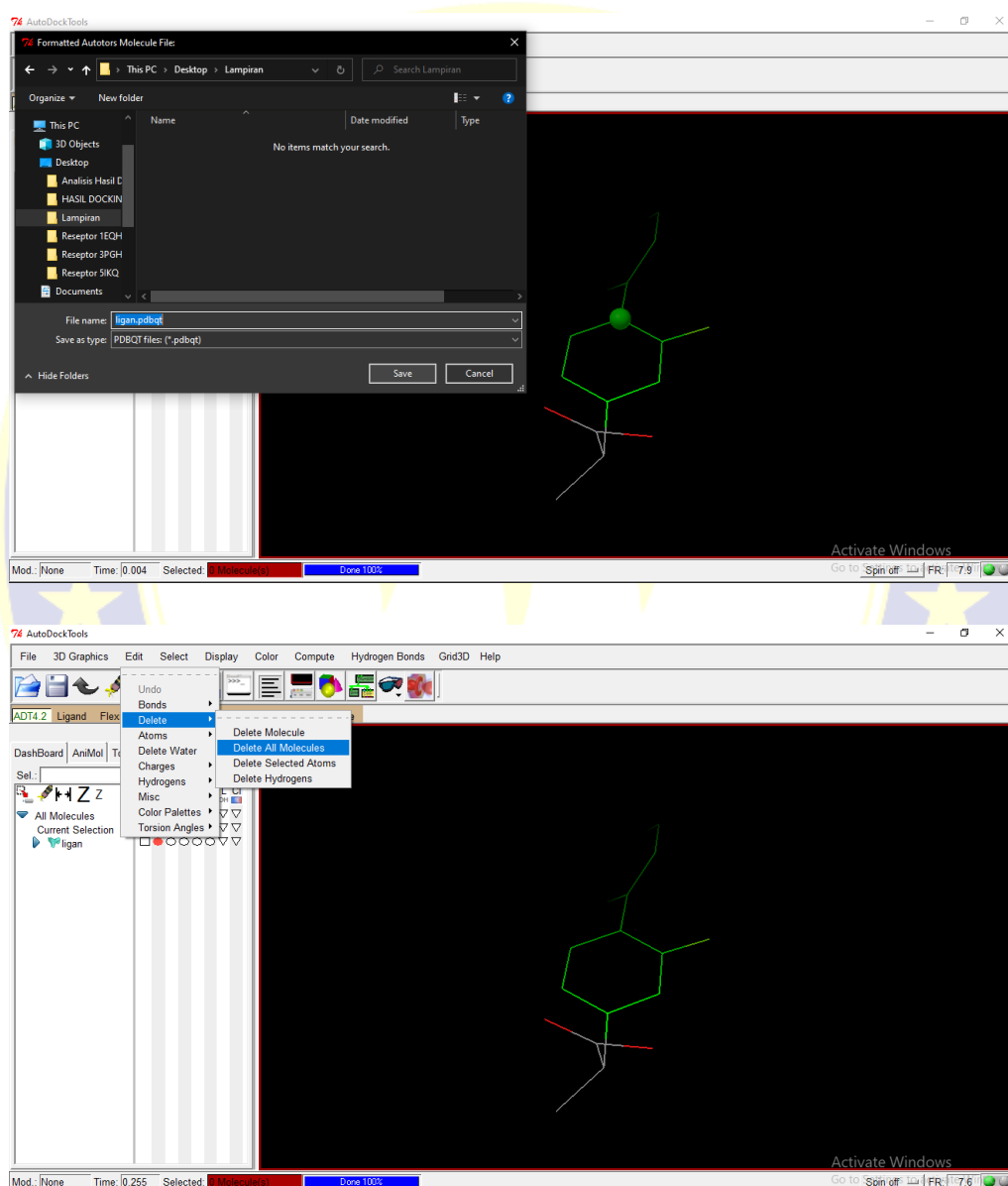
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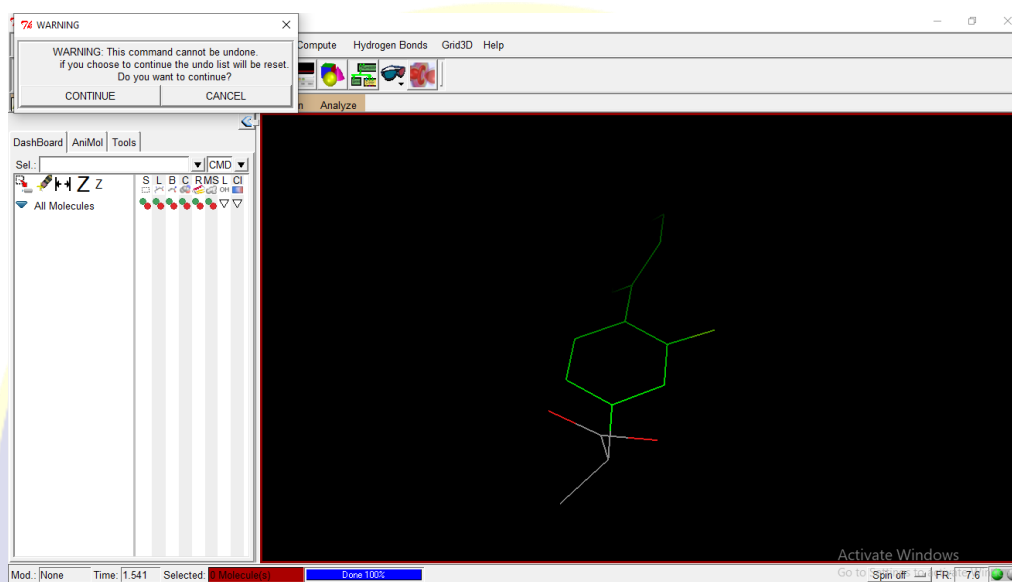
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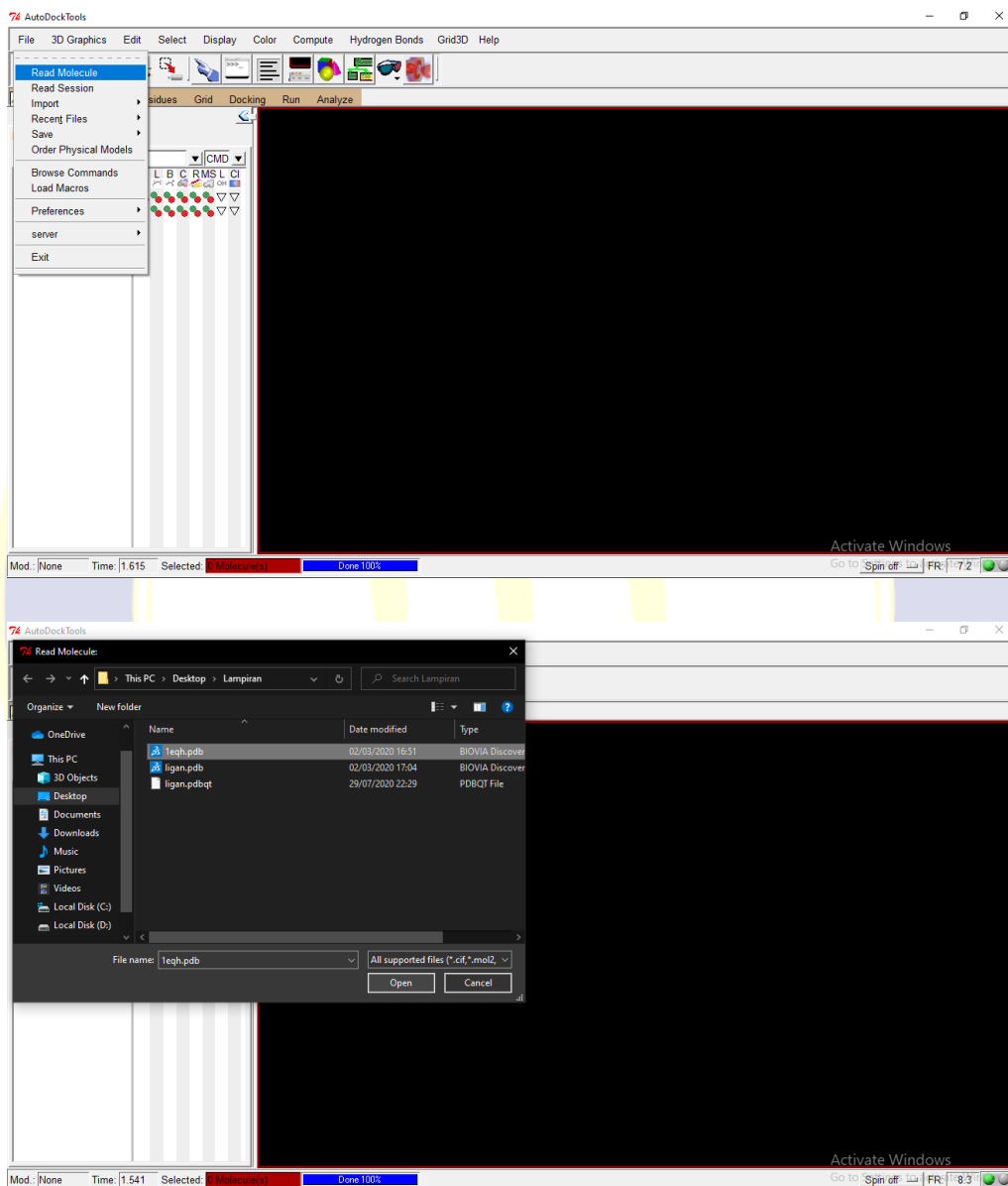
LAMPIRAN 3 (LANJUTAN)

LANGKAH – LANGKAH PREPARASI LIGAN DENGAN APLIKASI *AutoDock Tools*



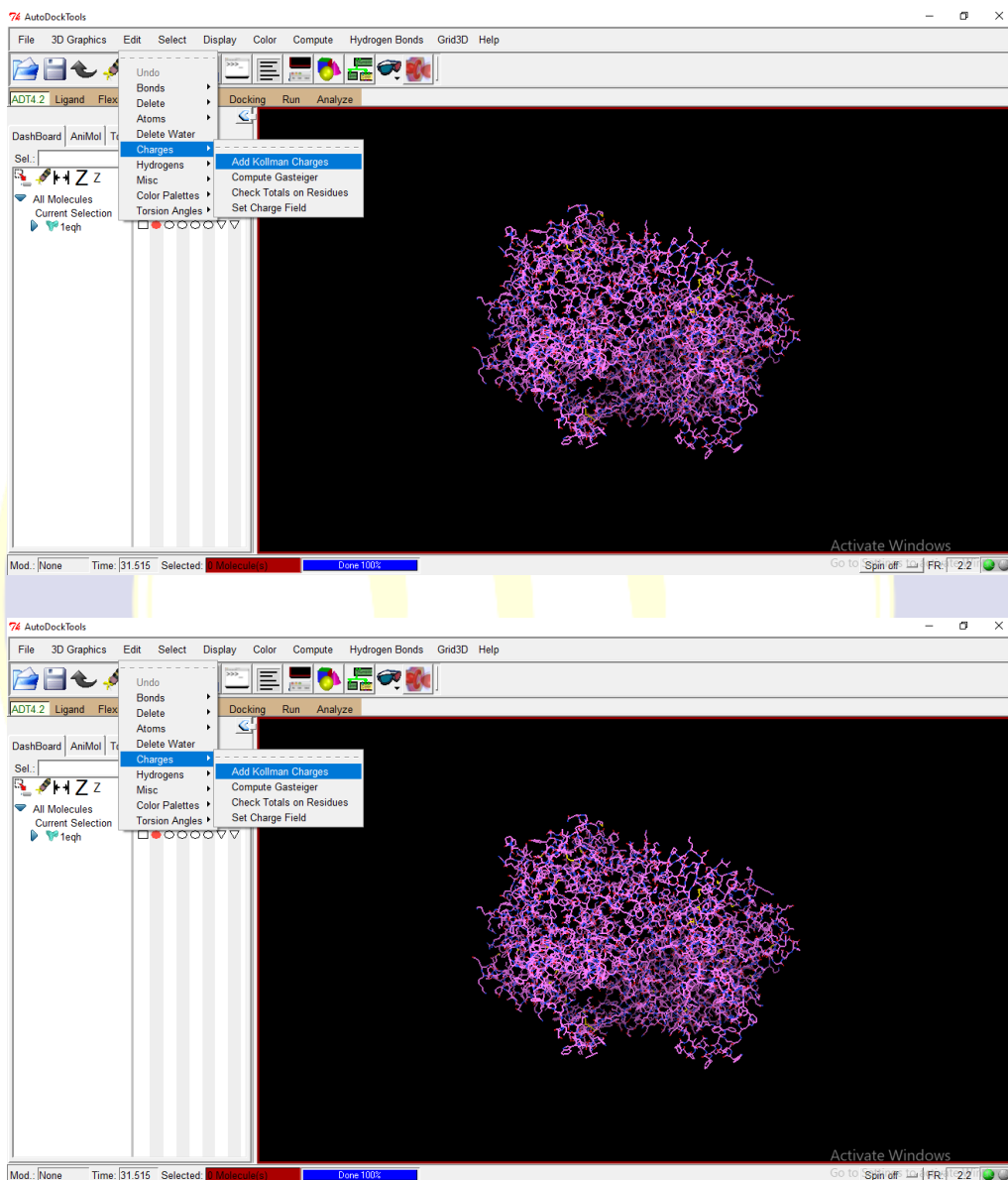
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LANGKAH-LANGKAH PREPARASI RESEPTOR DENGAN APLIKASI *AutoDock Tools*



