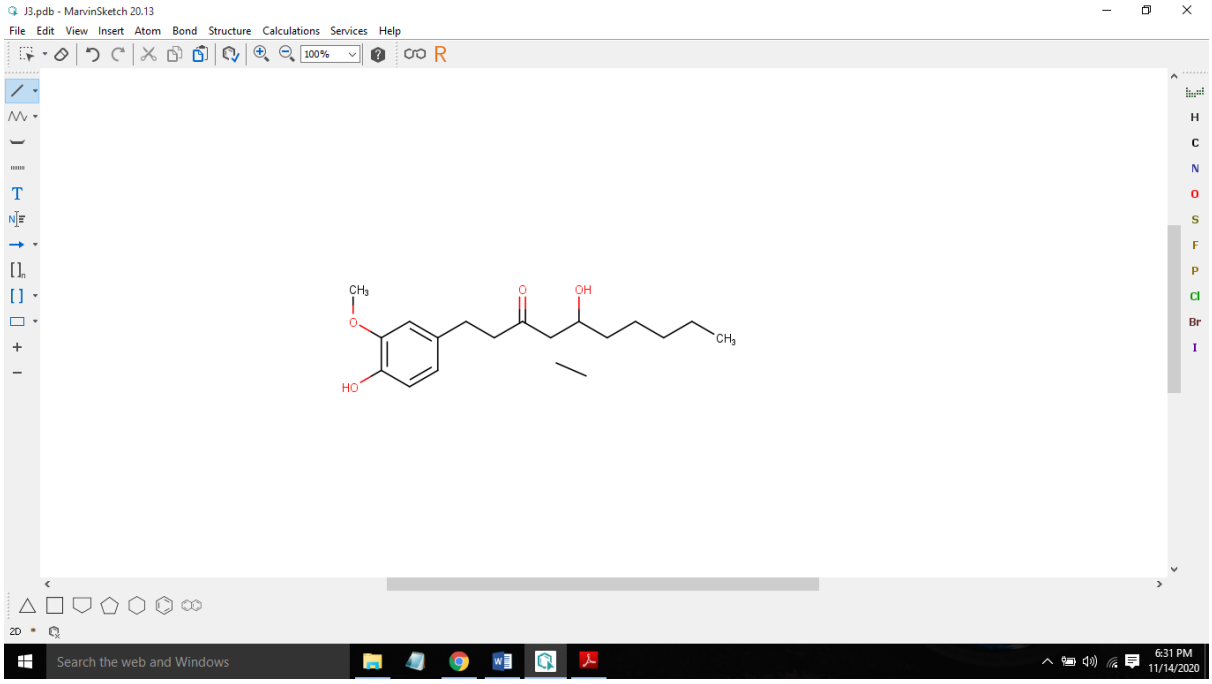
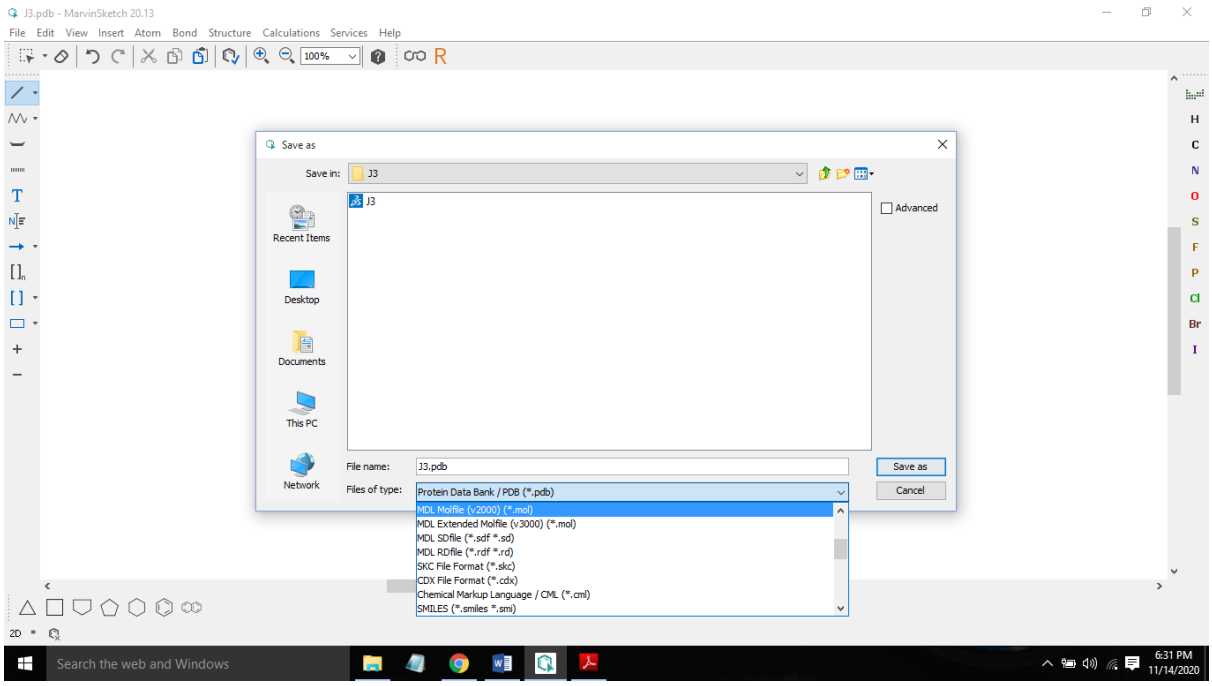
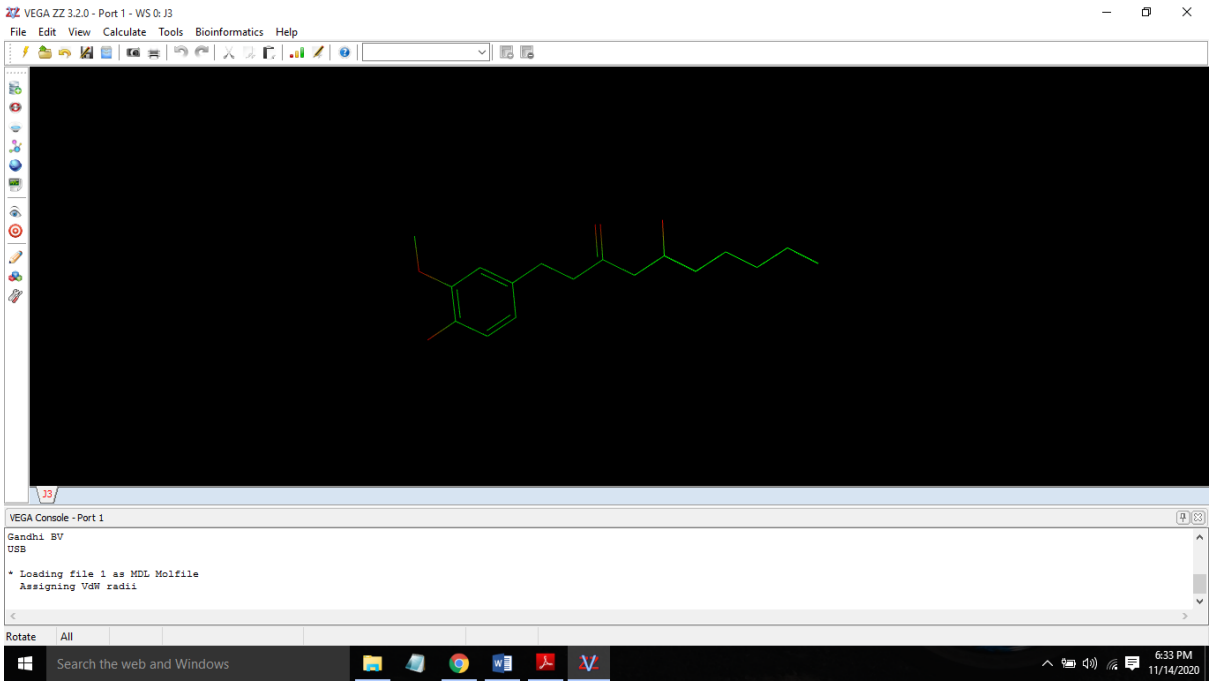
Lampiran

