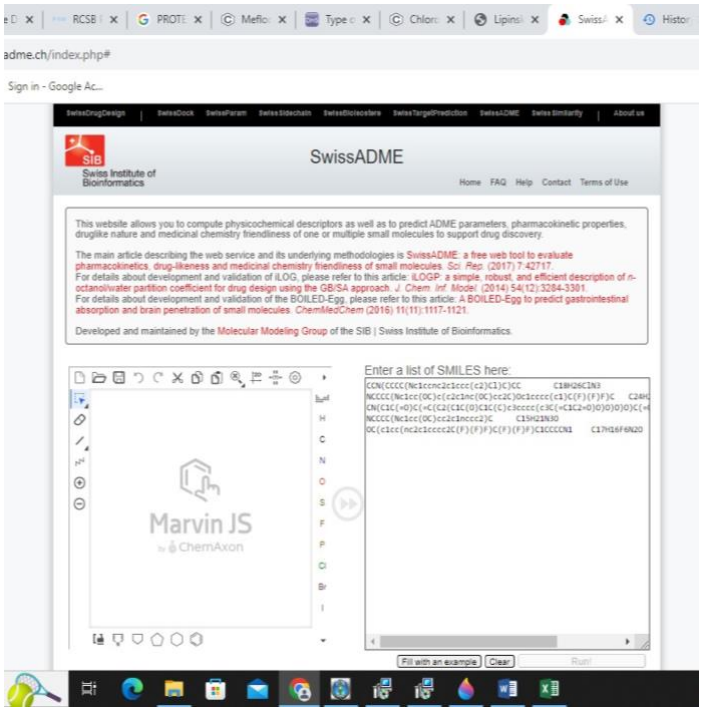
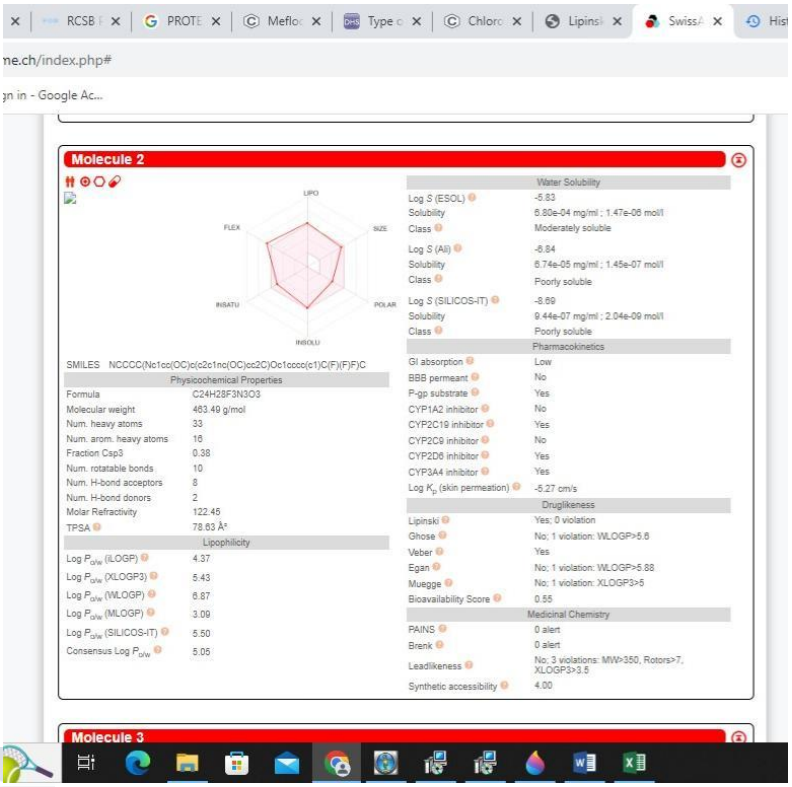