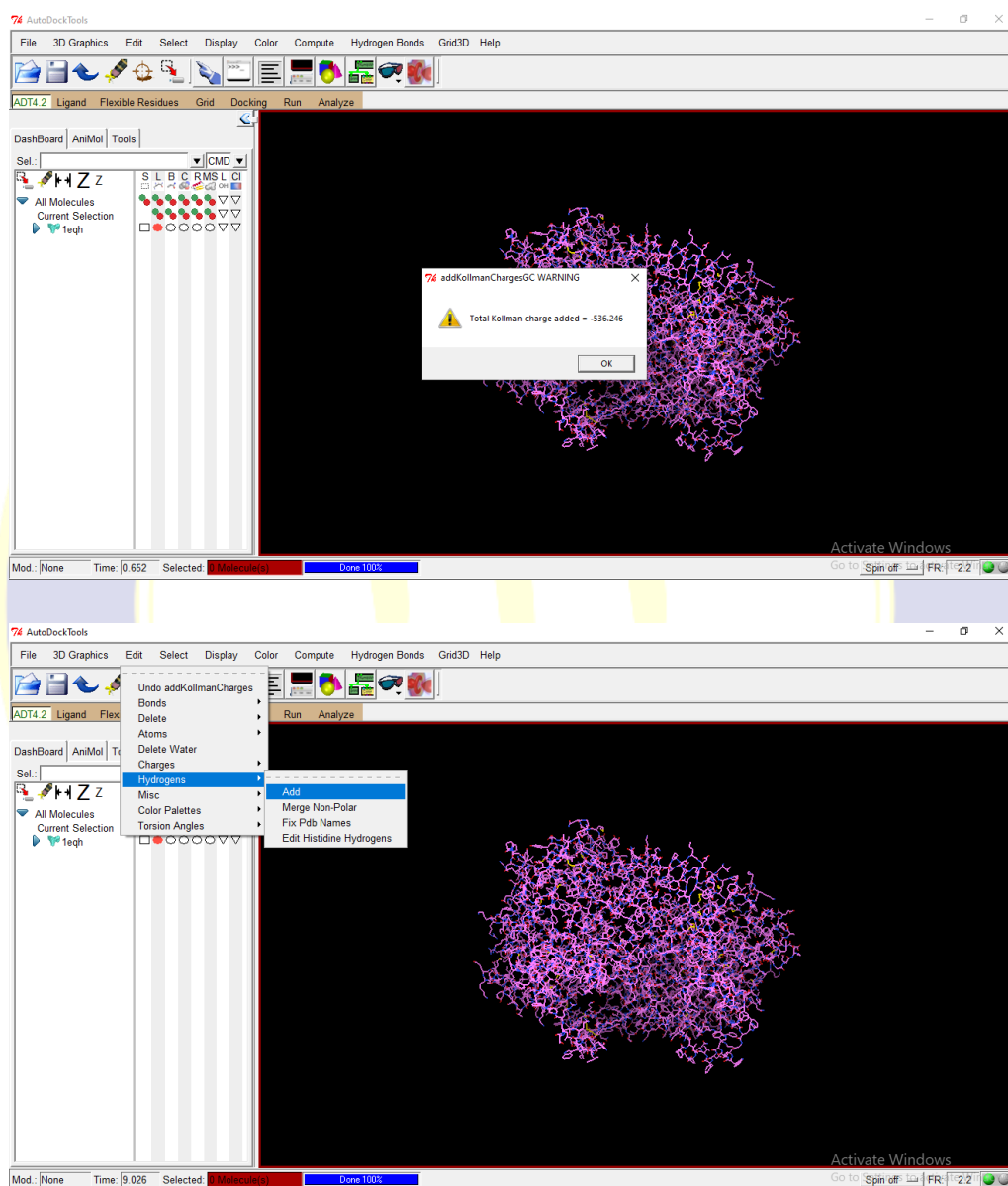
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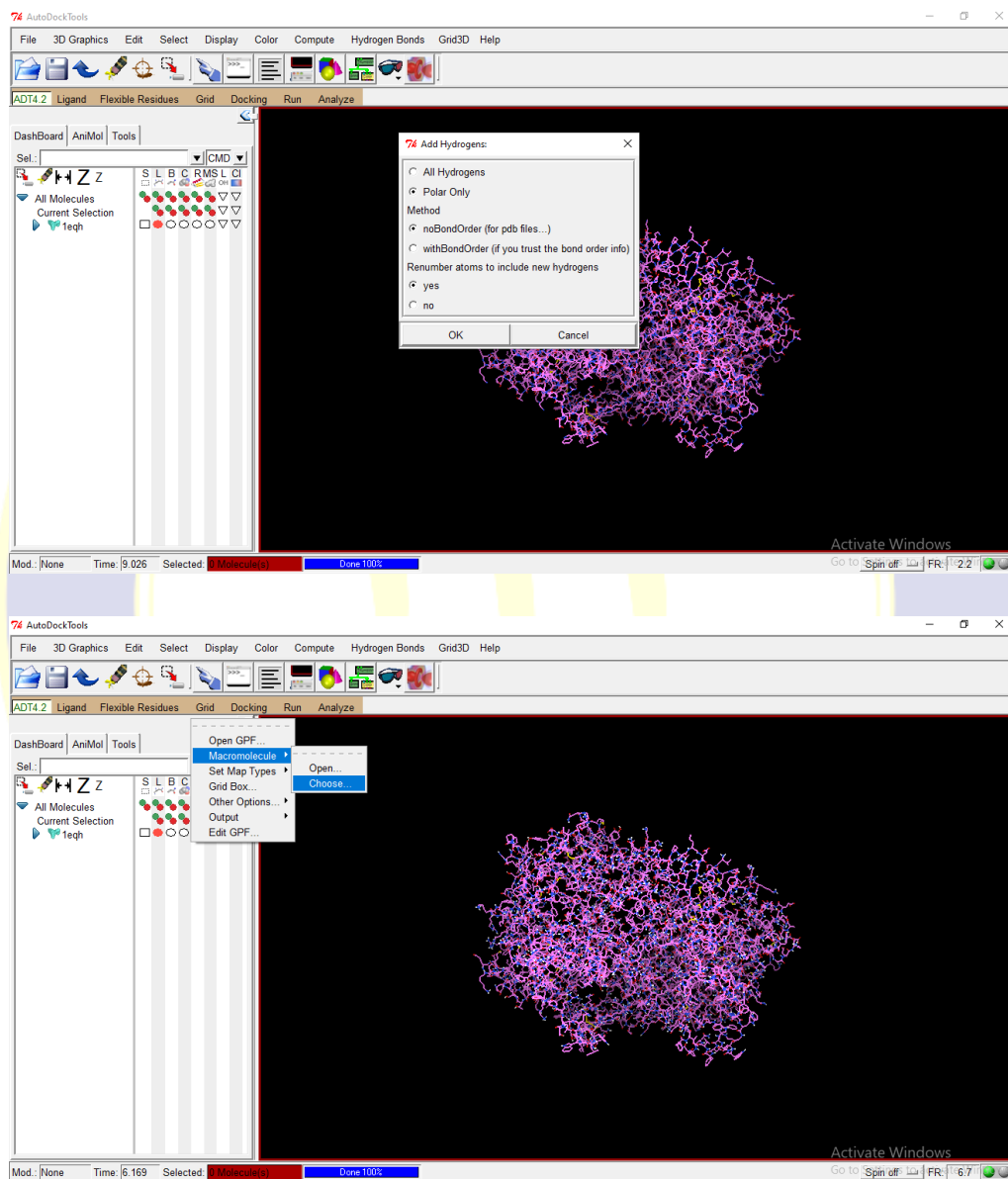
LAMPIRAN 4 (LANJUTAN)

LANGKAH-LANGKAH PREPARASI RESEPTOR DENGAN APLIKASI *AutoDock Tools*



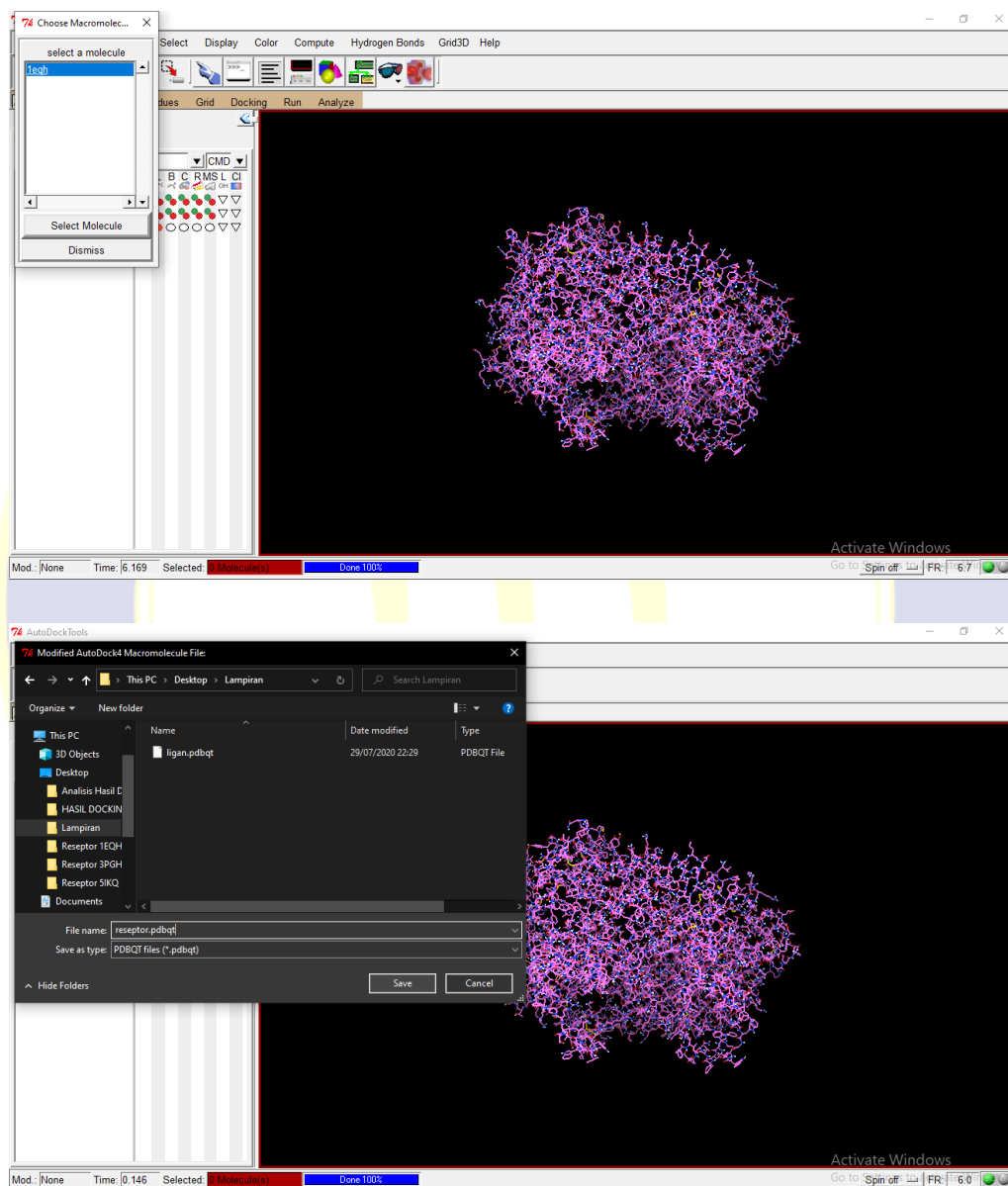
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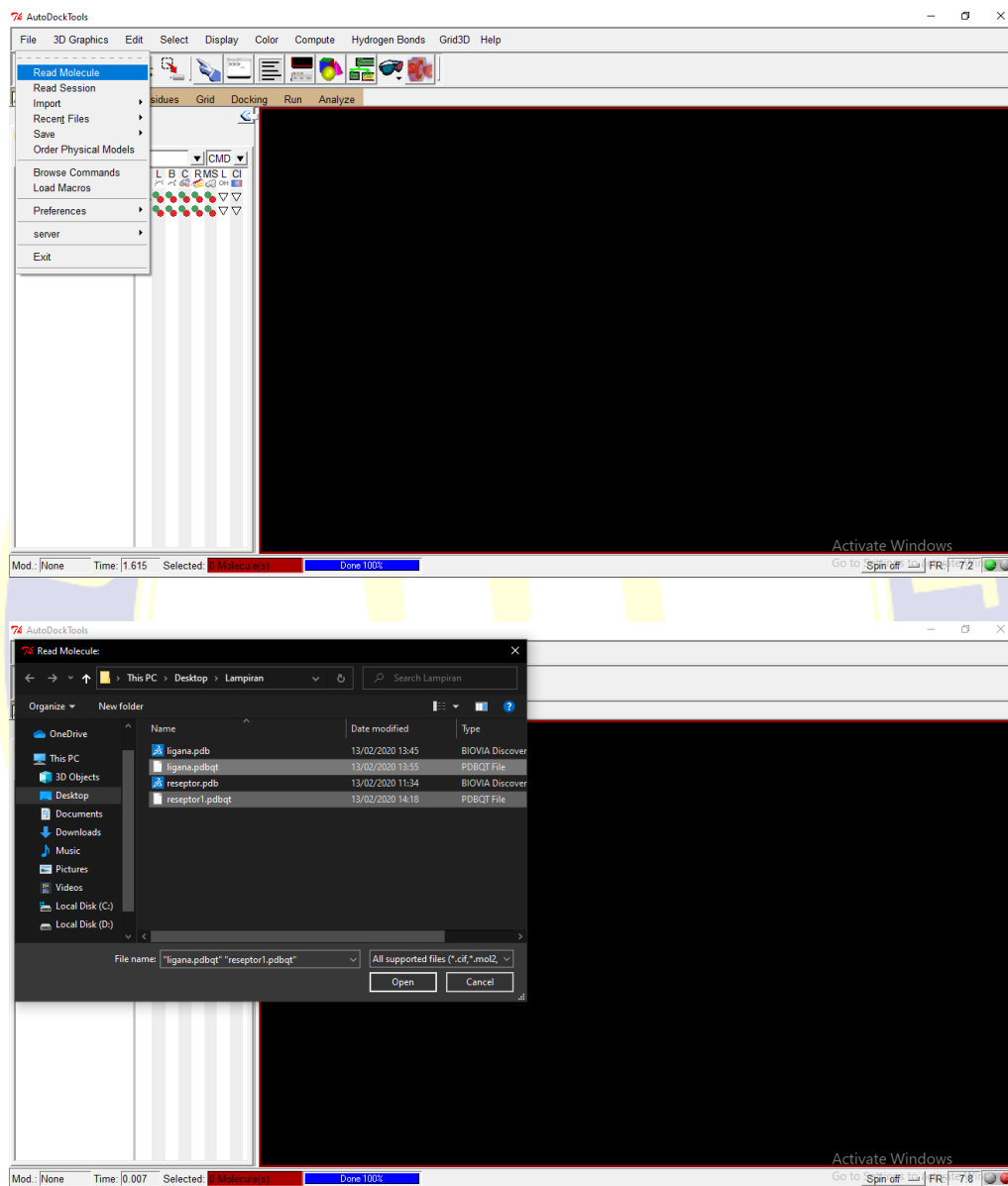
LAMPIRAN 4 (LANJUTAN)