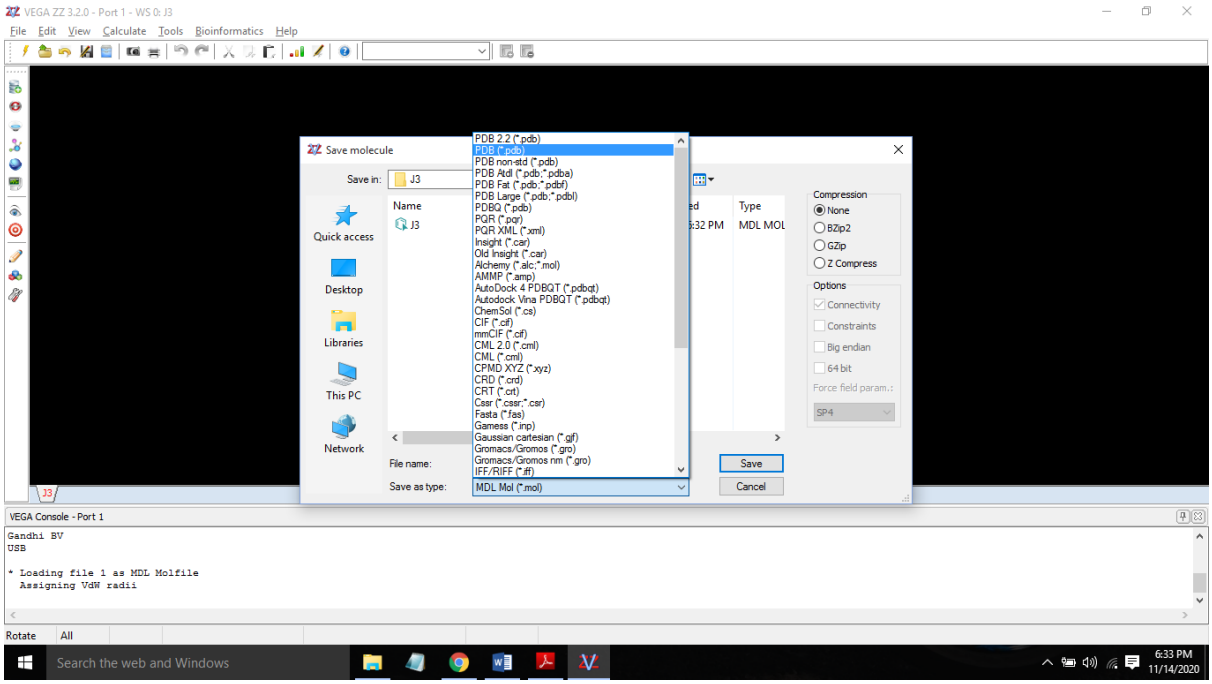
1. Menggambar 2 Dimensi Struktur



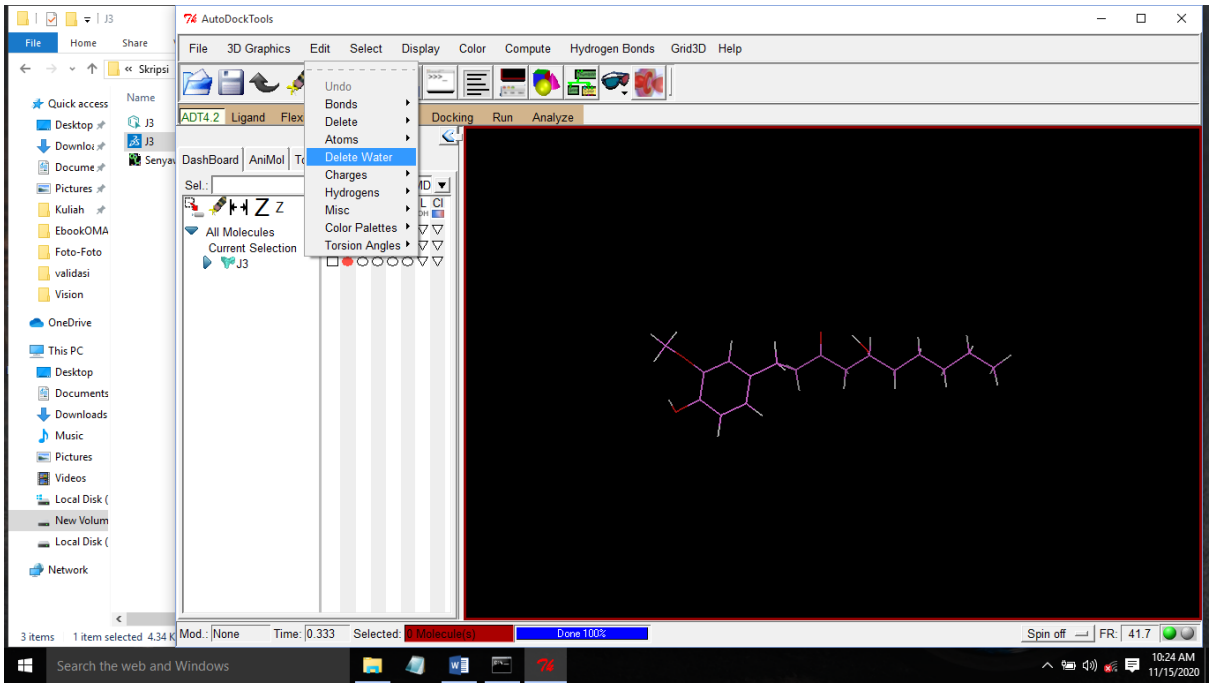


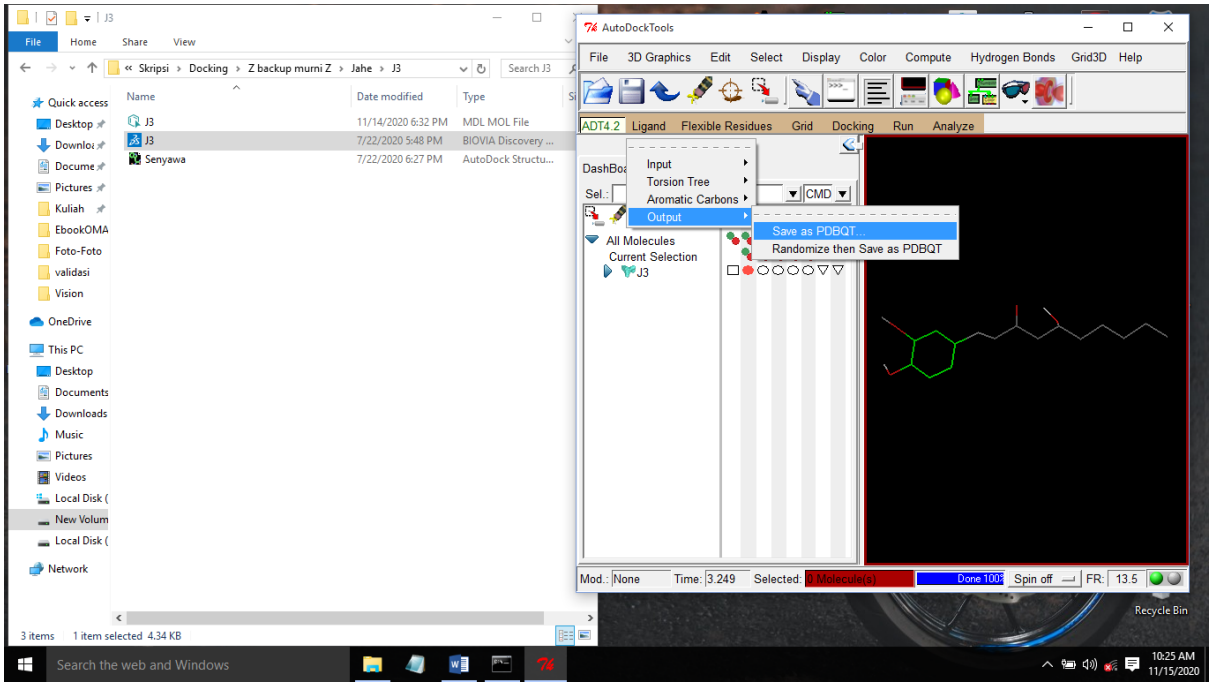
2. Konversi Struktur menjadi pdb



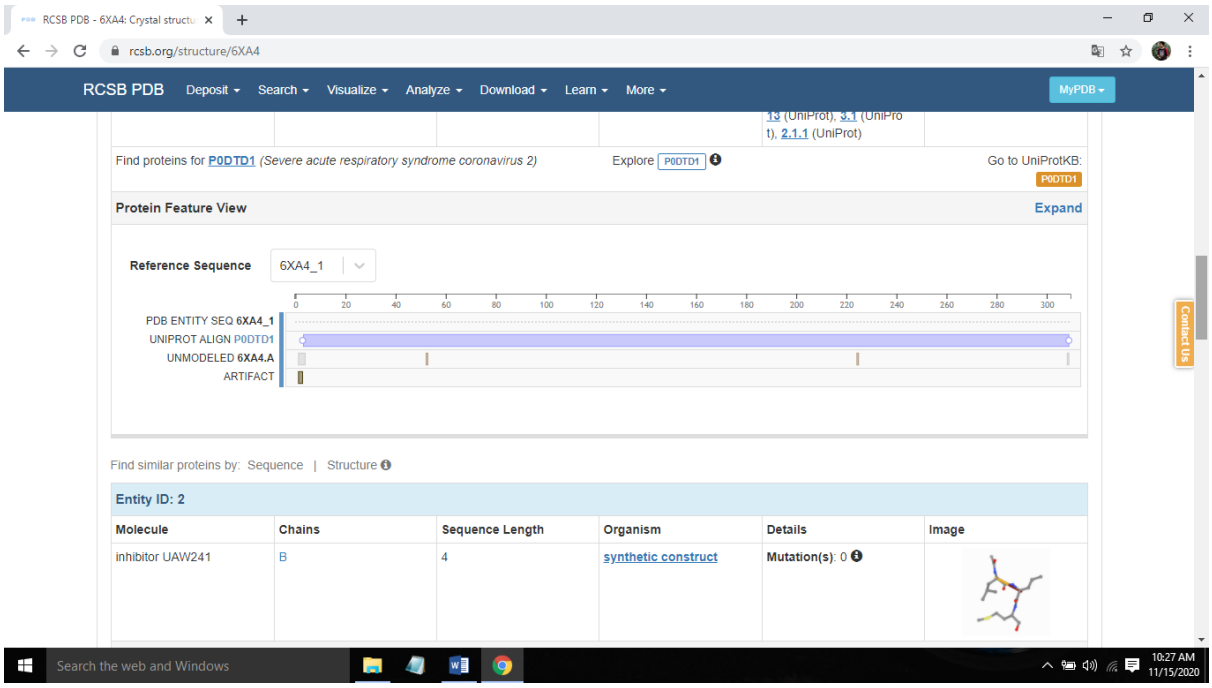


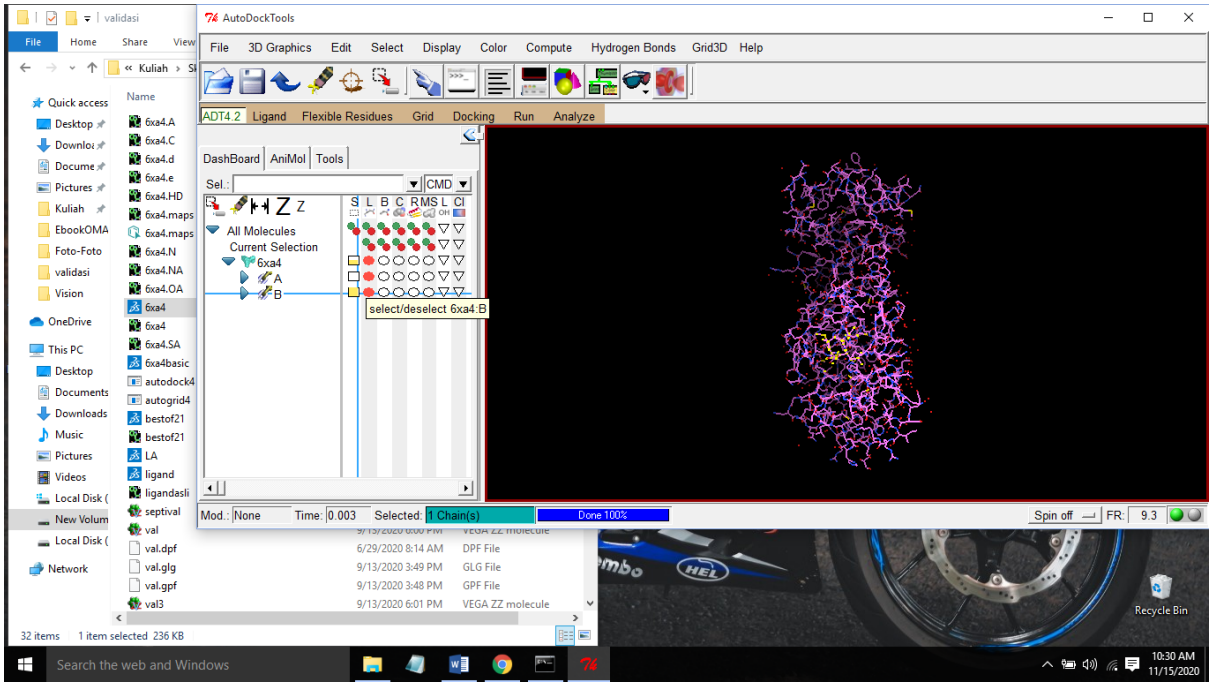
3. Preparasi Ligan uji

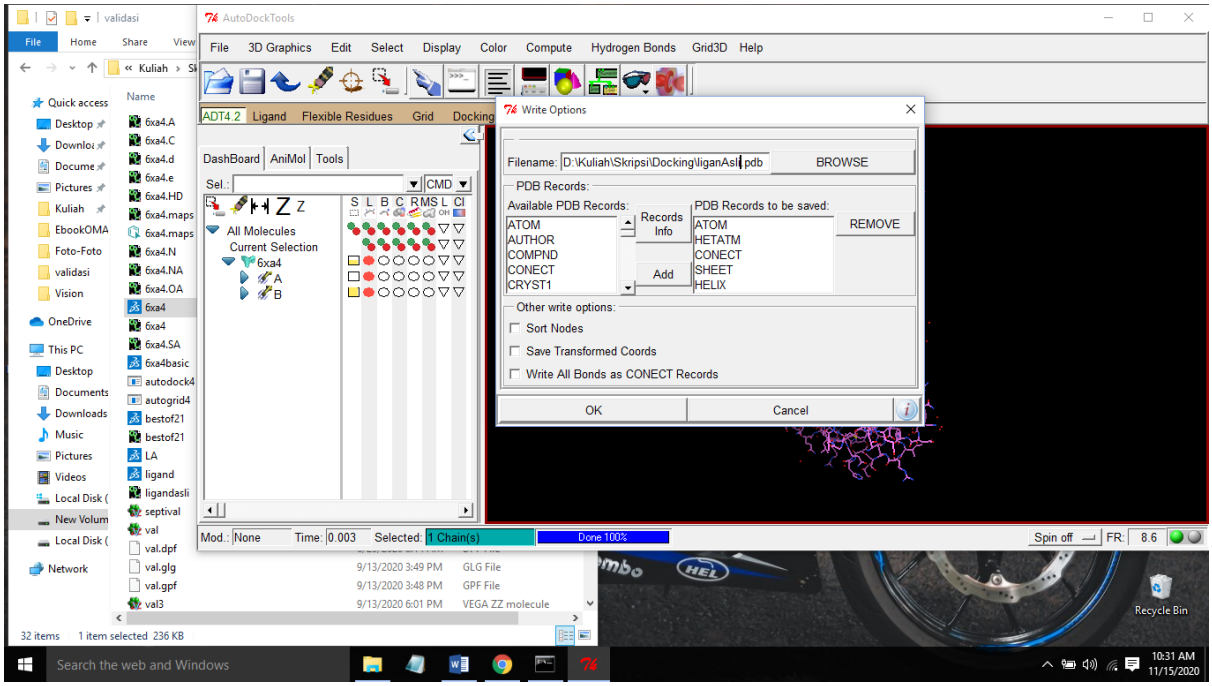




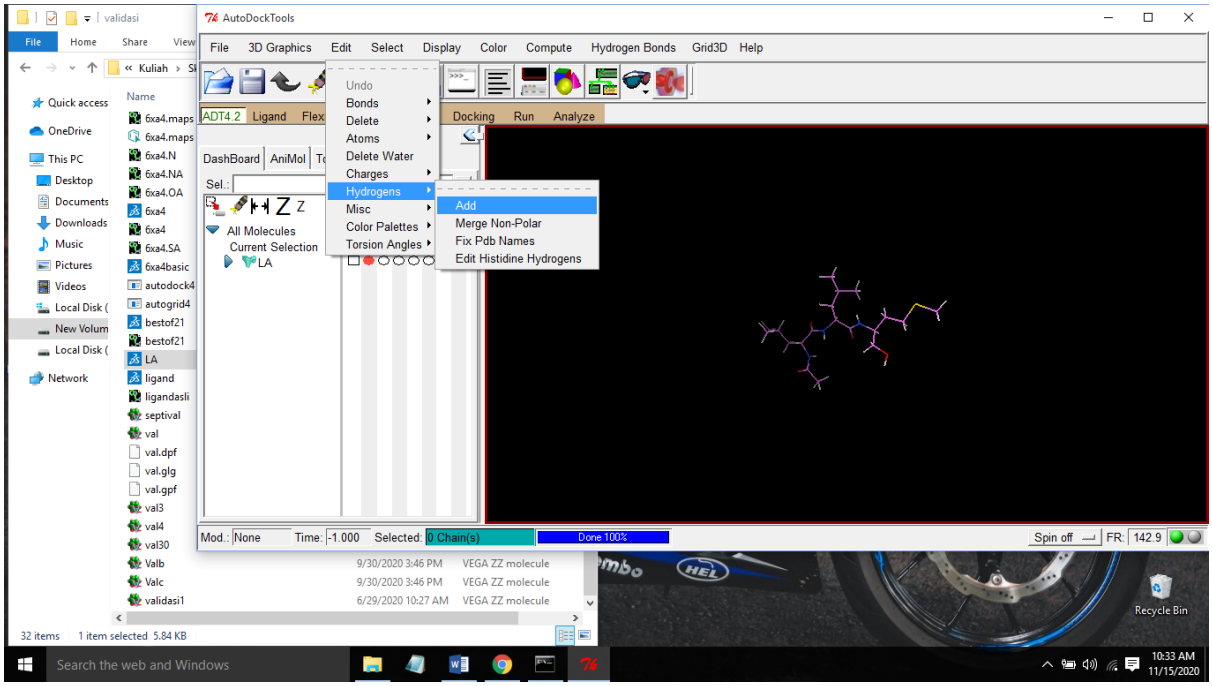
4. Mengetahui dan Memisahkan Ligan Asli

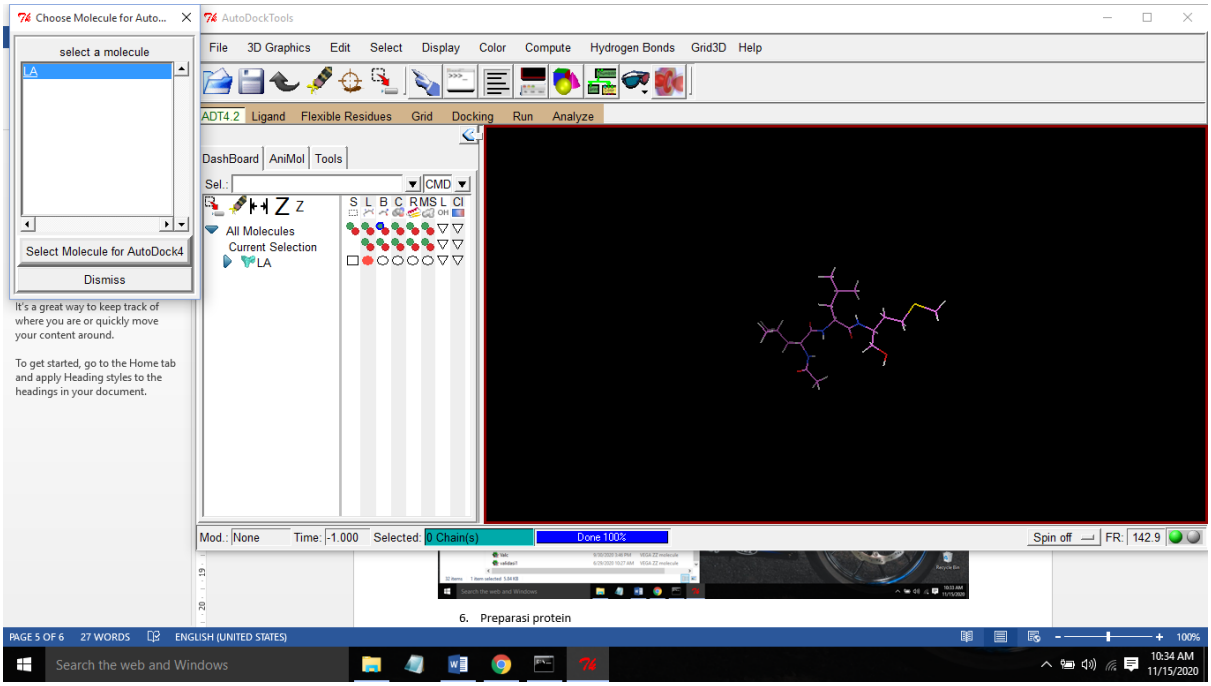




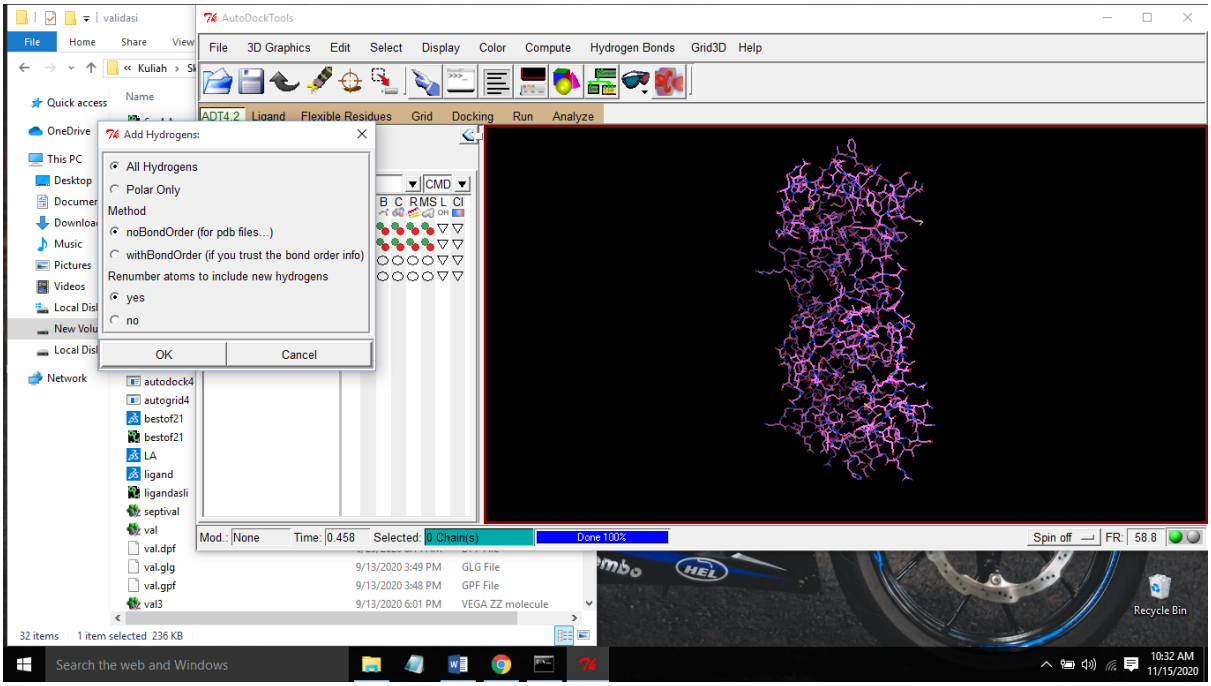


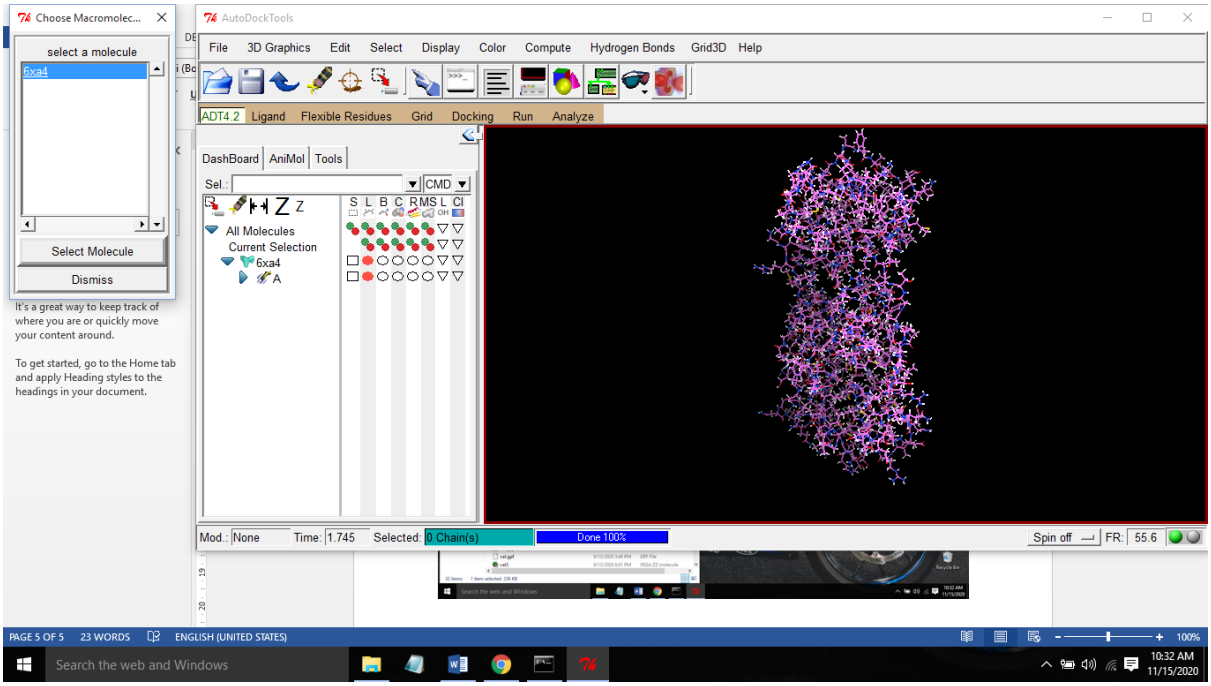
5. Preparasi ligan asli



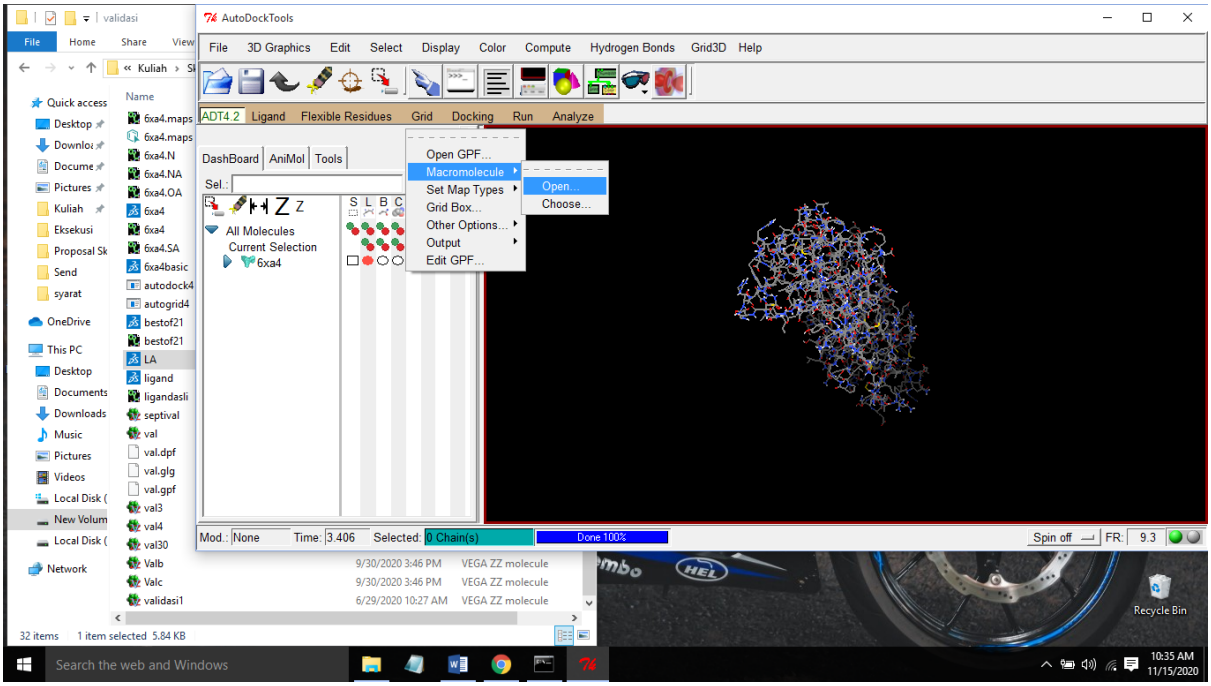


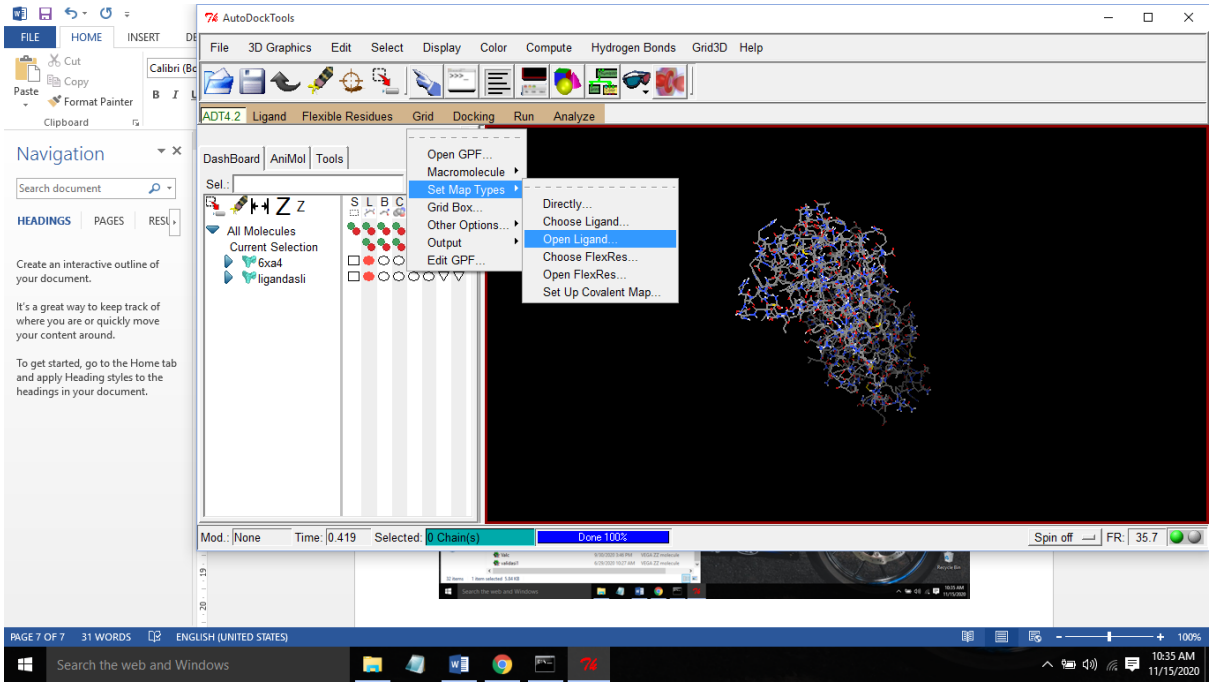
6. Preparasi protein





7. Preparasi grid validasi




AutoDockTools
File 3D Graphics Edit Select Display Color Compute Hydrogen Bonds Grid3D Help
ADT4.2 Ligand Flexible Residues Grid Docking Run Analyze
DashBoard AniMol Tools
Open GPF...
Macromolecule
Set Map Types
Grid Box...
Other Options...
Output
Edit GPF...
Directly...