LANGKAH-LANGKAH PREPARASI RESEPTOR DENGAN APLIKASI *AutoDock Tools*



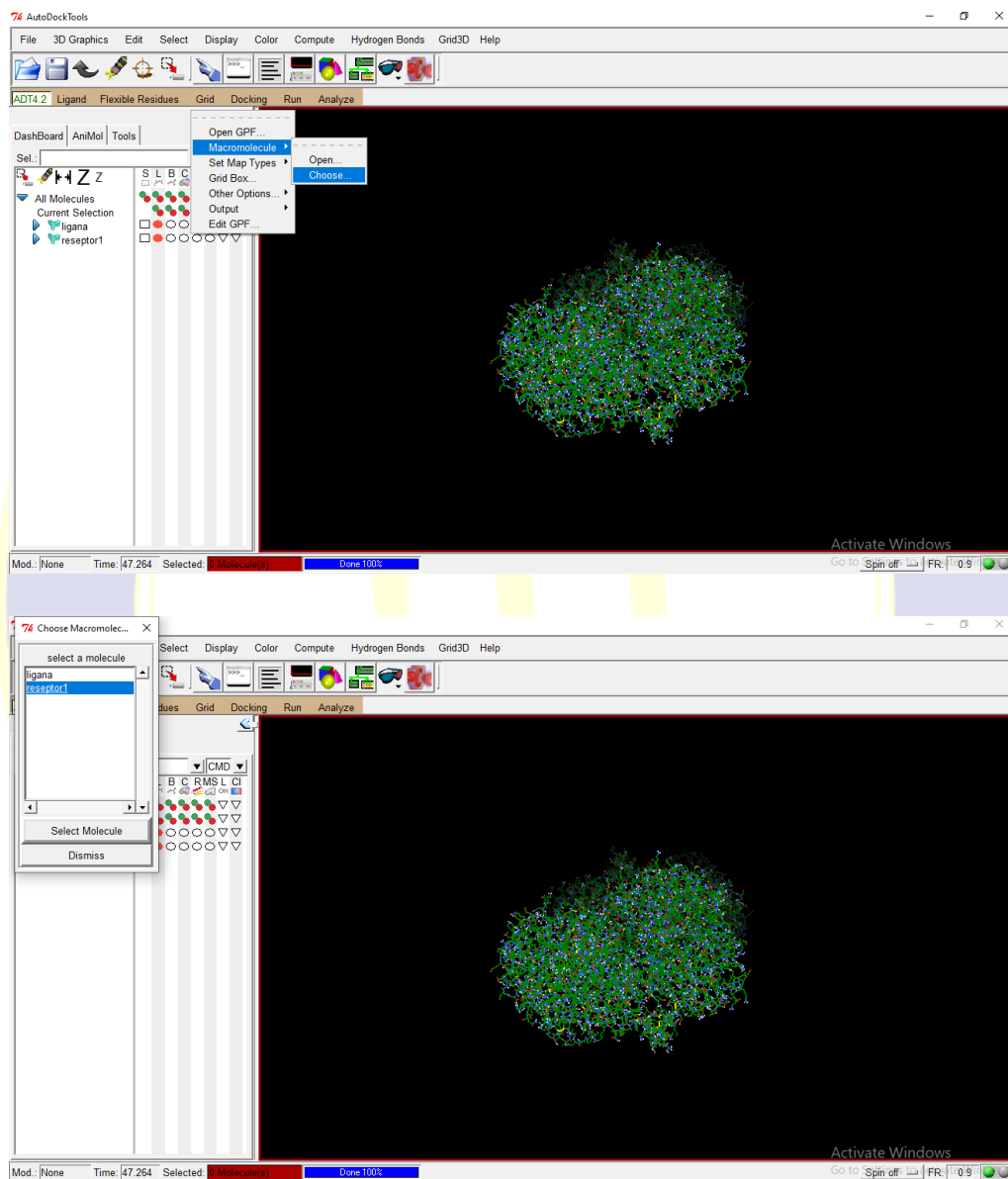
LAMPIRAN 5

LANGKAH-LANGKAH MOLECULAR DOCKING DENGAN APLIKASI *AutoDock Tools*



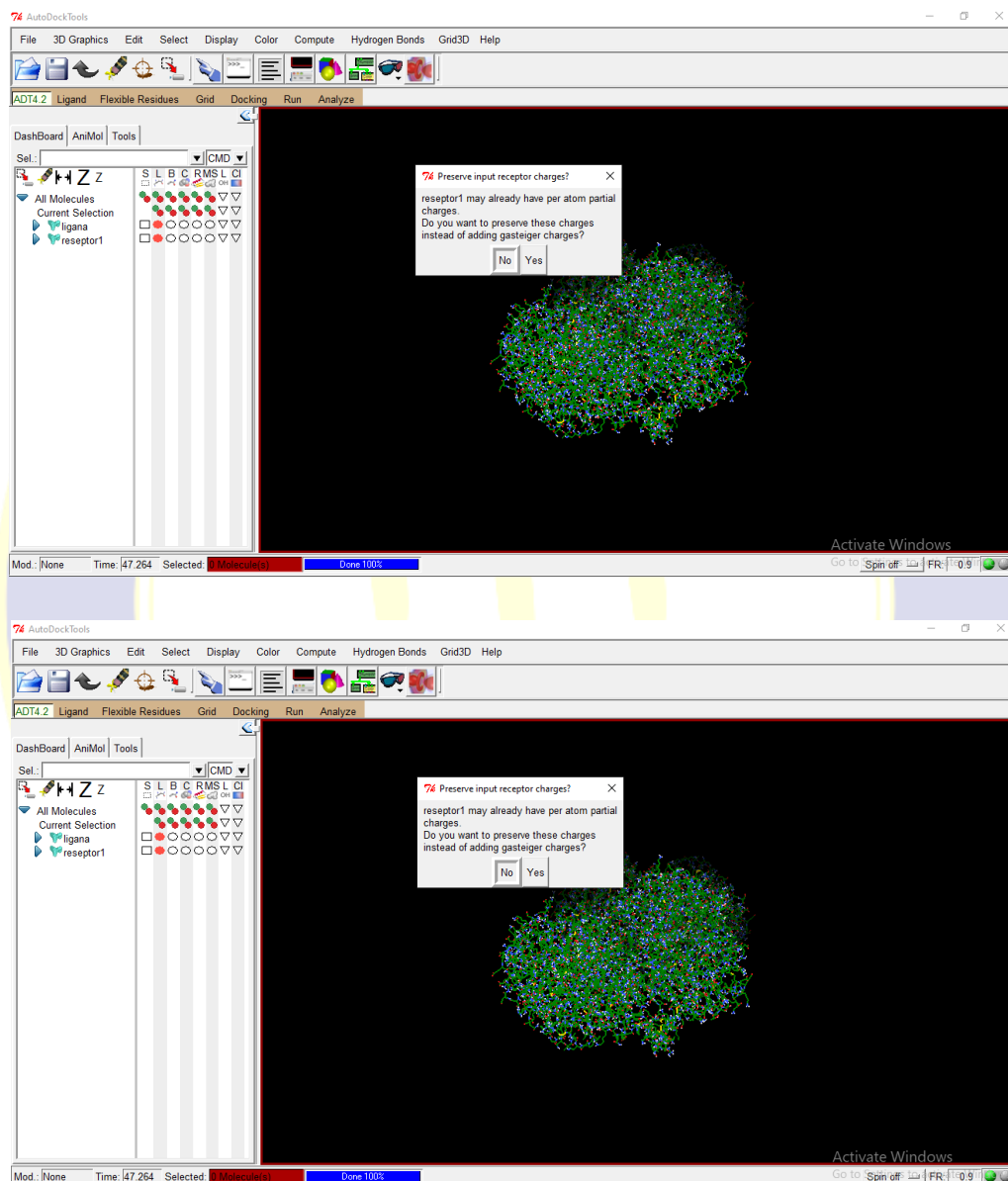
LAMPIRAN 5 (LANJUTAN)

LANGKAH-LANGKAH *MOLECUOLAR DOCKING* DENGAN APLIKASI *AutoDock Tools*



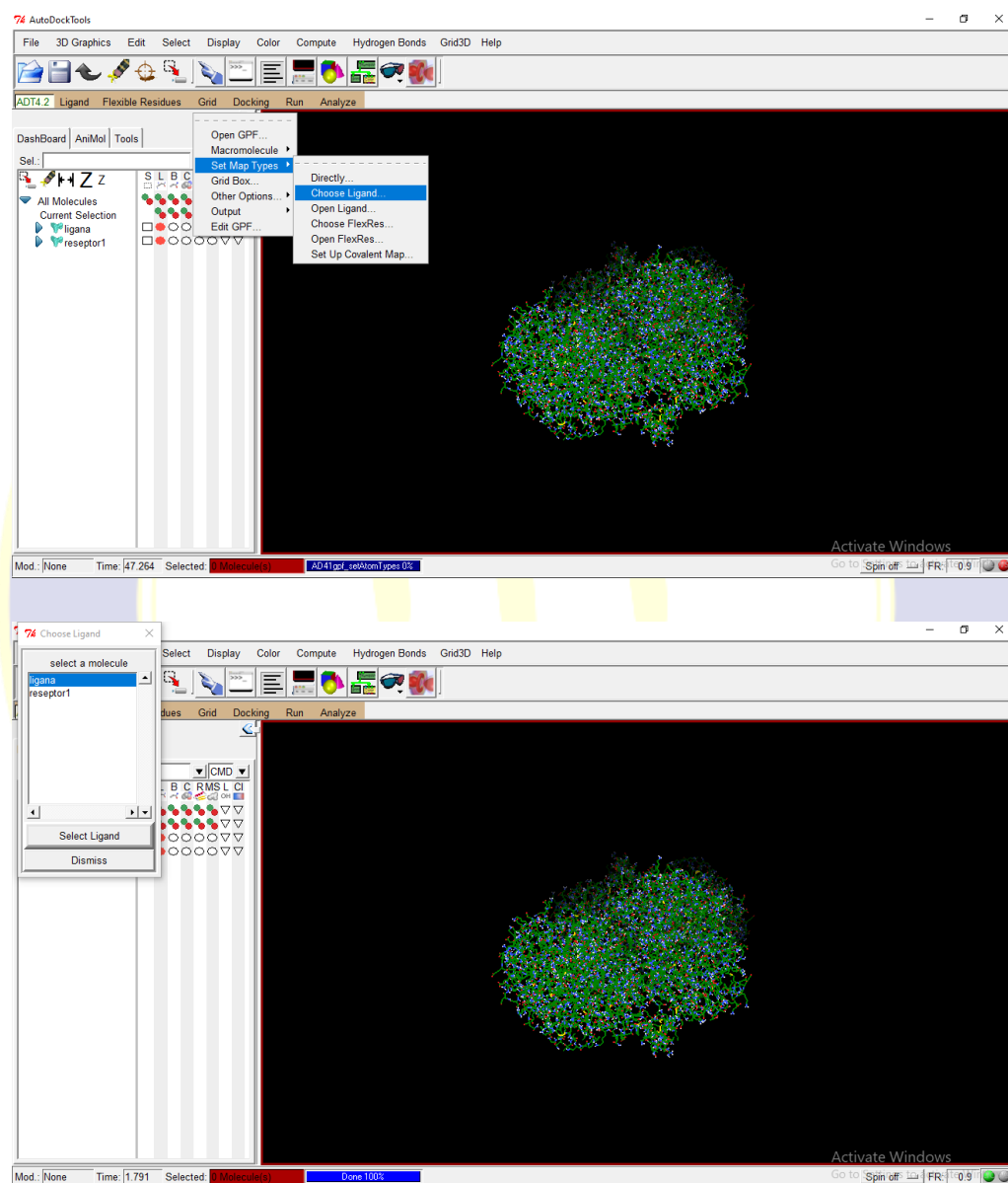
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LANGKAH-LANGKAH MOLECUOLAR DOCKING DENGAN APLIKASI *AutoDock Tools*



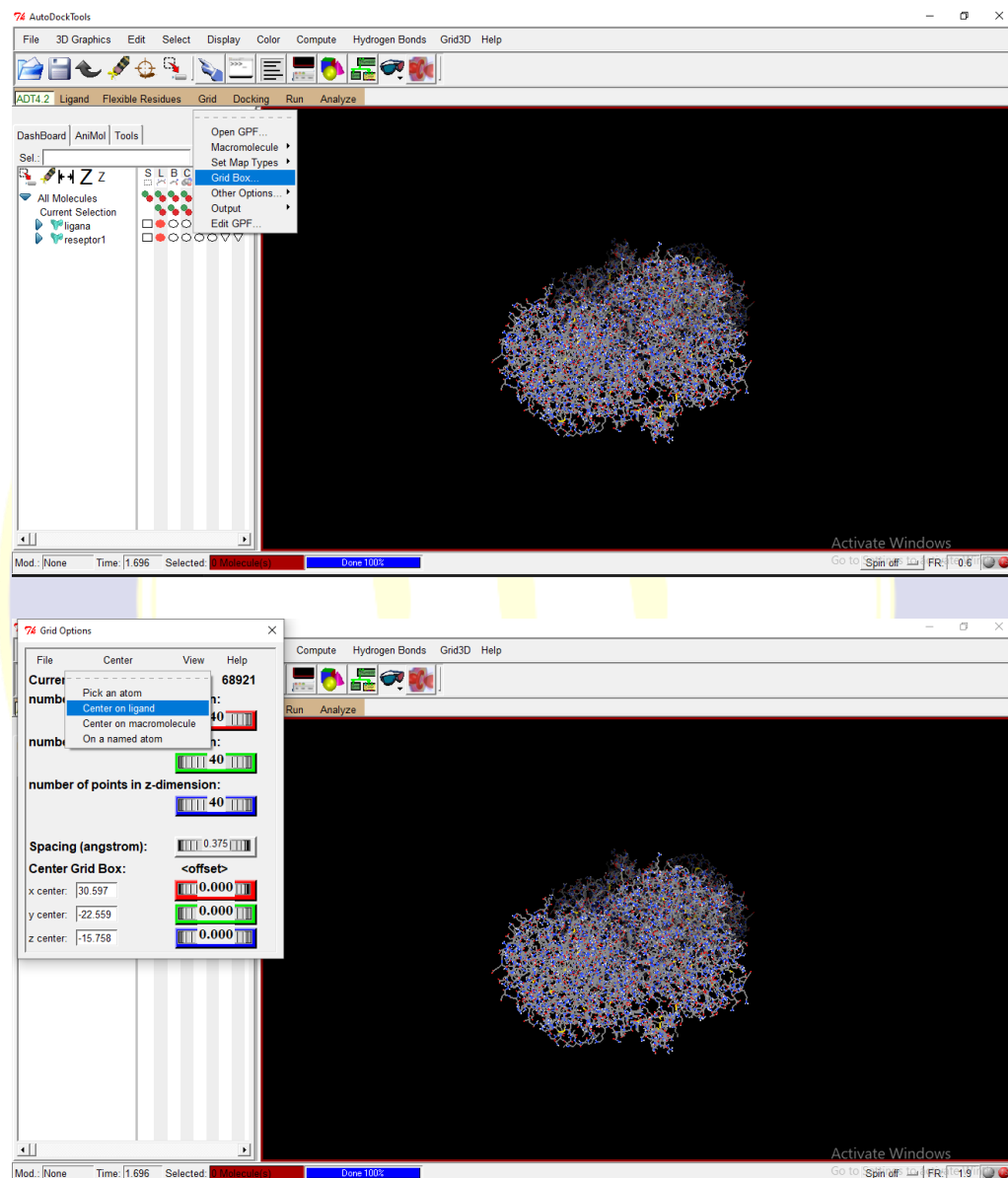
LAMPIRAN 5 (LANJUTAN)

LANGKAH-LANGKAH *MOLECUOLAR DOCKING* DENGAN APLIKASI *AutoDock Tools*



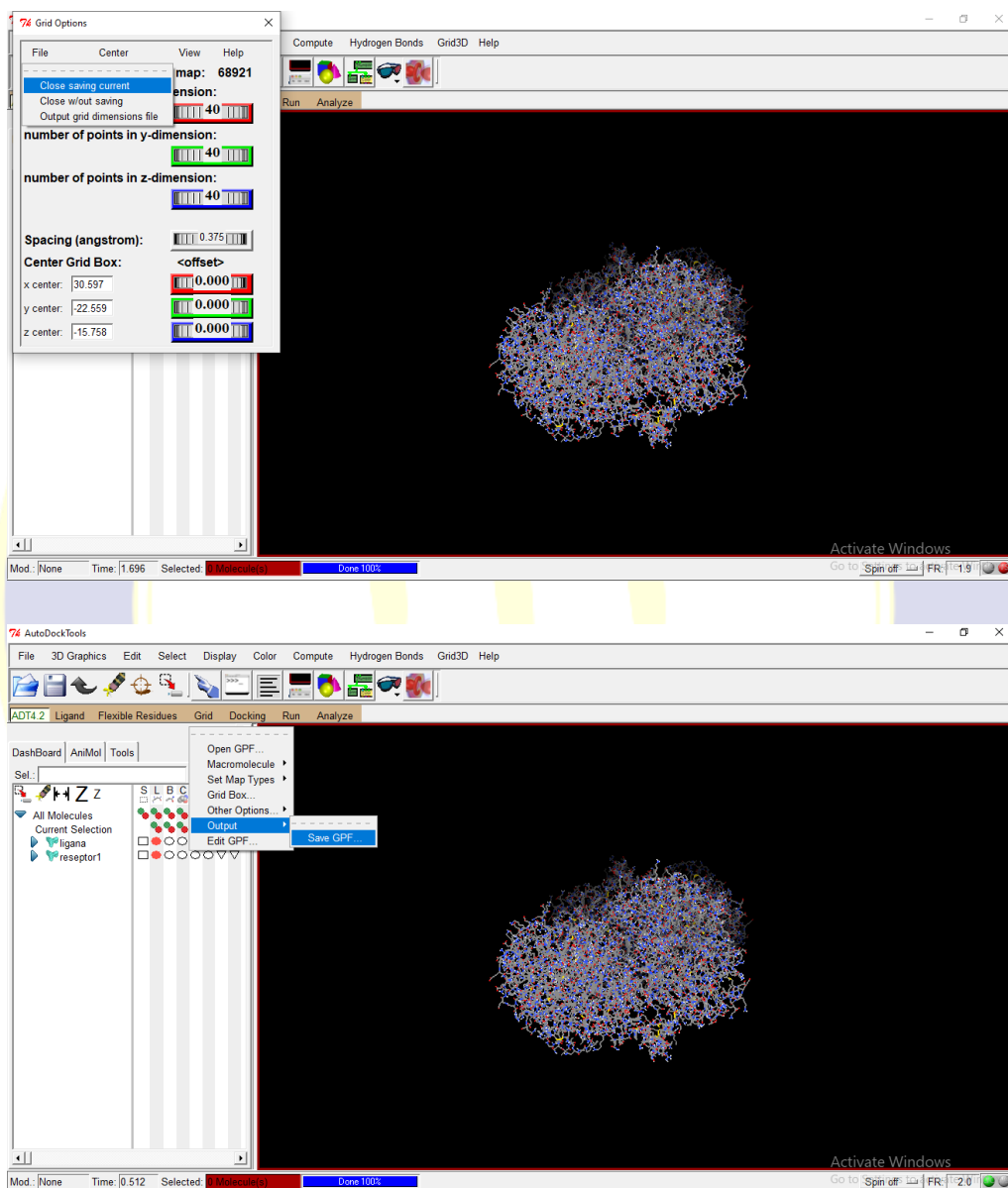
LAMPIRAN 5 (LANJUTAN)

LANGKAH-LANGKAH *MOLECUOLAR DOCKING* DENGAN APLIKASI *AutoDock Tools*



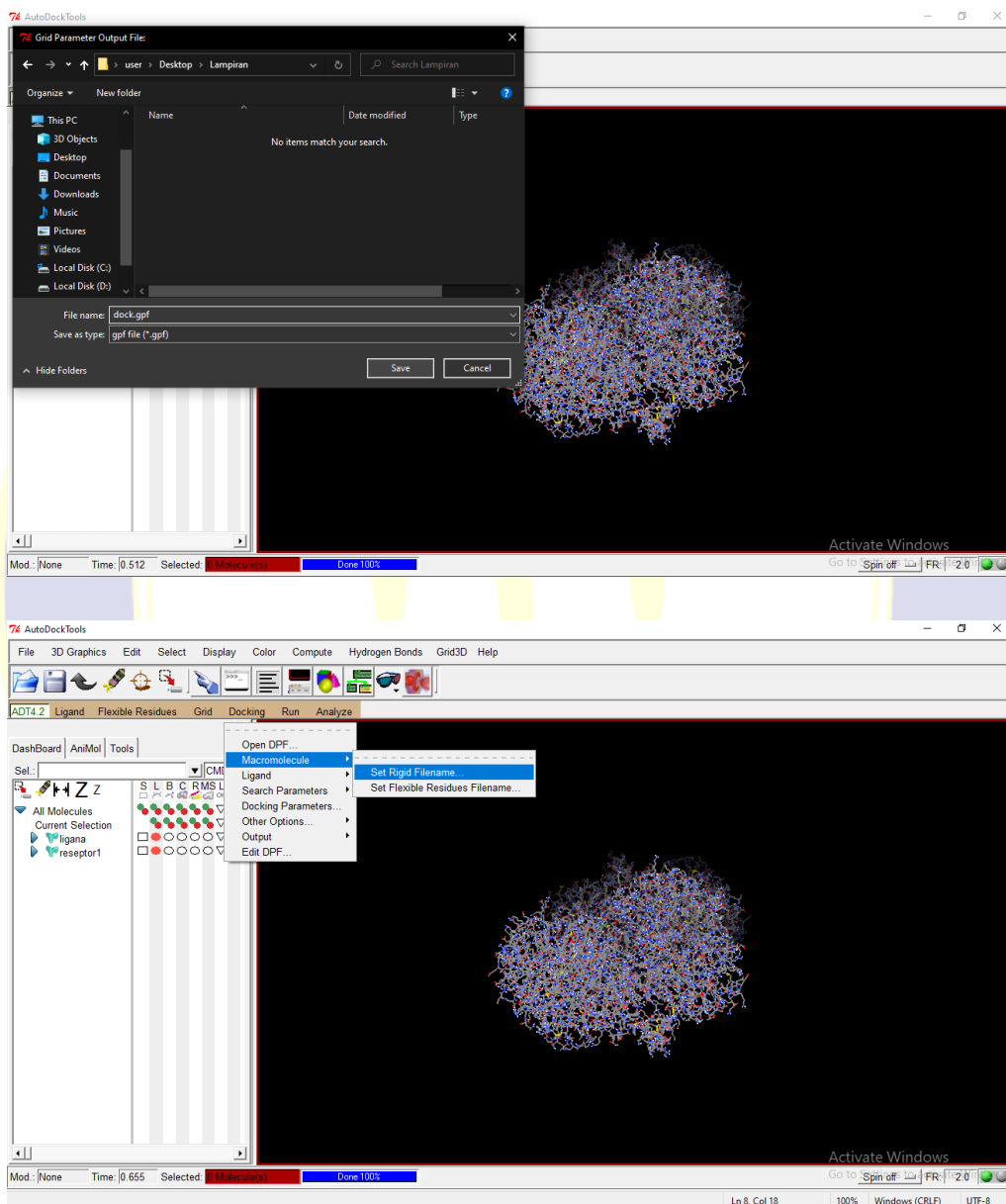
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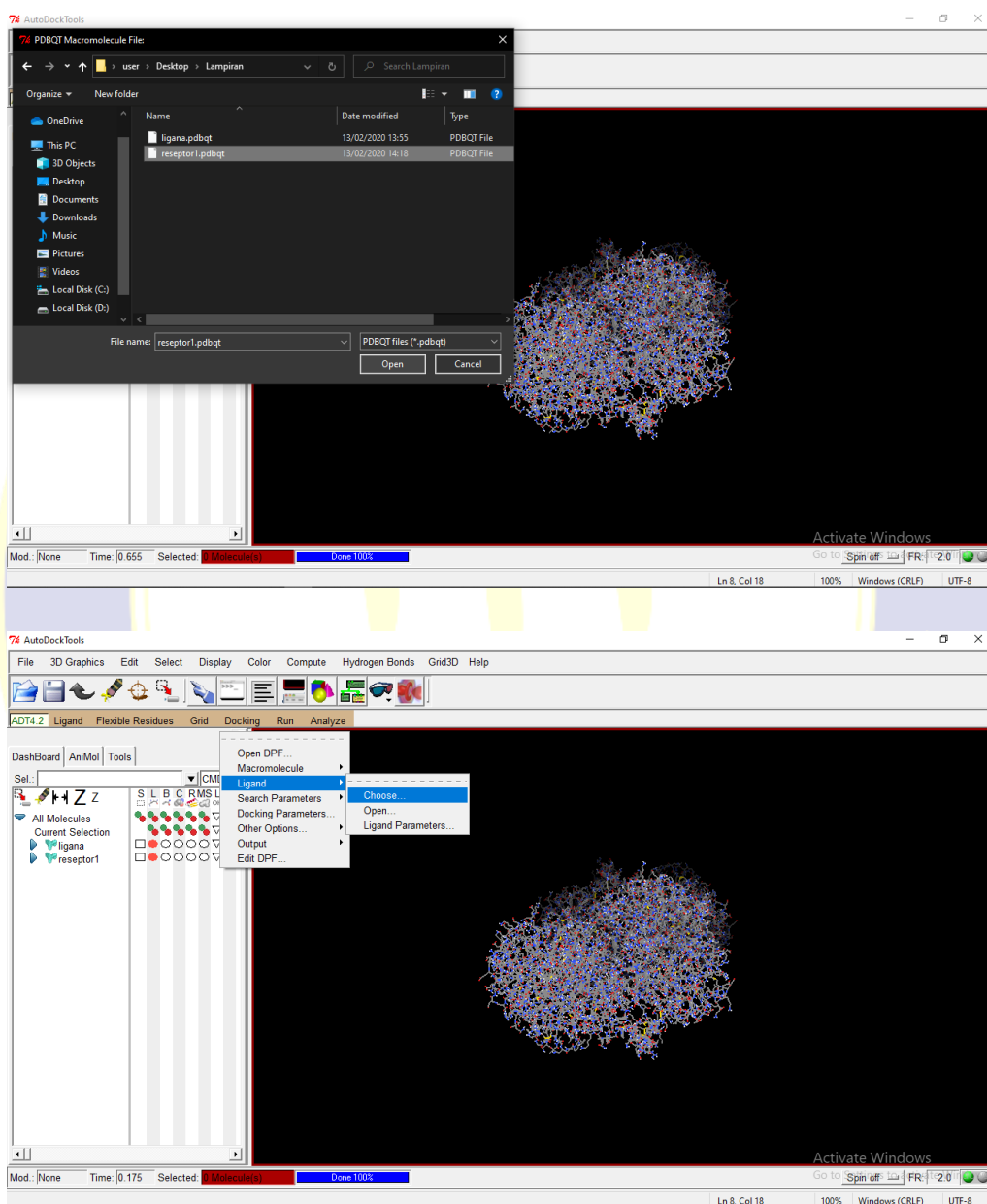
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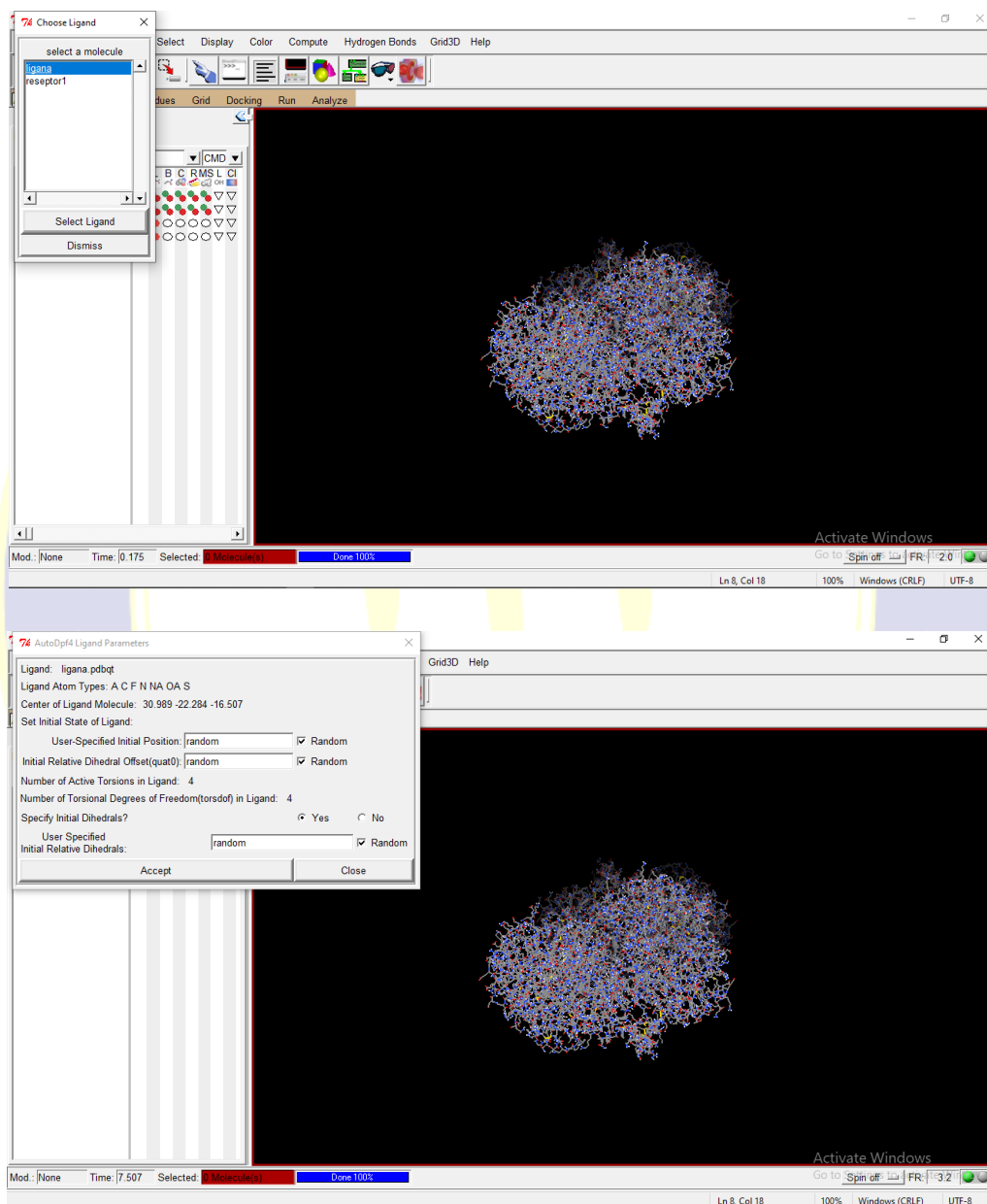
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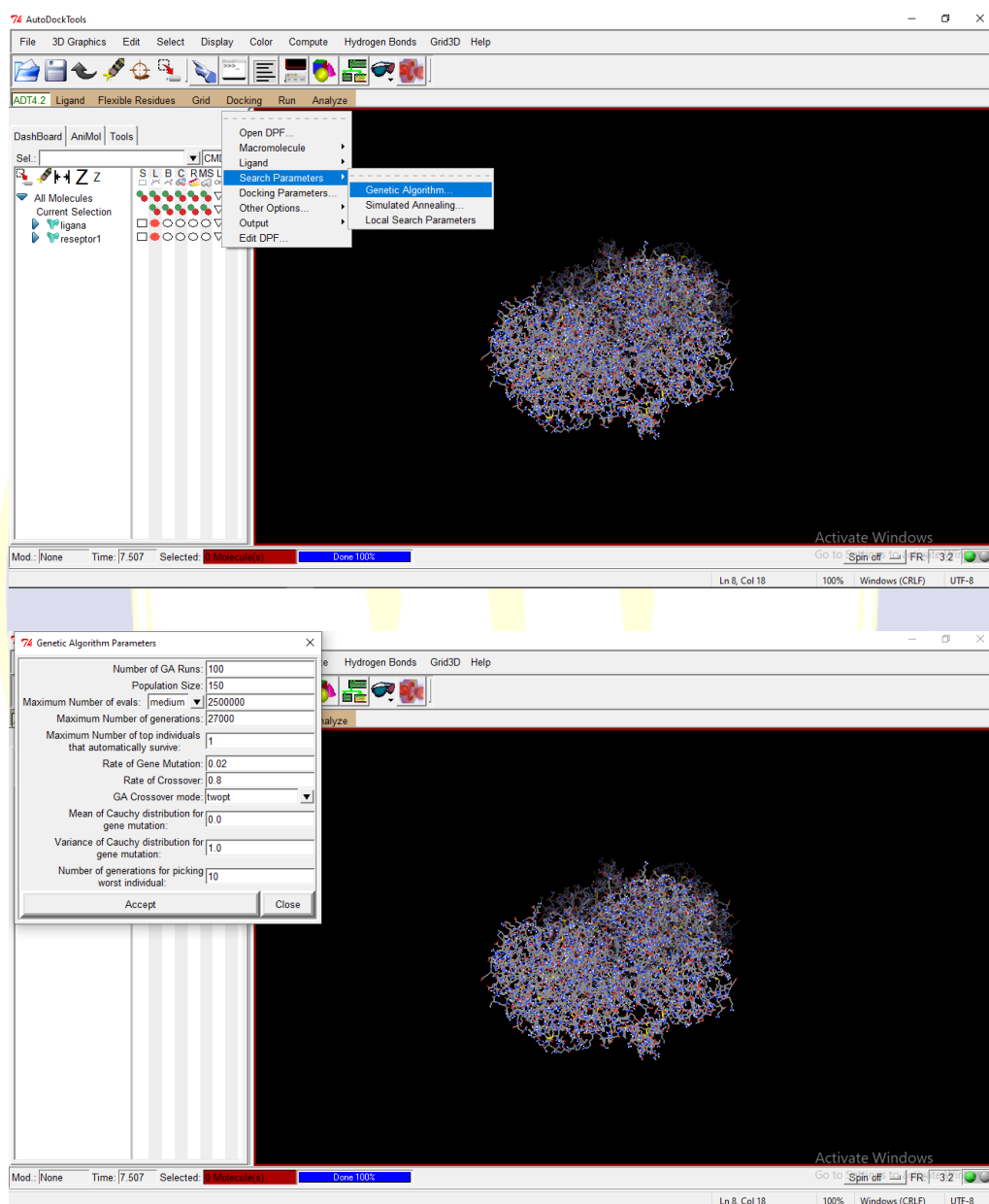
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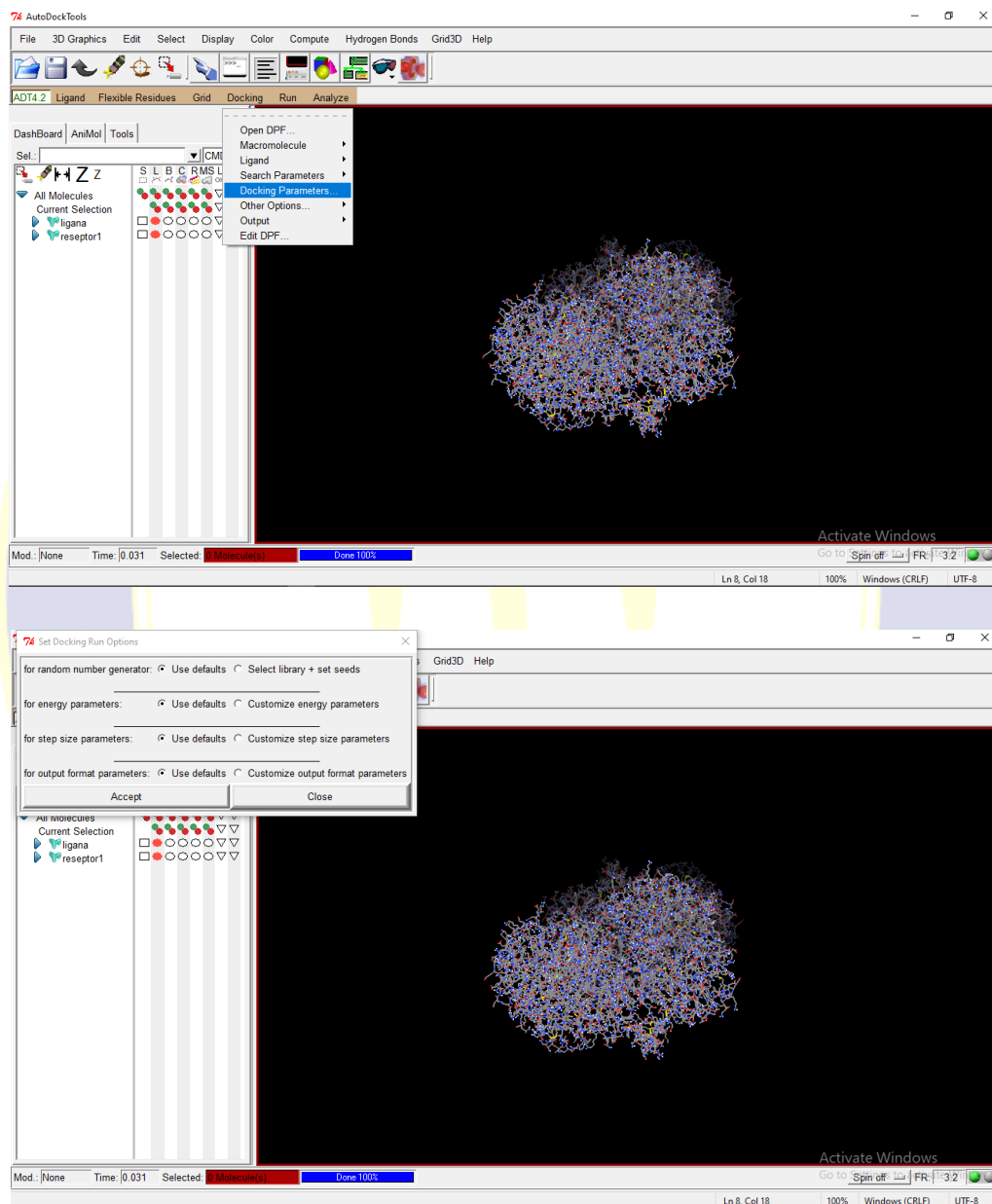
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LANGKAH-LANGKAH *MOLECULAR DOCKING* DENGAN APLIKASI *AutoDock Tools*