Choose Ligand...
Open Ligand...
Choose FlexRes...
Open FlexRes...
Set Up Covalent Map...
All Molecules
Current Selection
6xa4
ligandasli
Mod.: None Time: 0.419 Selected: 0 Chain(s) Done 100%
Spin off FR: 35.7
Navigation
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HEADINGS PAGES
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PAGE 7 OF 7 31 WORDS ENGLISH (UNITED STATES)
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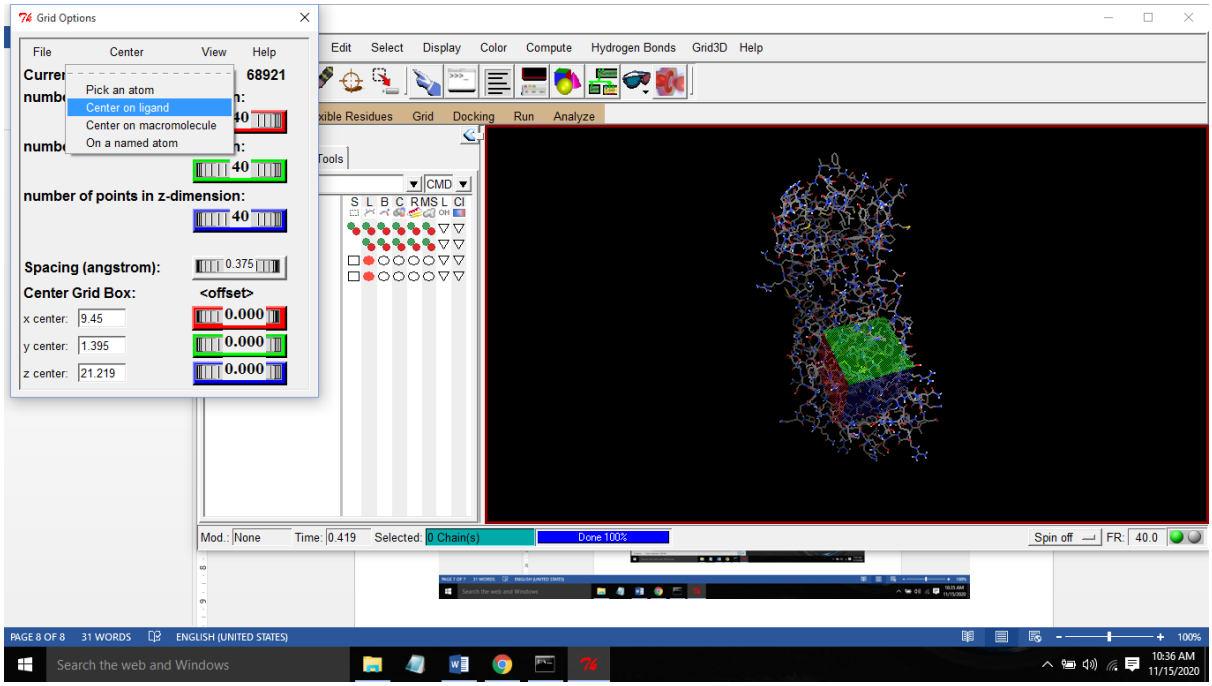
Grid Options
File Center View Help
Pick an atom
Center on ligand
Center on macromolecule
On a named atom
68921
40
40
number of points in z-dimension:
40
Spacing (angstrom):
0.375
Center Grid Box:
<offset>
x center: 9.45
y center: 1.395
z center: 21.219
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Edit Select Display Color Compute Hydrogen Bonds Grid3D Help
Grid Docking Run Analyze
CMD
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Spin off FR: 40.0
PAGE 8 OF 8 31 WORDS ENGLISH (UNITED STATES)