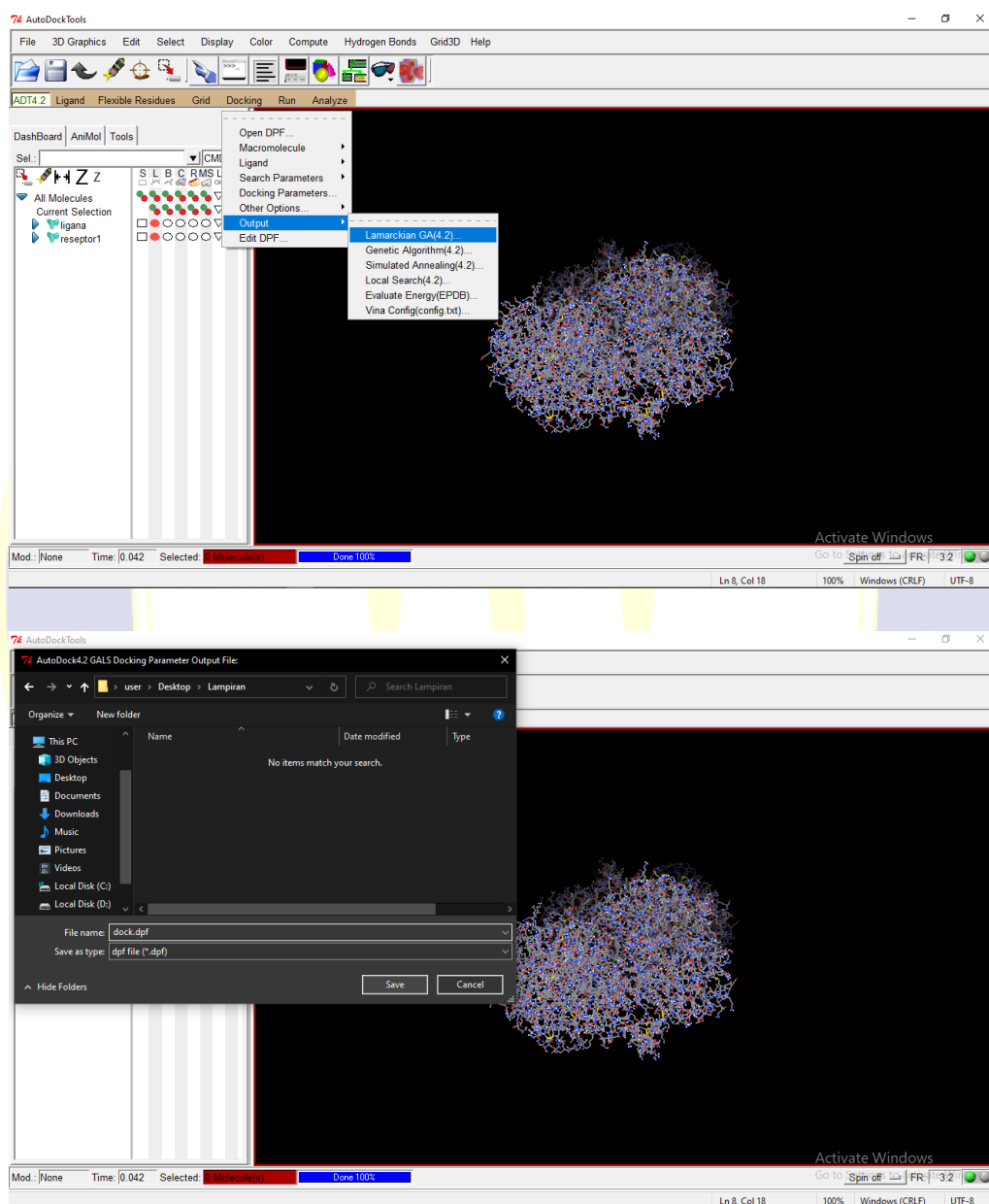
LAMPIRAN 5 (LANJUTAN)

LANGKAH-LANGKAH *MOLECULAR DOCKING* DENGAN APLIKASI *AutoDock Tools*



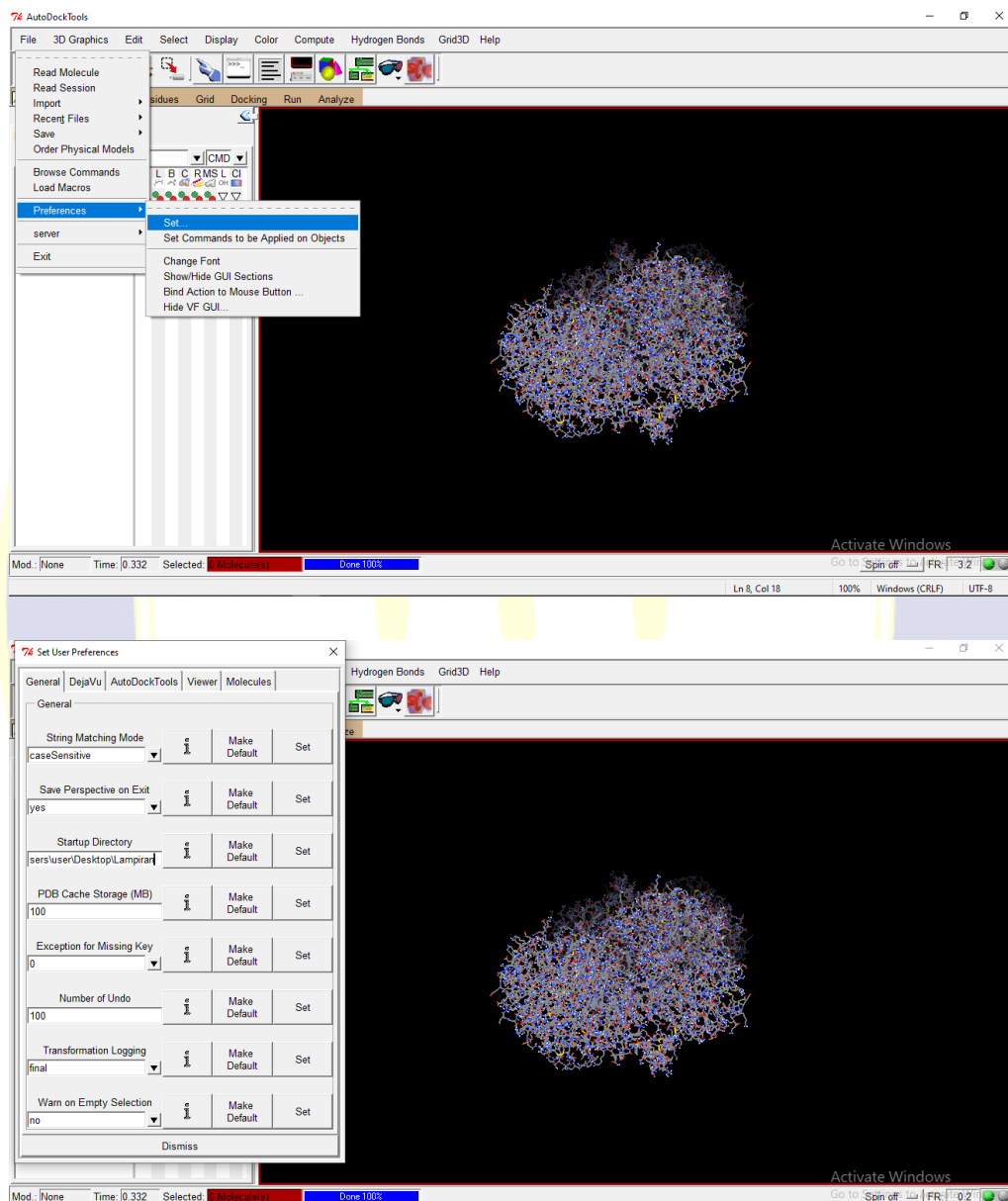
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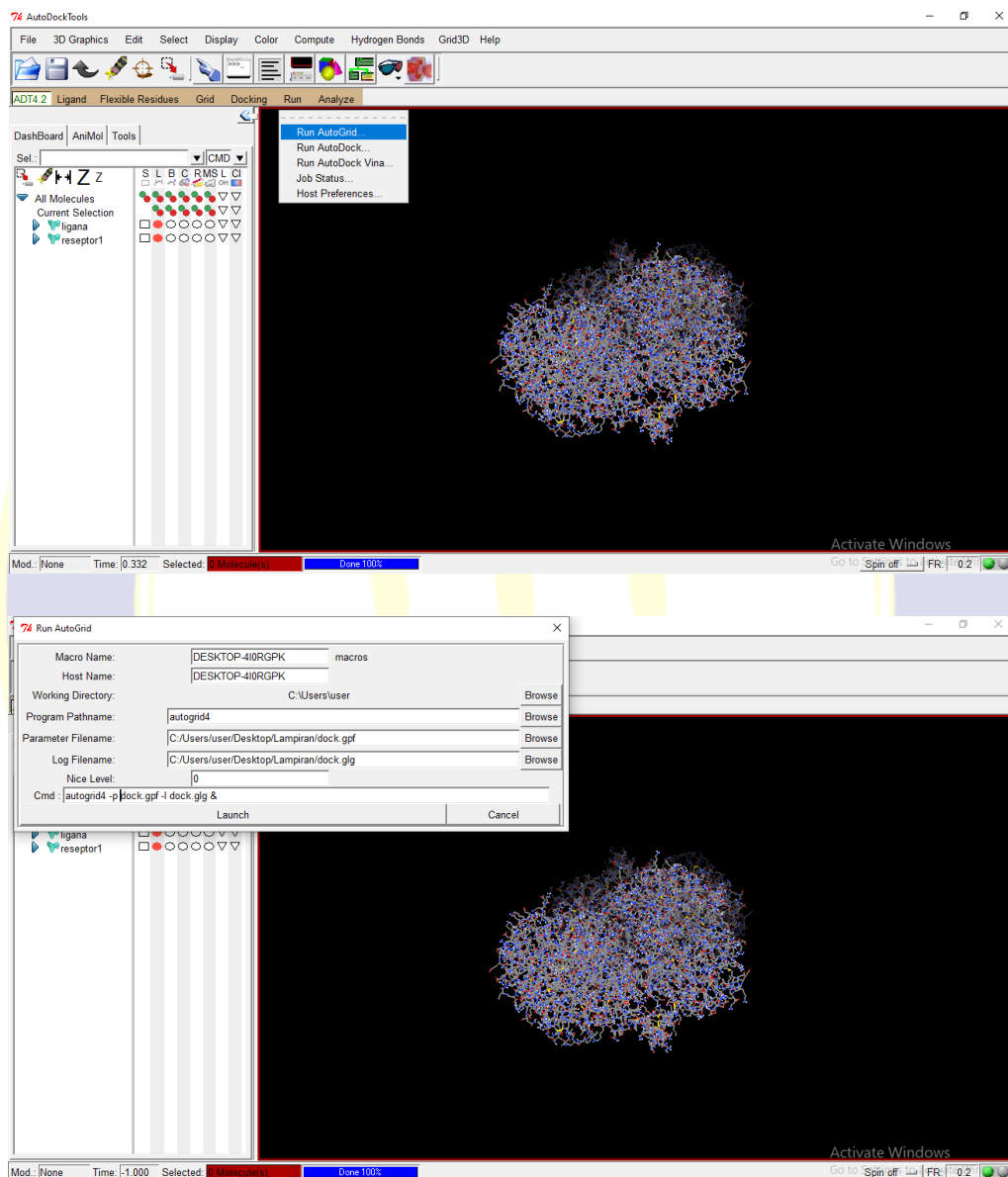
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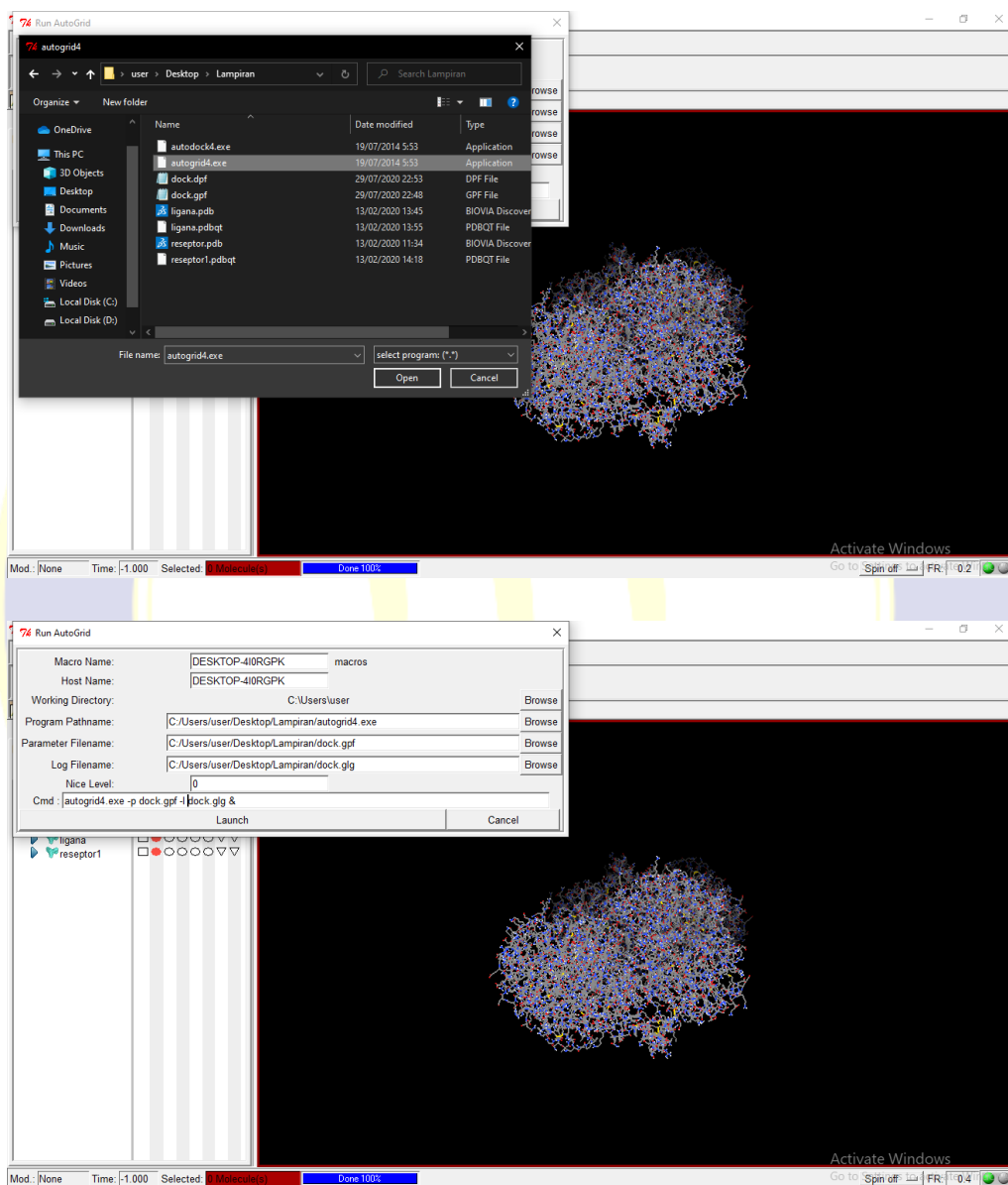
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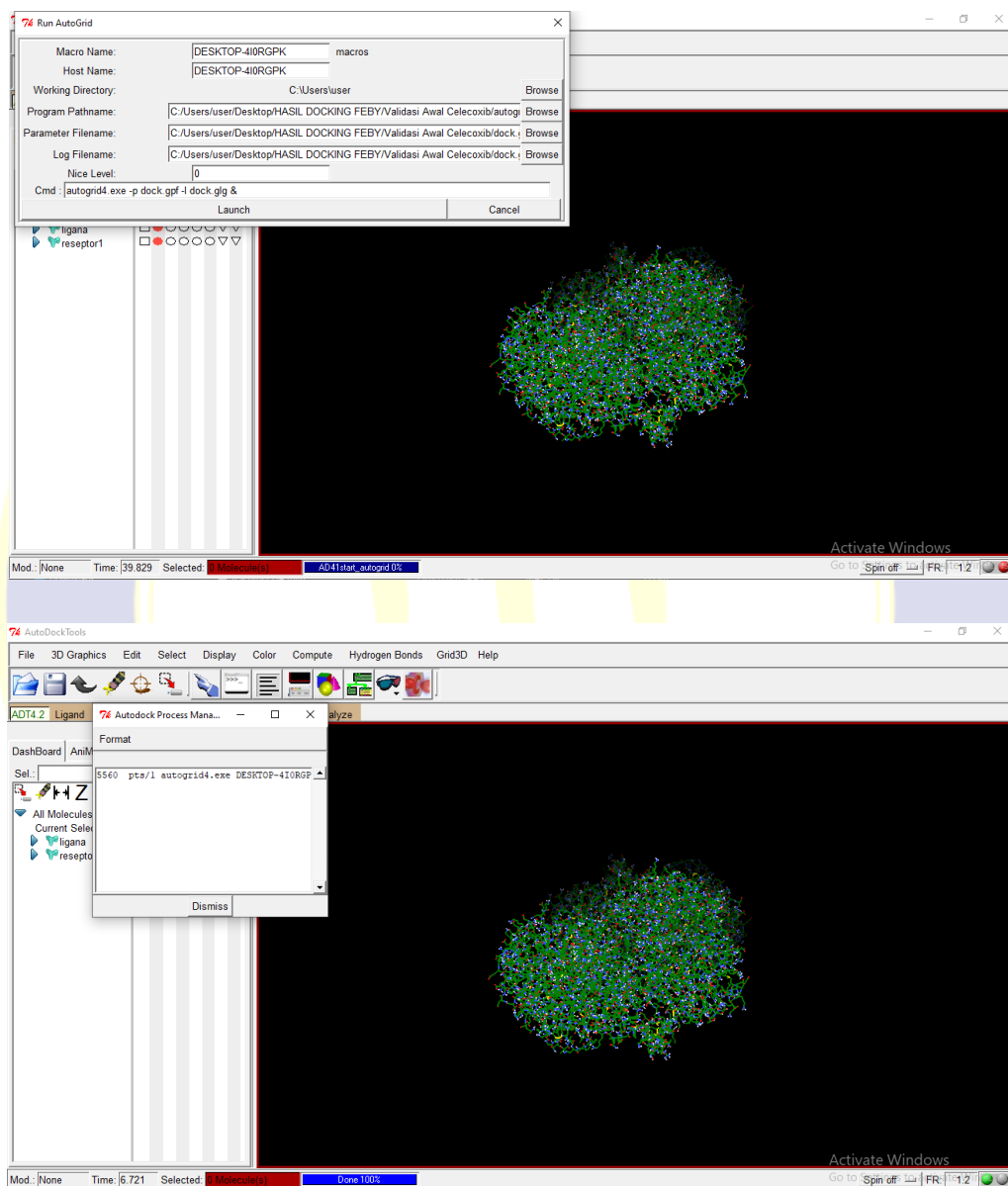
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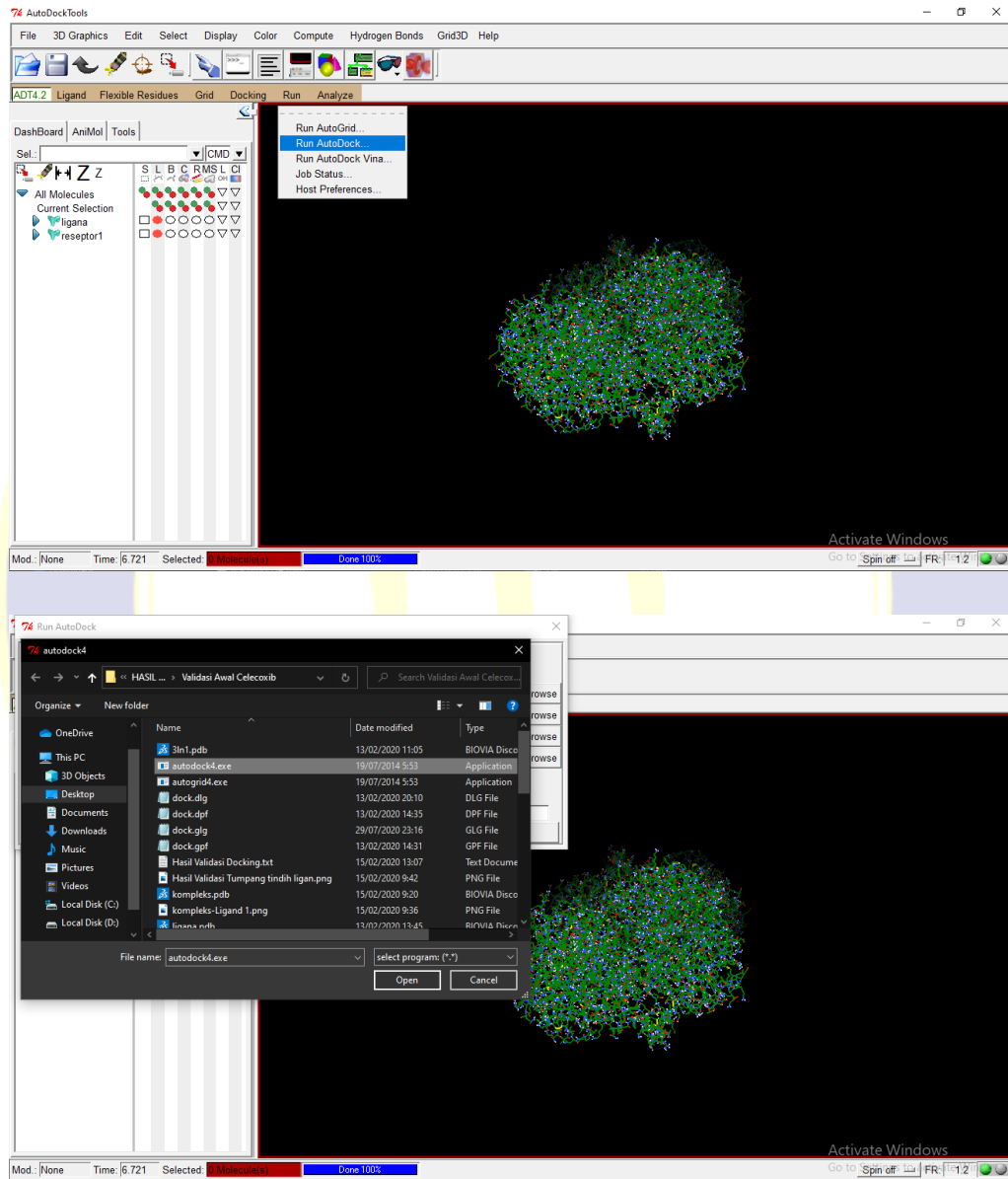
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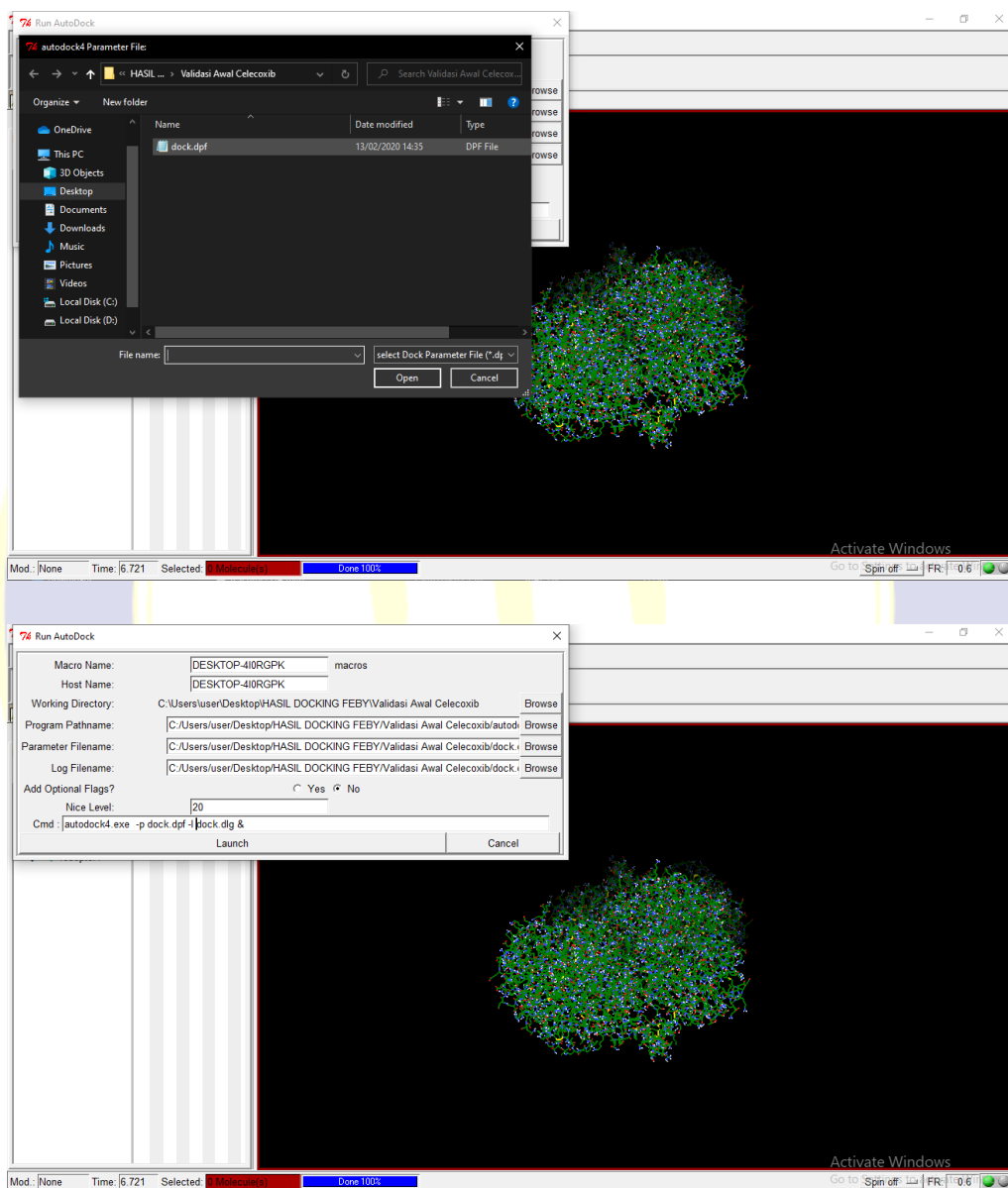
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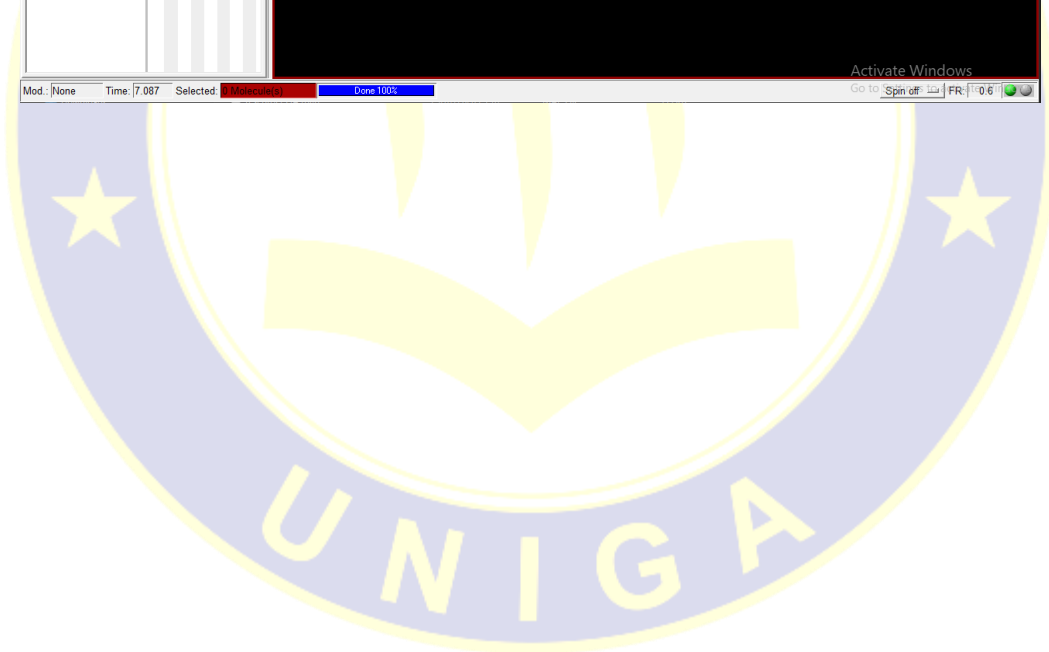
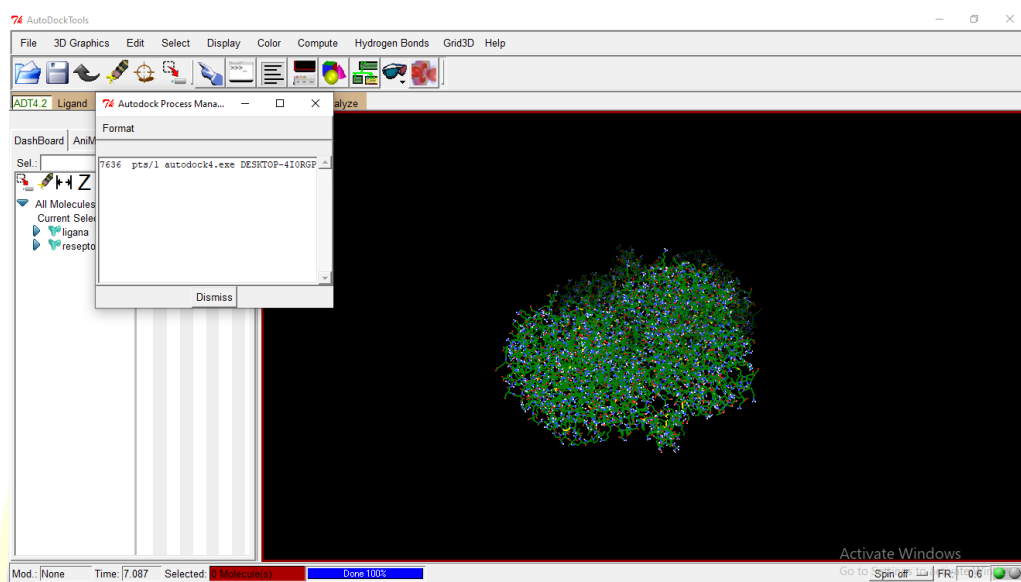
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LANGKAH-LANGKAH *MOLECULAR DOCKING* DENGAN APLIKASI *AutoDock Tools*