Search the web and Windows
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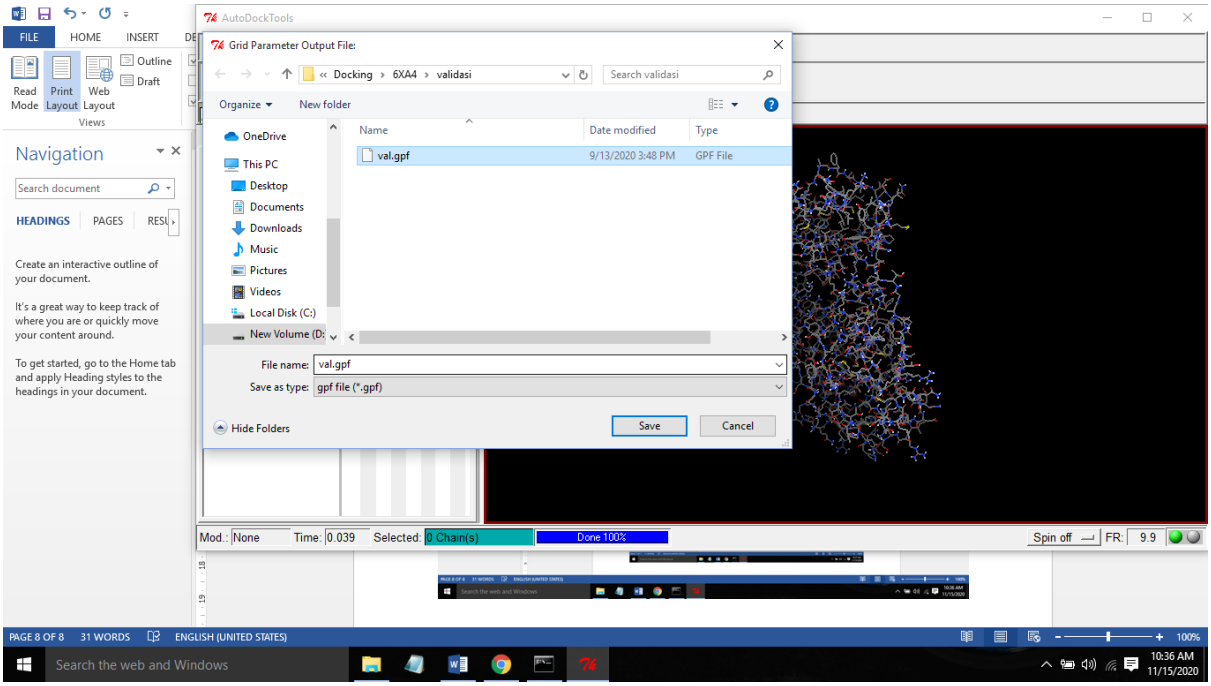
AutoDockTools
Grid Parameter Output File:
Docking › 6XA4 › validasi
Search validasi
Organize
New folder
OneDrive
This PC
Desktop
Documents
Downloads
Music
Pictures
Videos
Local Disk (C:)
New Volume (D:
Name
Date modified
Type
val.gpf
9/13/2020 3:48 PM
GPF File
File name: val.gpf
Save as type: gpf file (*.gpf)
Hide Folders
Save
Cancel
Navigation
Search document
HEADINGS
PAGES
Create an interactive outline of your document.
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Mod.: None
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Selected: 0 Chain(s)
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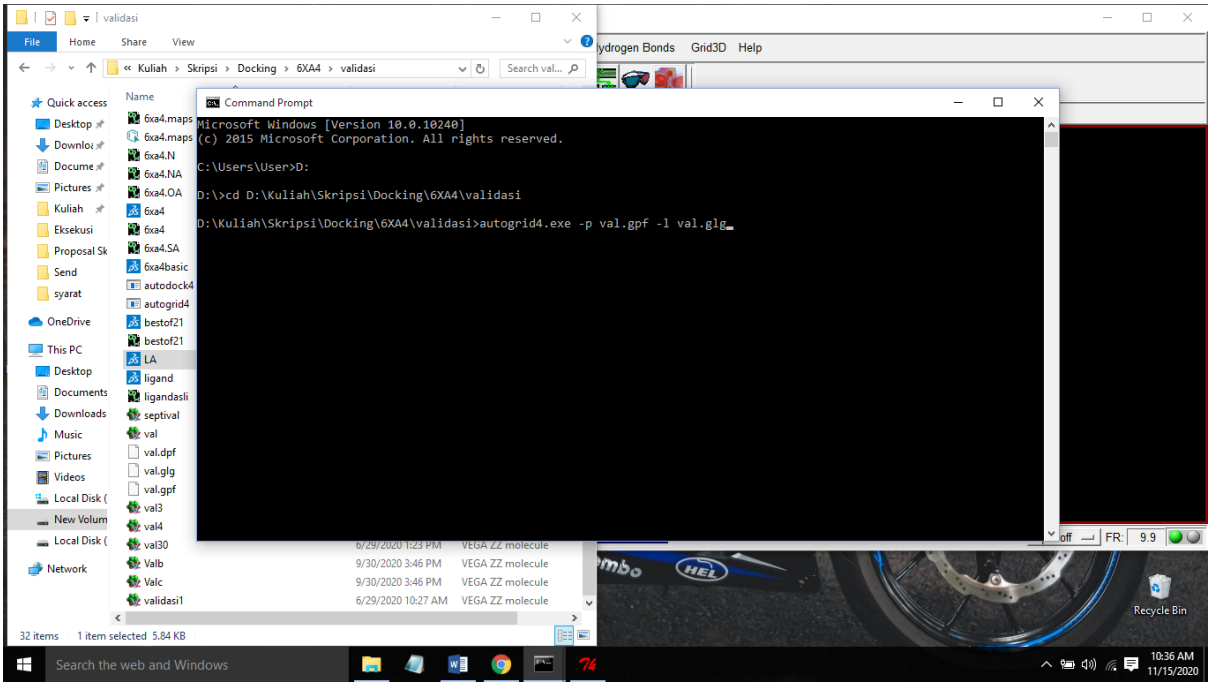
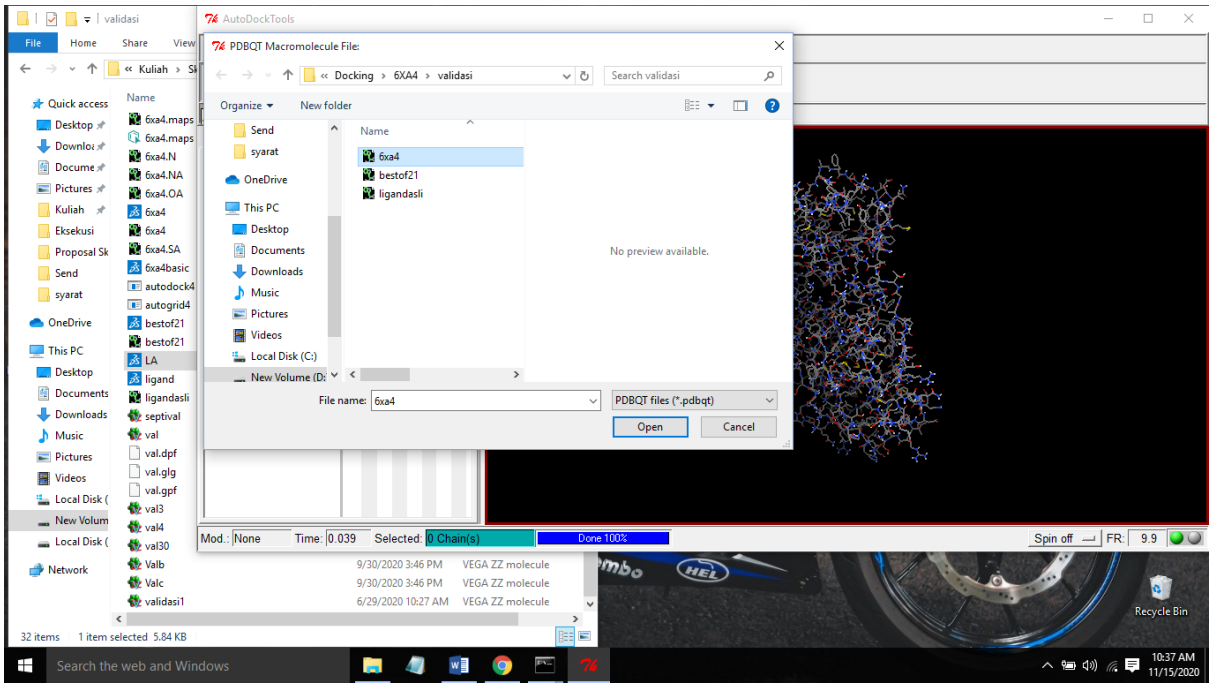
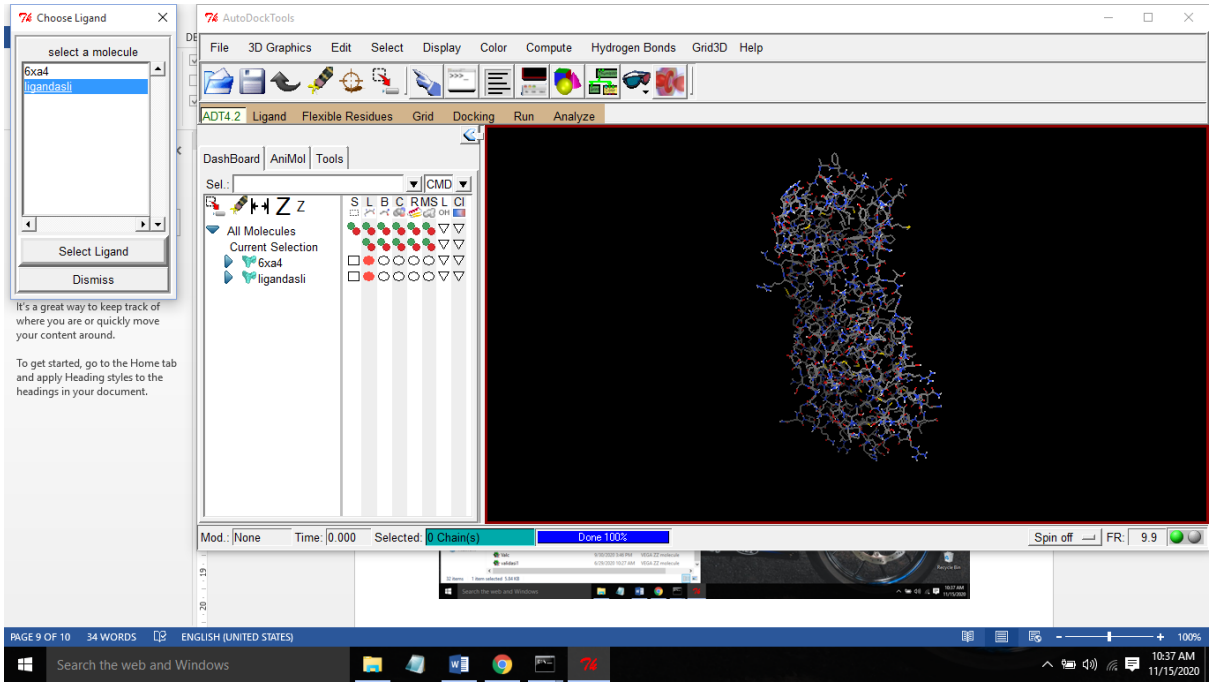
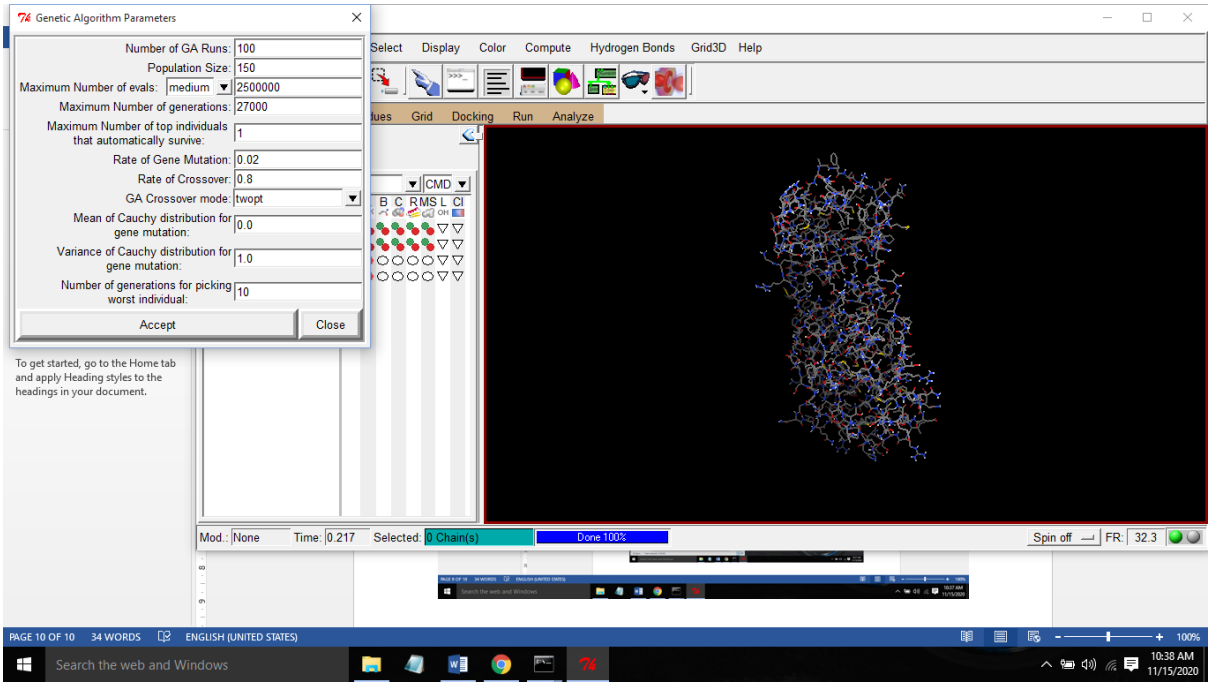
FR: 9.9
PAGE 8 OF 8
31 WORDS
ENGLISH (UNITED STATES)
Search the web and Windows
10:36 AM
11/15/2020