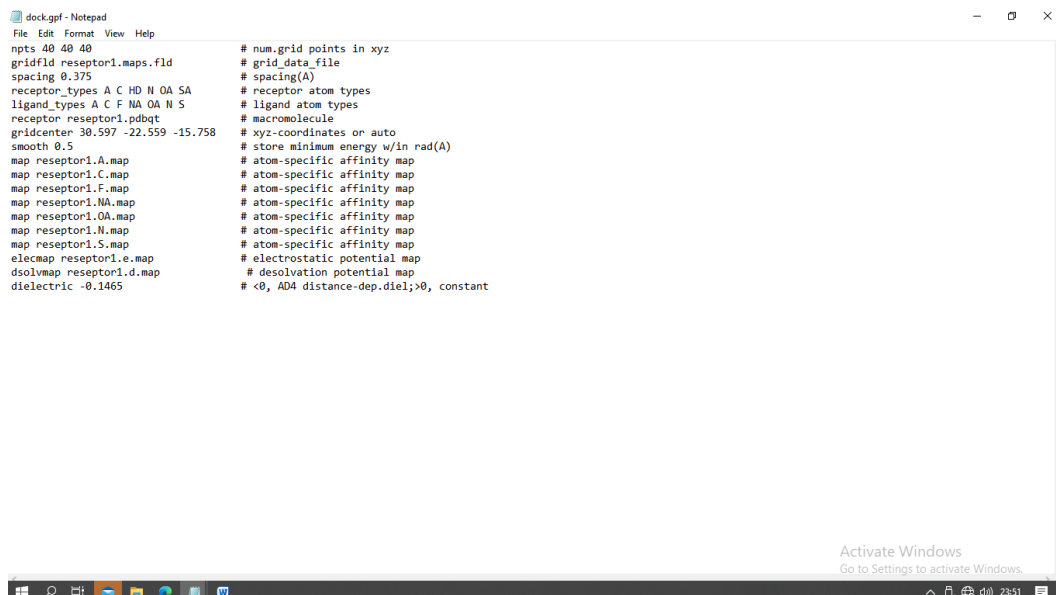
LAMPIRAN 5 (LANJUTAN)

LANGKAH-LANGKAH *MOLECULAR DOCKING* DENGAN APLIKASI *AutoDock Tools*



LAMPIRAN 6

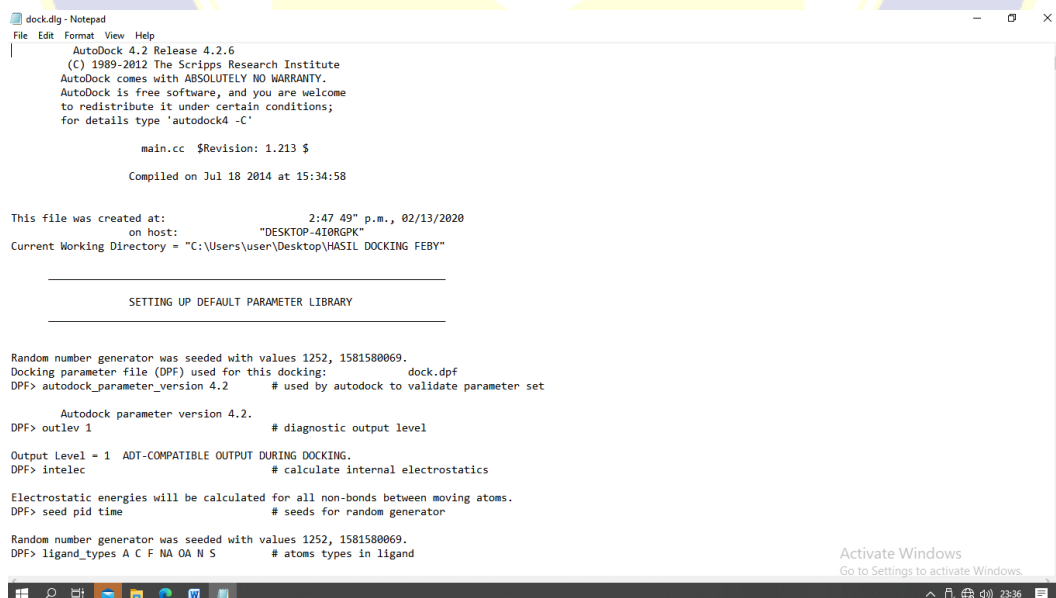
TAMPILAN APLIKASI *Notepad* RESEPTOR *Prostaglandin G/H Synthase 2* ID 3LN1



```

dock.gpf - Notepad
File Edit Format View Help
npts 40 40 40 # num.grid points in xyz
gridfld reseptor1.maps.fld # grid_data_file
spacing 0.375 # spacing(A)
receptor_types A C HD N OA SA # receptor atom types
ligand_types A C F NA OA N S # ligand atom types
receptor reseptor1.pdbqt # macromolecule
gridcenter 30.597 -22.559 -15.758 # xyz-coordinates or auto
smooth 0.5 # store minimum energy w/in rad(A)
map reseptor1.A.map # atom-specific affinity map
map reseptor1.C.map # atom-specific affinity map
map reseptor1.F.map # atom-specific affinity map
map reseptor1.NA.map # atom-specific affinity map
map reseptor1.OA.map # atom-specific affinity map
map reseptor1.N.map # atom-specific affinity map
map reseptor1.S.map # atom-specific affinity map
elecmap reseptor1.e.map # electrostatic potential map
dsolvmap reseptor1.d.map # desolvation potential map
dielectric -0.1465 # <0, AD4 distance-dep.diel;>0, constant
  
```

Gambar VII.3 Tampilan Aplikasi *Notepad* (dock.gpf) Ukuran *Gridbox* Reseptor *Prostaglandin G/H Synthase 2* ID 3LN1 Hasil Validasi



```

dock.dlg - Notepad
File Edit Format View Help
|
| AutoDock 4.2 Release 4.2.6
| (C) 1999-2012 The Scripps Research Institute
| AutoDock comes with ABSOLUTELY NO WARRANTY.
| AutoDock is free software, and you are welcome
| to redistribute it under certain conditions;
| for details type 'autodock4 -c'
|
| main.cc $Revision: 1.213 $
|
| Compiled on Jul 18 2014 at 15:34:58
|
| This file was created at: 2:47 49" p.m., 02/13/2020
| on host: "DESKTOP-410RGPK"
| Current Working Directory = "C:\Users\user\Desktop\HASIL DOCKING FEBY"
|
|-----
| SETTING UP DEFAULT PARAMETER LIBRARY
|-----
|
| Random number generator was seeded with values 1252, 1581580069.
| Docking parameter file (DPF) used for this docking: dock.dpf
| DPF> autodock_parameter_version 4.2 # used by autodock to validate parameter set
|
| Autodock parameter version 4.2.
| DPF> outlev 1 # diagnostic output level
|
| Output Level = 1 ADT-COMPATIBLE OUTPUT DURING DOCKING.
| DPF> intelc # calculate internal electrostatics
|
| Electrostatic energies will be calculated for all non-bonds between moving atoms.
| DPF> seed pid time # seeds for random generator
|
| Random number generator was seeded with values 1252, 1581580069.
| DPF> ligand_types A C F NA OA N S # atoms types in ligand
  
```

Gambar VII.4 Tampilan Aplikasi *Notepad* (dock.dlg) Hasil Validasi *Molecular Docking* Reseptor *Prostaglandin G/H Synthase 2* ID 3LN1

LAMPIRAN 6 (LANJUTAN)

TAMPILAN APLIKASI *Notepad* RESEPTOR *Prostaglandin G/H Synthase 2* ID 3LN1

```

dock.dlg - Notepad
File Edit Format View Help

CLUSTER ANALYSIS OF CONFORMATIONS

Number of conformations = 100

RMSD cluster analysis will be performed using the ligand atoms only (26 / 26 total atoms).

Outputting structurally similar clusters, ranked in order of increasing energy.

-----

Number of distinct conformational clusters found = 1, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

-----
Clus-   Lowest   Run   Mean   Num   Histogram
-ter   Binding   |     | Mean   in   |
Rank   Energy   |     | Bind- | Clus | 5   10  15  20  25  30  35
      |         |     | ding |     | :   :   :   :   :   :   :
  1   | -11.11 | 78 | -10.92 | 100 | #####
      |         |     |         |     |
-----

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

RMSD TABLE

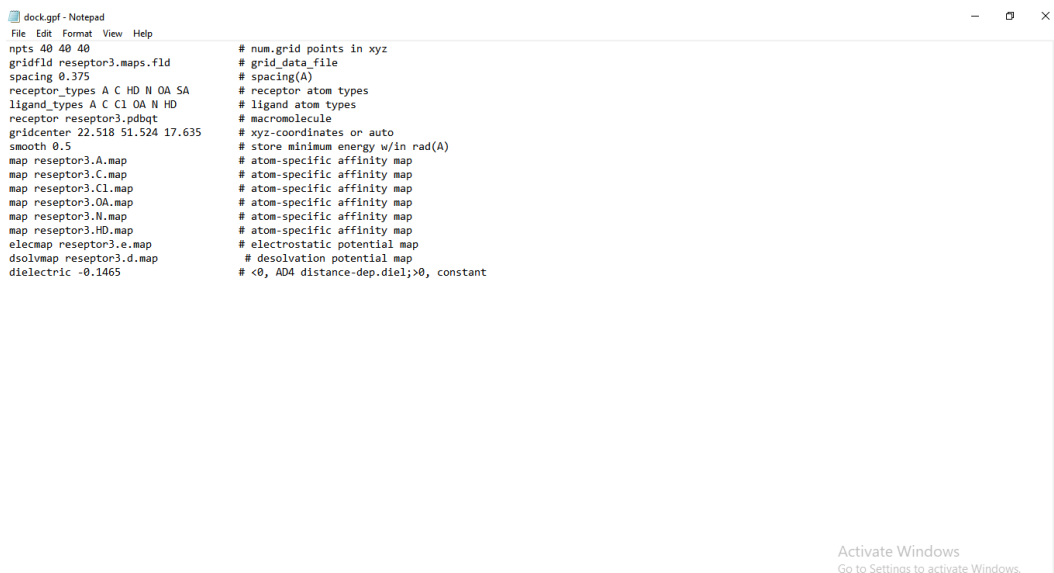
-----

```

Gambar VII.5 Tampilan *Notepad* (dock.dlg) Nilai Cluster Rank, ΔG dan Histogram Hasil Validasi *Molecular Docking* Reseptor *Prostaglandin G/H Synthase 2* ID 3LN1

LAMPIRAN 7

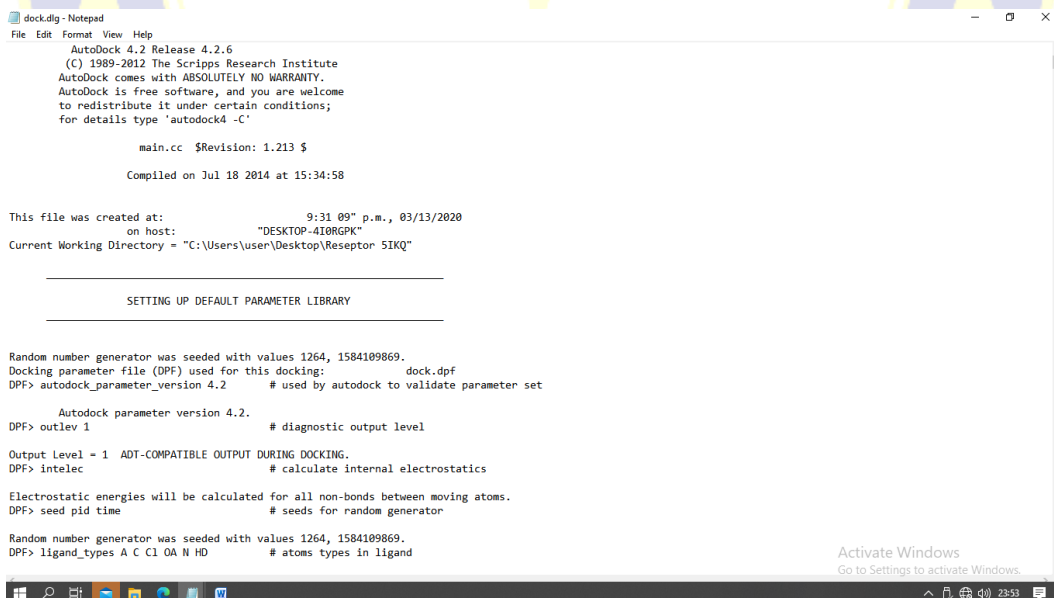
TAMPILAN APLIKASI *Notepad* RESEPTOR *Prostaglandin G/H Synthase 2* ID 5IKQ



```

dock.gpf - Notepad
File Edit Format View Help
npts 40 40 40 # num.grid points in xyz
gridfld reseptor3.maps.fld # grid_data_file
spacing 0.375 # spacing(A)
receptor_types A C HD N OA SA # receptor atom types
ligand_types A C Cl OA N HD # ligand atom types
receptor reseptor3.pdbqt # macromolecule
gridcenter 22.518 51.524 17.635 # xyz-coordinates or auto
smooth 0.5 # store minimum energy w/in rad(A)
map reseptor3.A.map # atom-specific affinity map
map reseptor3.C.map # atom-specific affinity map
map reseptor3.Cl.map # atom-specific affinity map
map reseptor3.OA.map # atom-specific affinity map
map reseptor3.N.map # atom-specific affinity map
map reseptor3.HD.map # atom-specific affinity map
elecmap reseptor3.e.map # electrostatic potential map
dsolvmap reseptor3.d.map # desolvation potential map
dielectric -0.1465 # <0, AD4 distance-dep.diel;>0, constant
  
```

Gambar VII.6 Tampilan Aplikasi *Notepad* (dock.gpf) Ukuran *Gridbox* Reseptor *Prostaglandin G/H Synthase 2* ID 5IKQ Hasil Validasi



```

dock.dlg - Notepad
File Edit Format View Help
AutoDock 4.2 Release 4.2.6
(C) 1999-2012 The Scripps Research Institute
AutoDock comes with ABSOLUTELY NO WARRANTY.
AutoDock is free software, and you are welcome
to redistribute it under certain conditions;
for details type 'autodock4 -c'

main.cc $Revision: 1.213 $

Compiled on Jul 18 2014 at 15:34:58

This file was created at:          9:31 09" p.m., 03/13/2020
on host:                          "DESKTOP-410RGPK"
Current Working Directory = "C:\Users\user\Desktop\Reseptor 5IKQ"

-----
SETTING UP DEFAULT PARAMETER LIBRARY
-----

Random number generator was seeded with values 1264, 1584109869.
Docking parameter file (DPF) used for this docking: dock.dpf
DPF> autodock_parameter_version 4.2 # used by autodock to validate parameter set

Autodock parameter version 4.2.
DPF> outlev 1 # diagnostic output level

Output Level = 1 ADT-COMPATIBLE OUTPUT DURING DOCKING.
DPF> intelc # calculate internal electrostatics

Electrostatic energies will be calculated for all non-bonds between moving atoms.
DPF> seed pid time # seeds for random generator

Random number generator was seeded with values 1264, 1584109869.
DPF> ligand_types A C Cl OA N HD # atoms types in ligand
  
```

Gambar VII.7 Tampilan Aplikasi *Notepad* (dock.dlg) Hasil Validasi *Molecular Docking* Reseptor *Prostaglandin G/H Synthase 2* ID 5IKQ

LAMPIRAN 7 (LANJUTAN)

TAMPILAN APLIKASI *Notepad* RESEPTOR *Prostaglandin G/H Synthase 2* ID 5IKQ

```

dock.dlg - Notepad
File Edit Format View Help
Outputting structurally similar clusters, ranked in order of increasing energy.

Number of distinct conformational clusters found = 1, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank | Lowest Binding Energy | Run | Mean Binding Energy | Num in Clus | Histogram
-----|-----|-----|-----|-----|-----
1 | -8.36 | 18 | -8.34 | 100 | #####

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

RMSD TABLE

Rank | Sub-Rank | Run | Binding Energy | Cluster RMSD | Reference RMSD | Grep Pattern
-----|-----|-----|-----|-----|-----|-----
1 | 1 | 18 | -8.36 | 0.00 | 0.63 | RANKING
1 | 2 | 19 | -8.36 | 0.02 | 0.62 | RANKING
1 | 3 | 50 | -8.36 | 0.06 | 0.60 | RANKING
1 | 4 | 81 | -8.35 | 0.12 | 0.59 | RANKING
1 | 5 | 21 | -8.35 | 0.05 | 0.60 | RANKING
1 | 6 | 33 | -8.35 | 0.15 | 0.52 | RANKING

```

Gambar VII.8 Tampilan *Notepad* (dock.dlg) Nilai Cluster Rank, ΔG dan Histogram Hasil Validasi *Molecular Docking* Reseptor *Prostaglandin G/H Synthase 2* ID 5IKQ


```

dock.dlg - Notepad
File Edit Format View Help

CLUSTER ANALYSIS OF CONFORMATIONS

Number of conformations = 100
RMSD cluster analysis will be performed using the ligand atoms only (18 / 18 total atoms).
Outputting structurally similar clusters, ranked in order of increasing energy.

Number of distinct conformational clusters found = 1, out of 100 runs,
Using an rmsd-tolerance of 2.0 A

CLUSTERING HISTOGRAM

Clus-ter Rank | Lowest Binding Energy | Run | Mean Binding Energy | Num in Clus | Histogram
-----|-----|-----|-----|-----|-----
1 | -8.76 | 72 | -8.73 | 100 | #####

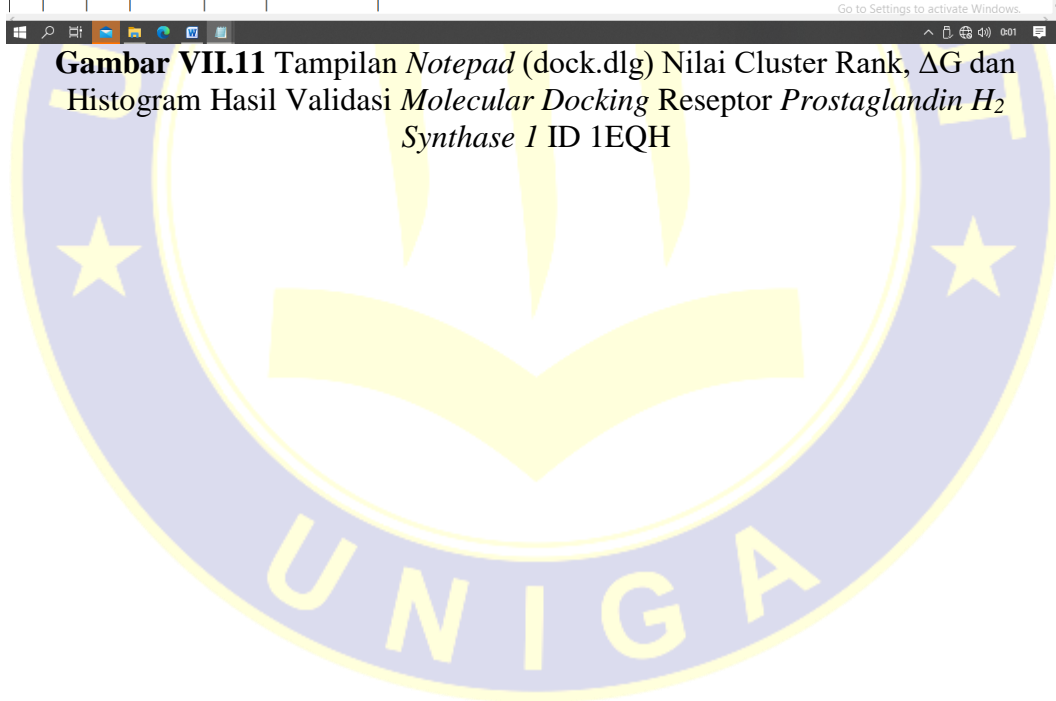
```

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

RMSD TABLE

Activate Windows
Go to Settings to activate Windows.

Gambar VII.11 Tampilan *Notepad* (dock.dlg) Nilai Cluster Rank, ΔG dan Histogram Hasil Validasi *Molecular Docking* Reseptor *Prostaglandin H₂ Synthase 1* ID 1EQH



CURRICULUM VITAE



Personal Detail

Nama : Pebi Astriani
 Tempat, Tanggal Lahir : Garut, 25 Februari 1998
 Jenis Kelamin : Perempuan
 Sekolah : UNIVERSITAS GARUT
 Program Keahlian : Farmasi
 Agama : Islam
 Status : Belum Menikah
 Tinggi, Berat Badan : 168 cm / 50 kg
 Alamat : Kp. Cinunuk Tengah Rt.
 03 Rw. 07 Desa Wanaraja Kecamatan Wanaraja
 Kab. Garut
 No.Telp / HP : 088806300562
 E-mail : astrianipebi@gmail.com

Pendidikan Formal

- 2016 – 2020 : UNIVERSITAS GARUT
- 2013 – 2016 : SMK YBKP3 GARUT
- 2010 – 2013 : SMPN 1 WANARAJA
- 2004 - 2010 : SDN WANARAJA 3

Pengalaman Praktik Kerja

Tahun 2020 : Apotek Assyfa

Tahun 2015 : Puskesmas DTP Wanaraja

Tahun 2015 : Apotek Sadahurip