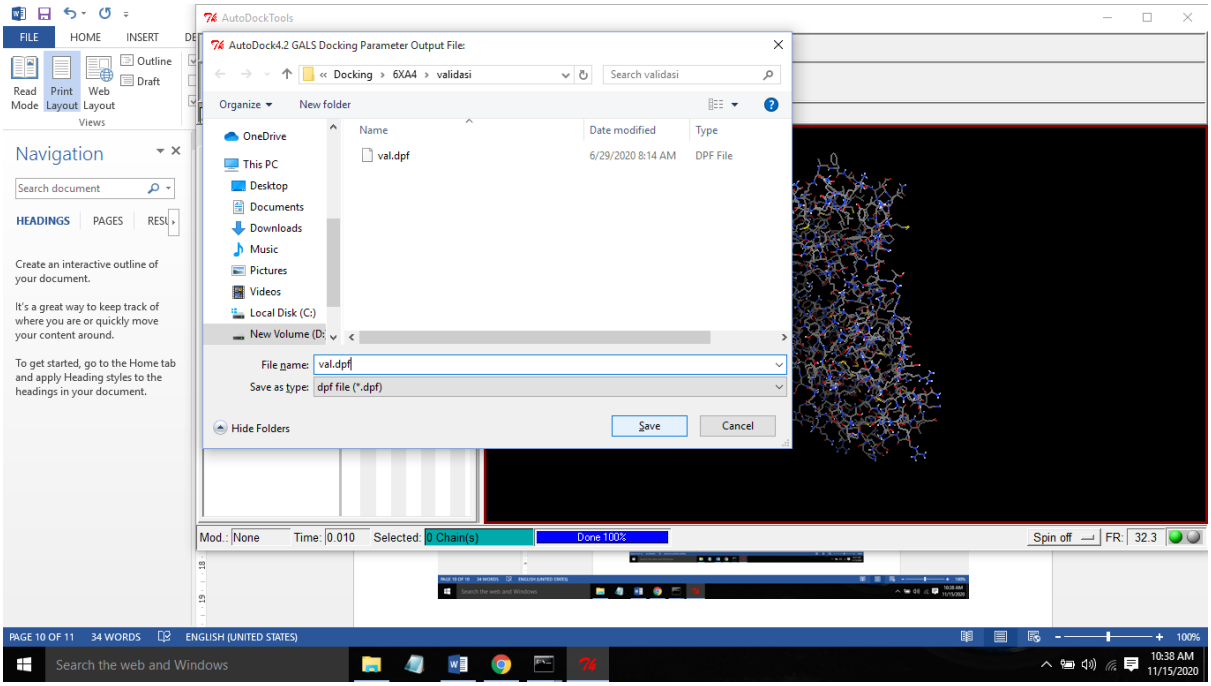

validasi
File
Home
Share
View
Kuliah › Skripsi › Docking › 6XA4 › validasi
Search val...
Quick access
Desktop
Documents
Pictures
Kuliah
Eksekusi
Proposal Sk
Send
syarat
OneDrive
This PC
Desktop
Documents
Downloads
Music
Pictures
Videos
Local Disk (
New Volum
Local Disk (
Network
Name
6xa4.maps
6xa4.maps
6xa4.N
6xa4.NA
6xa4.OA
6xa4
6xa4
6xa4.SA
6xa4basic
autodock4
autogrid4
bestof21
bestof21
LA
ligand
ligandasli
septival
val
val.dpf
val.glg
val.gpf
val3
val4
val30
Valb
Valc
validasi1
9/30/2020 3:46 PM
VEGA ZZ molecule
9/30/2020 3:46 PM
VEGA ZZ molecule
6/29/2020 10:27 AM
VEGA ZZ molecule
32 items
1 item selected 5.84 KB
Command Prompt
Microsoft Windows [Version 10.0.10240]
(c) 2015 Microsoft Corporation. All rights reserved.
C:\Users\User>D:
D:\>cd D:\Kuliah\Skripsi\Docking\6XA4\validasi
D:\Kuliah\Skripsi\Docking\6XA4\validasi>autogrid4.exe -p val.gpf -l val.glg
ydrogen Bonds
Grid3D
Help
FR: 9.9
Recycle Bin
Search the web and Windows
10:36 AM
11/15/2020

8. Validasi docking






Genetic Algorithm Parameters
Number of GA Runs: 100
Population Size: 150
Maximum Number of evals: medium 2500000
Maximum Number of generations: 27000
Maximum Number of top individuals that automatically survive: 1
Rate of Gene Mutation: 0.02
Rate of Crossover: 0.8
GA Crossover mode: twopt
Mean of Cauchy distribution for gene mutation: 0.0
Variance of Cauchy distribution for gene mutation: 1.0
Number of generations for picking worst individual: 10
Accept
Close
Select Display Color Compute Hydrogen Bonds Grid3D Help
Grid Docking Run Analyze
Mod.: None Time: 0.217 Selected: 0 Chain(s) Done 100%
Spin off FR: 32.3
PAGE 10 OF 10 34 WORDS ENGLISH (UNITED STATES)
Search the web and Windows
10:38 AM 11/15/2020


AutoDockTools
AutoDock4.2 GALS Docking Parameter Output File:
Docking 6XA4 validasi
Search validasi
Organize New folder
OneDrive
This PC
Desktop
Documents
Downloads
Music
Pictures
Videos
Local Disk (C:)
New Volume (D:
Name Date modified Type
val.dpf 6/29/2020 8:14 AM DPF File
File name: val.dpf
Save as type: dpf file (*.dpf)
Hide Folders
Save
Cancel
Navigation
Search document
HEADINGS PAGES
Create an interactive outline of your document.
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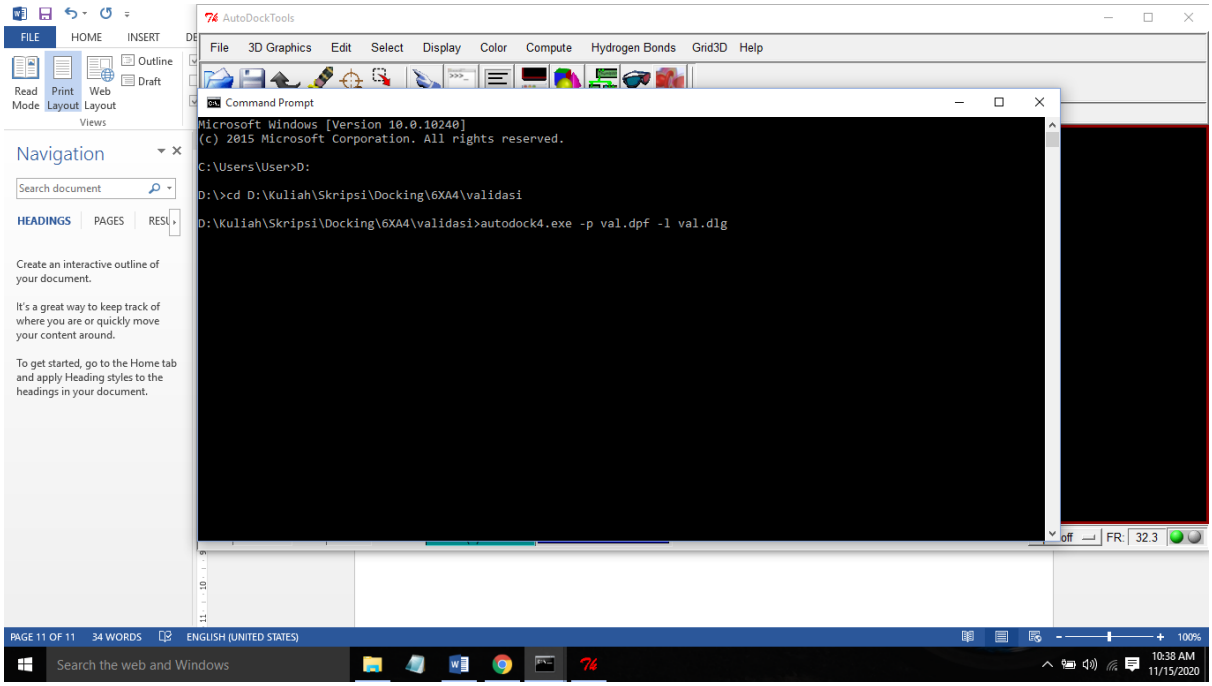
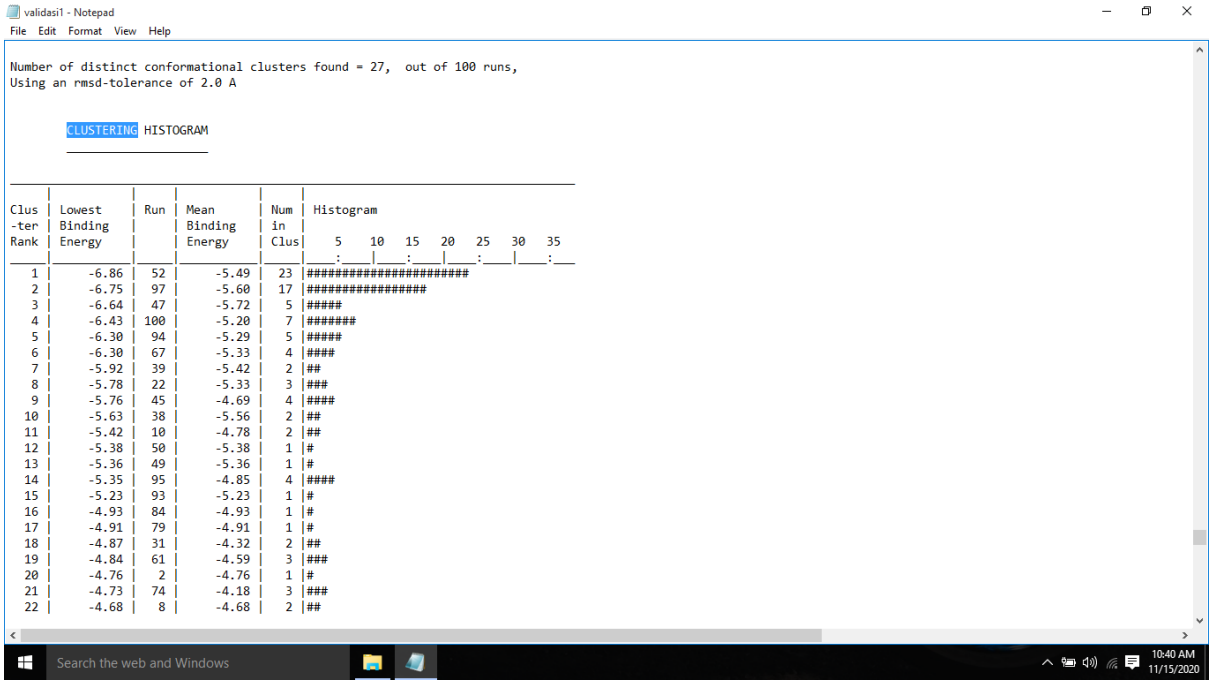
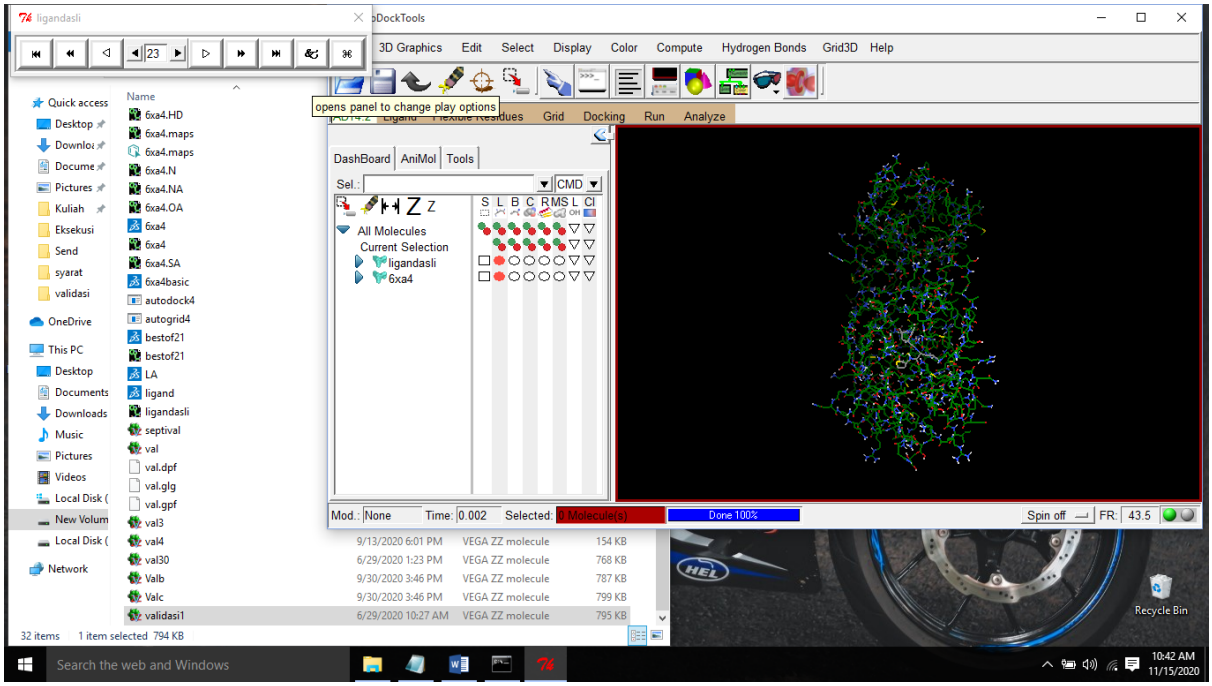
Mod.: None Time: 0.010 Selected: 0 Chain(s) Done 100%
Spin off FR: 32.3
PAGE 10 OF 11 34 WORDS ENGLISH (UNITED STATES)
Search the web and Windows
10:38 AM 11/15/2020

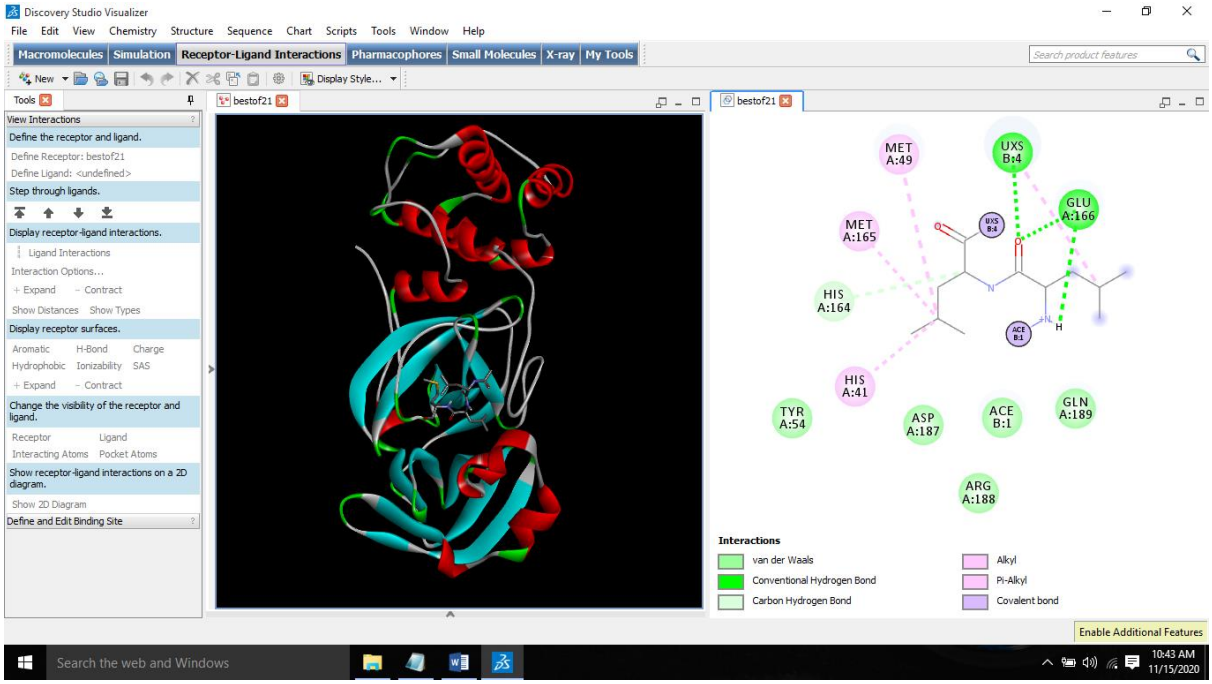


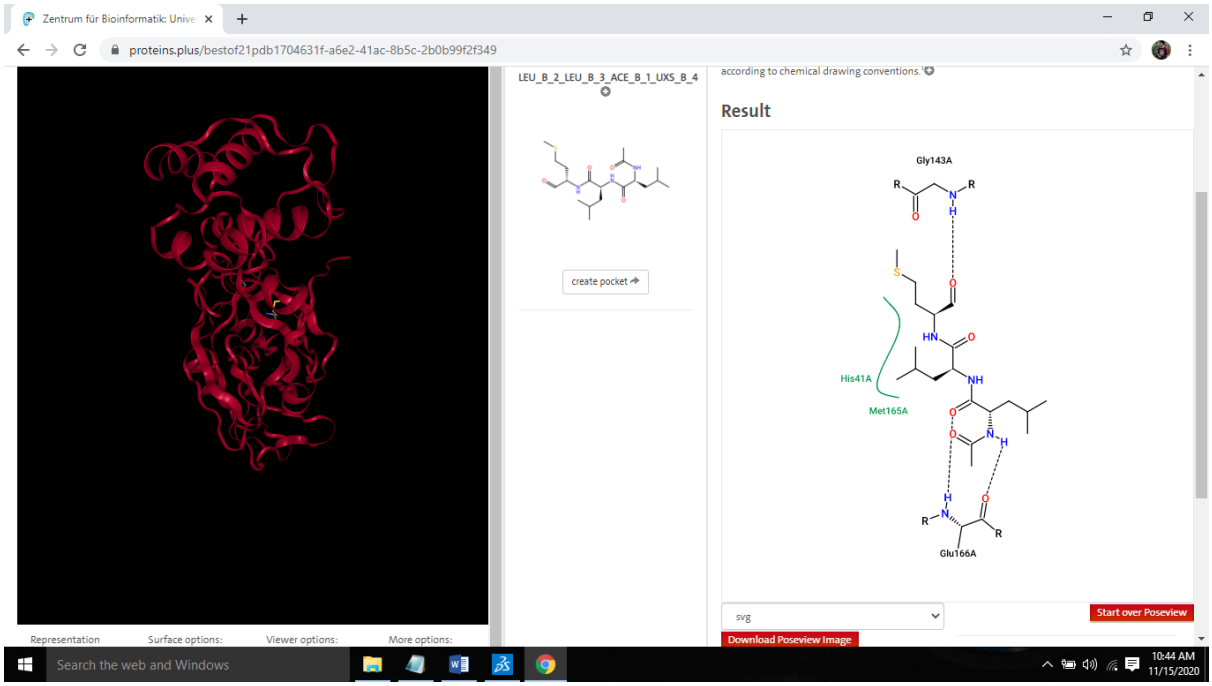
9. Pemilihan energi ikatan terbaik



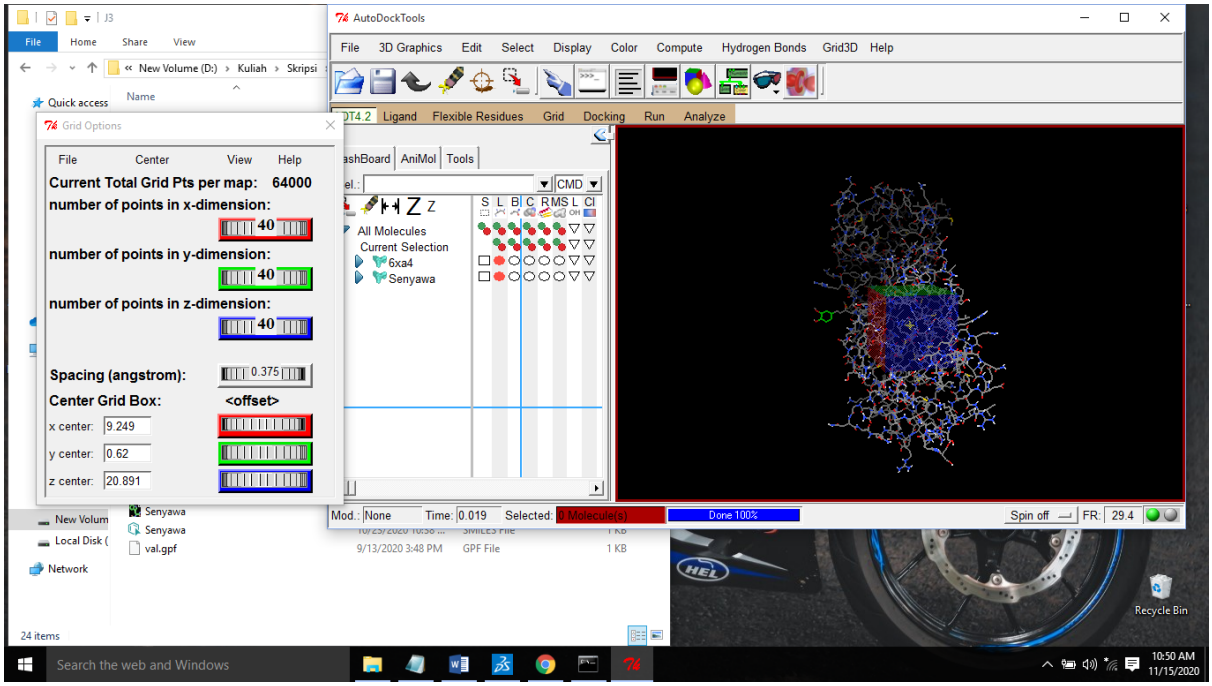


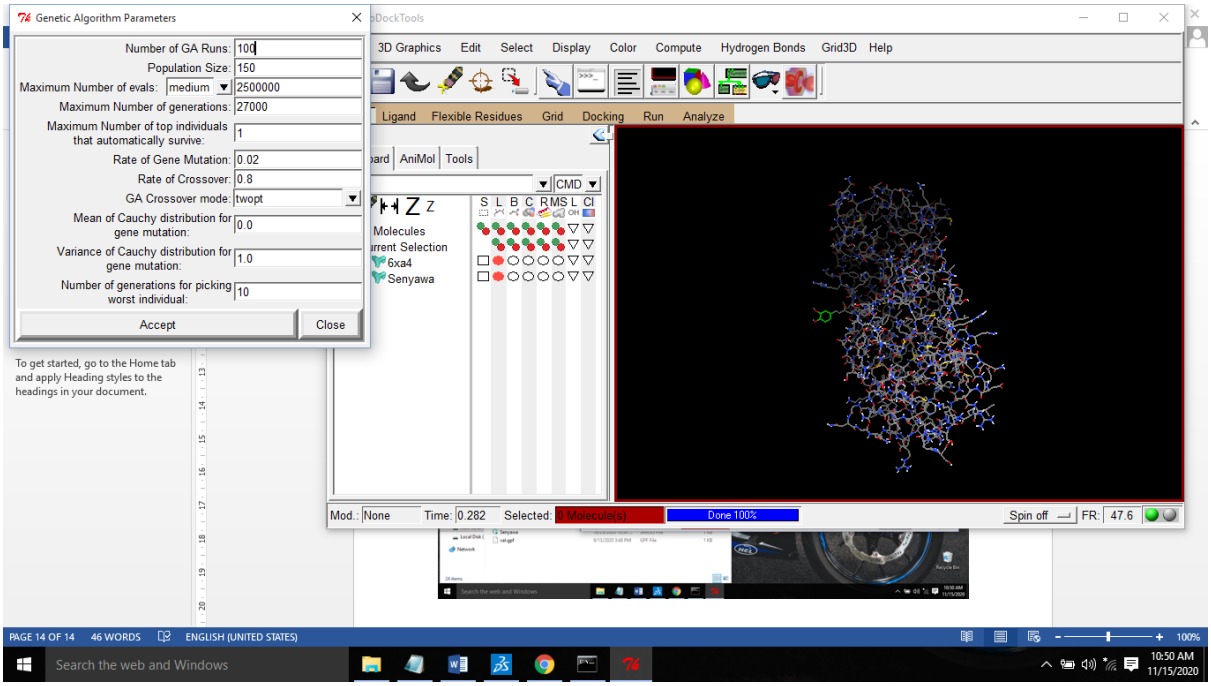
10. Visualisasi



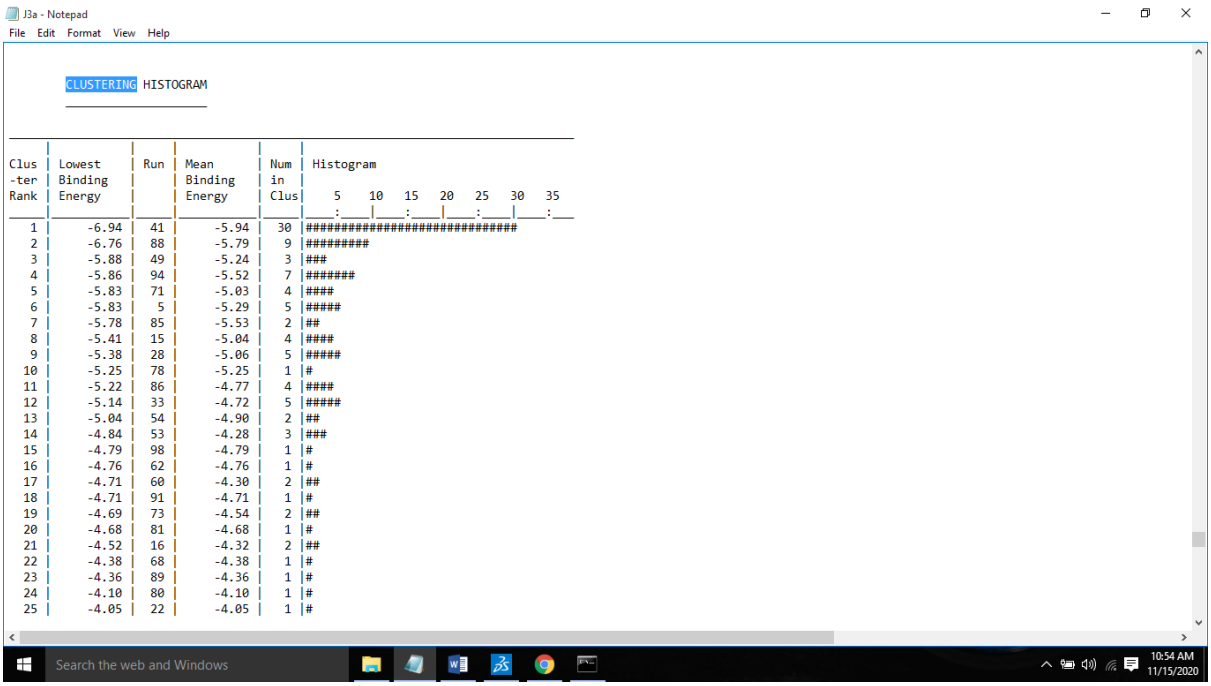


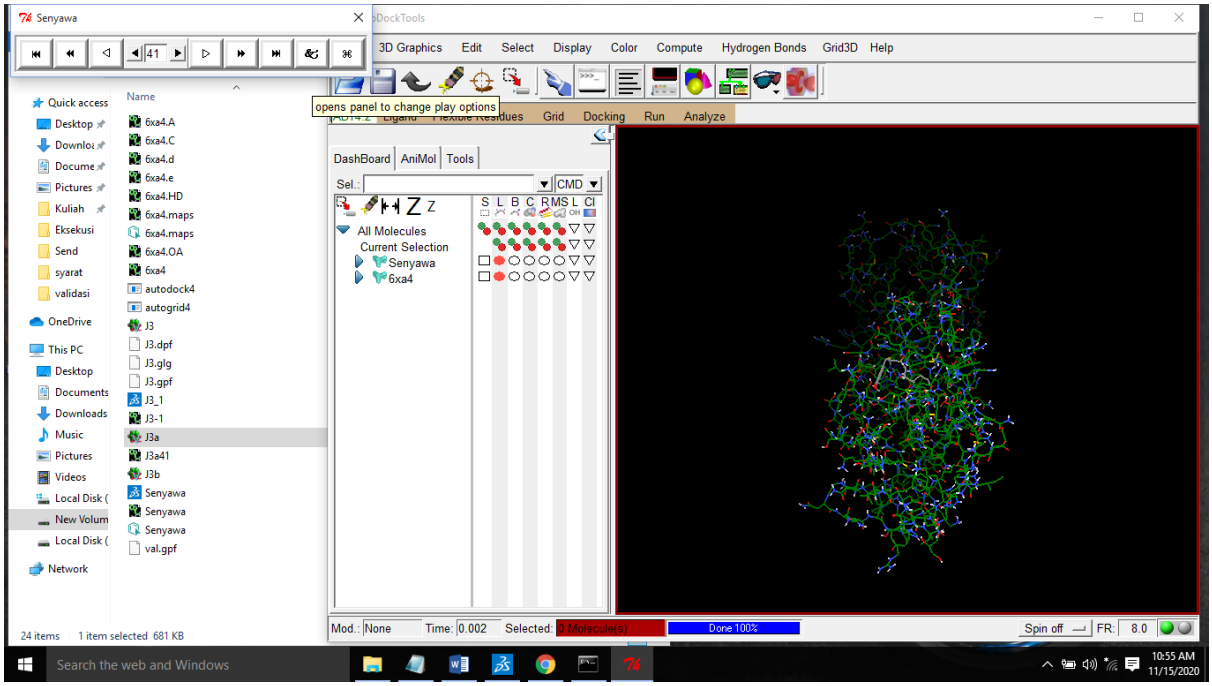
11. Docking dengan ligan uji

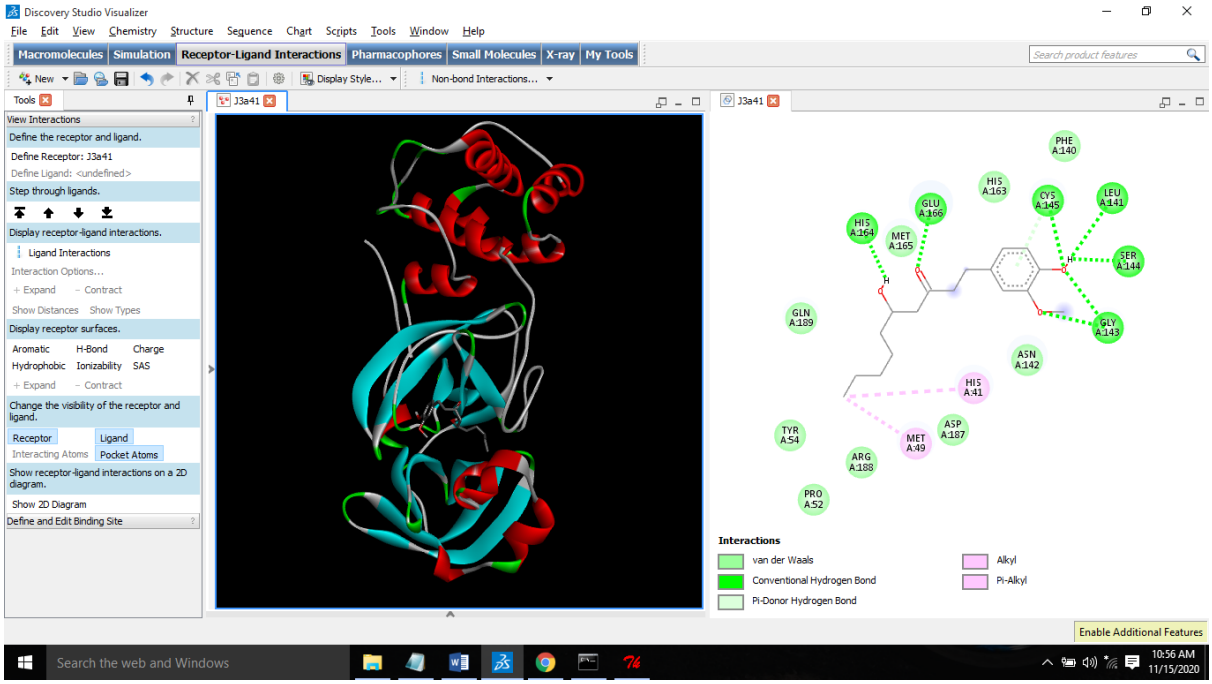




12. Visualisasi hasil docking




Senyawa
DockTools
3D Graphics
Edit
Select
Display
Color
Compute
Hydrogen Bonds
Grid3D
Help
opens panel to change play options
Grid
Docking
Run
Analyze
DashBoard
AniMol
Tools
All Molecules
Current Selection
Senyawa
6xa4
Mod.: None
Time: 0.002
Selected:
Done 100%
Spin off
FR: 8.0
24 items
1 item selected 681 KB
Search the web and Windows
10:55 AM
11/15/2020


Discovery Studio Visualizer
File Edit View Chemistry Structure Sequence Chart Scripts Tools Window Help
Macromolecules
Simulation
Receptor-Ligand Interactions
Pharmacophores
Small Molecules
X-ray
My Tools
Search product features
Tools
View Interactions
Define the receptor and ligand.
Define Receptor: J3a41
Define Ligand: <undefined>
Step through ligands.
Display receptor-ligand interactions.
Ligand Interactions
Interaction Options...
Expand
Contract
Show Distances
Show Types
Display receptor surfaces.
Aromatic
H-Bond
Charge
Hydrophobic
Ionizability
SAS
Change the visibility of the receptor and ligand.
Receptor
Ligand
Interacting Atoms
Pocket Atoms
Show receptor-ligand interactions on a 2D diagram.
Show 2D Diagram
Define and Edit Binding Site
J3a41
PHE A:140
HIS A:163
CYS A:145
LEU A:141
GLU A:166
HIS A:164
MET A:165
SER A:144
GLN A:189
GLY A:143
ASN A:142
HIS A:41
TYR A:54
MET A:49
ASP A:187
ARG A:188
PRO A:52
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Donor Hydrogen Bond
Alkyl
Pi-Alkyl
Enable Additional Features
Search the web and Windows
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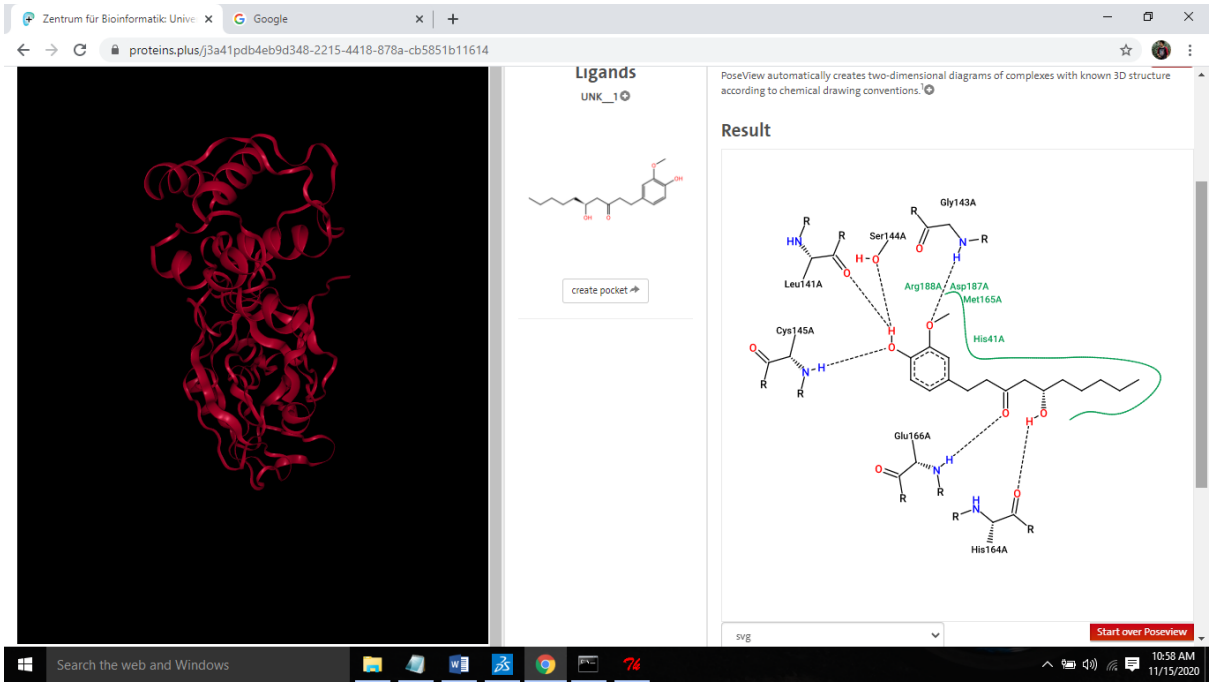
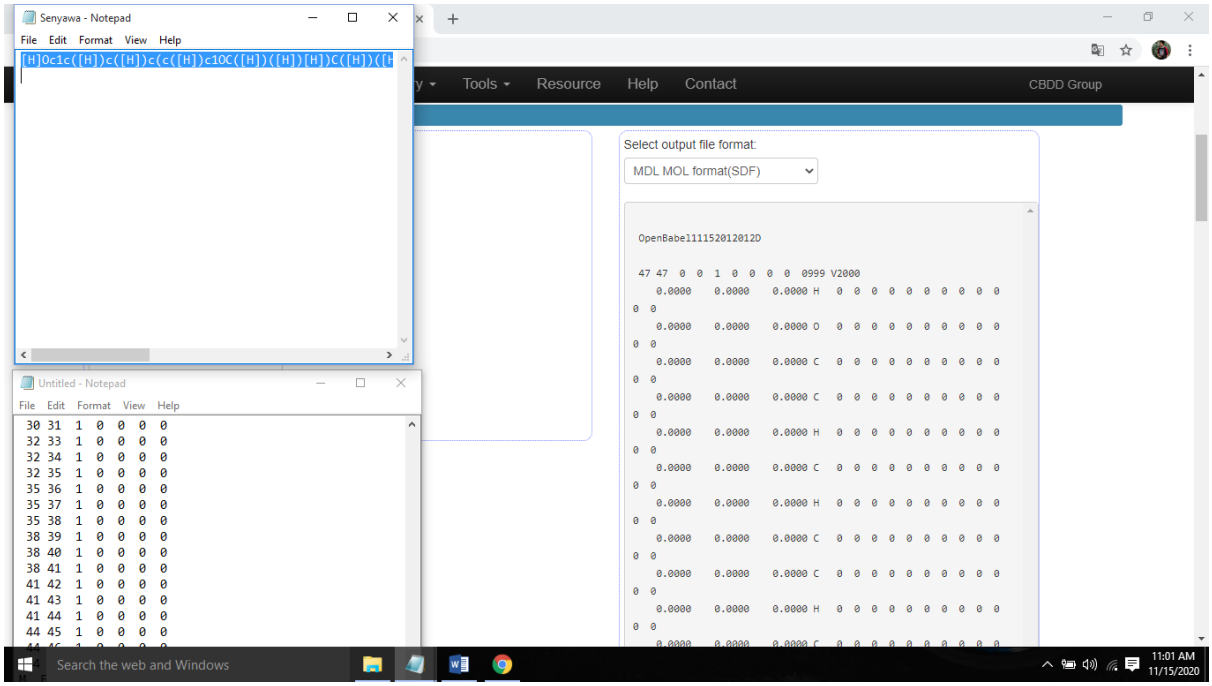
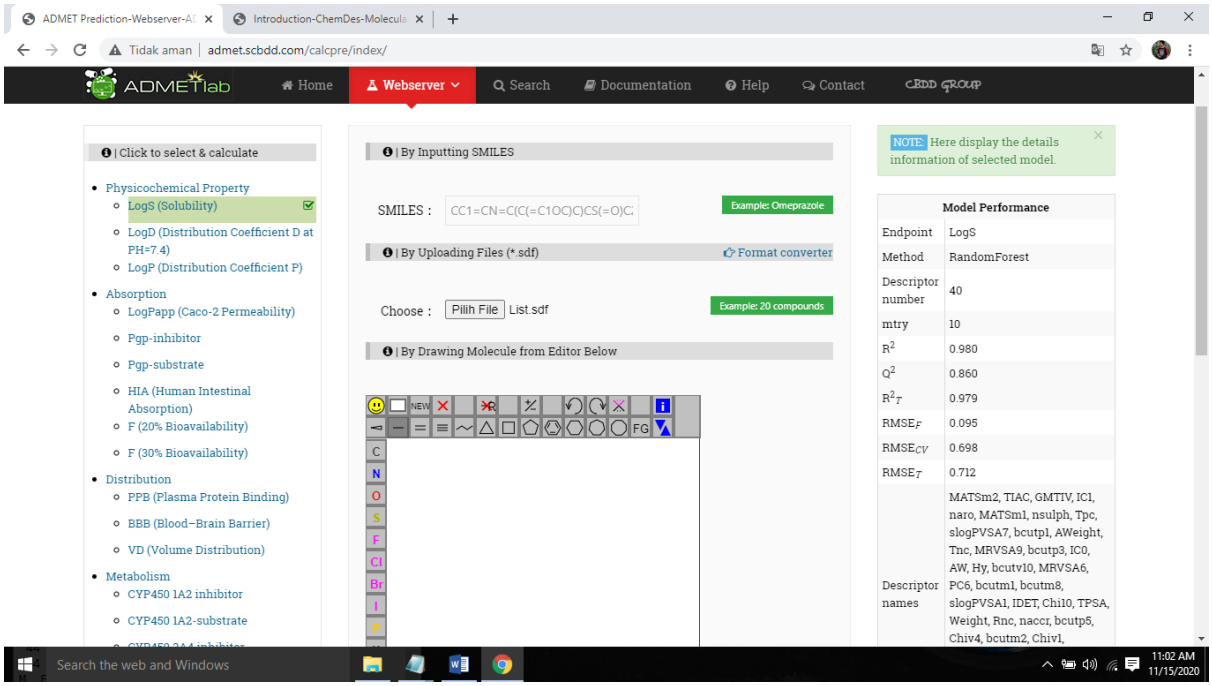


13. Pembacaan prediksi farmakokinetik




ADMET Prediction-Webserver-A
Introduction-ChemDes-Molecula
Tidak aman | admet.scbdd.com/calcpre/index/
ADMETlab
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Webserver
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Documentation
Help
Contact
CBDD GROUP
| Click to select & calculate
Physicochemical Property
LogS (Solubility)
LogD (Distribution Coefficient D at PH=7.4)
LogP (Distribution Coefficient P)
Absorption
LogPapp (Caco-2 Permeability)
Pgp-inhibitor
Pgp-substrate
HIA (Human Intestinal Absorption)
F (20% Bioavailability)
F (30% Bioavailability)
Distribution
PPB (Plasma Protein Binding)
BBB (Blood–Brain Barrier)
VD (Volume Distribution)
Metabolism
CYP450 1A2 inhibitor
CYP450 1A2-substrate
| By Inputting SMILES
SMILES :
CC1=CN=C(C(=C1OC)C)CS(=O)C
Example: Omeprazole
| By Uploading Files (*.sdf)
Format converter
Choose :
Pilih File
List.sdf
Example: 20 compounds
| By Drawing Molecule from Editor Below
NOTE: Here display the details information of selected model.
Model Performance
Endpoint
LogS
Method
RandomForest
Descriptor number
40
mtry
10
R2
0.980
Q2
0.860
R2T
0.979
RMSEF
0.095
RMSECV
0.698
RMSET
0.712
Descriptor names
MATSm2, TIAC, GMTIV, IC1, naro, MATSm1, nsulph, Tpc, slogPVSA7, bcutp1, AWeight, Tnc, MRVSA9, bcutp3, IC0, AW, Hy, bcutv10, MRVSA6, PC6, bcutm1, bcutm8, slogPVSA1, IDET, Chi10, TPSA, Weight, Rnc, naccr, bcutp5, Chiv4, bcutm2, Chiv1,
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11/15/2020