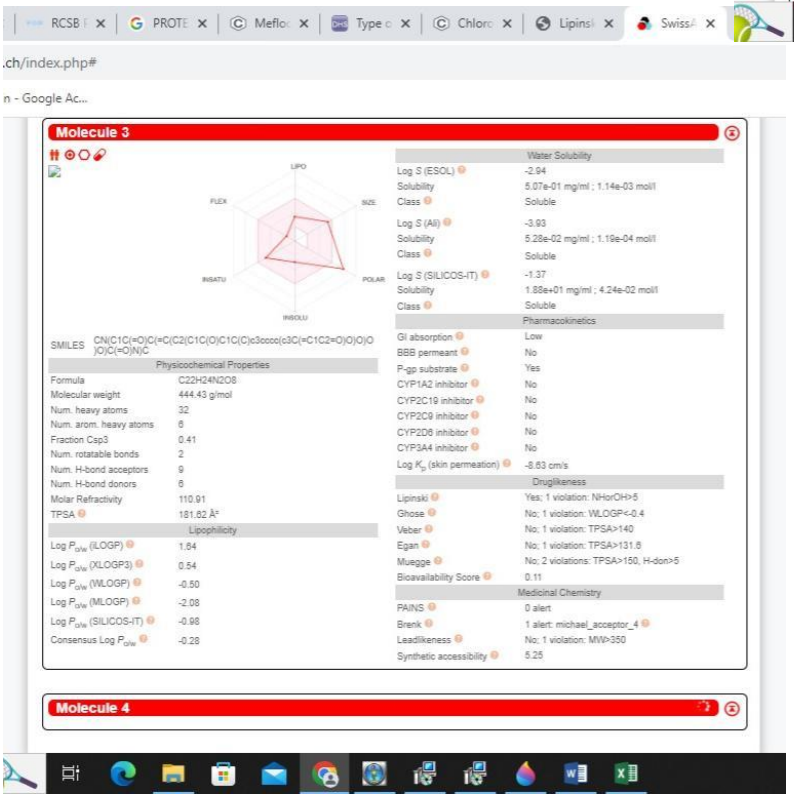
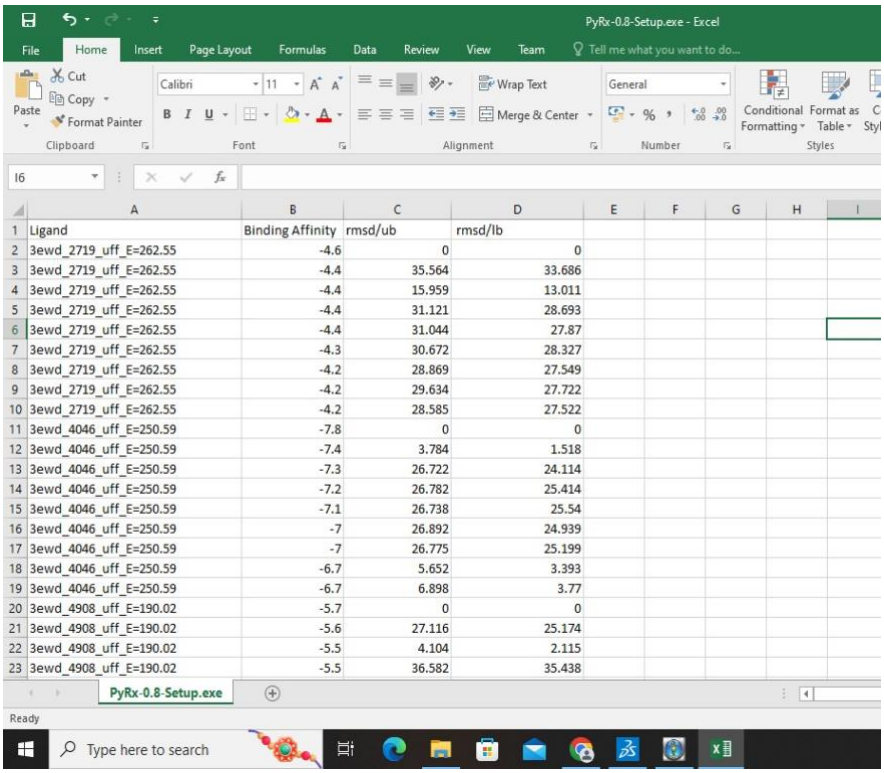
Molecular docking Antimalarial drugs



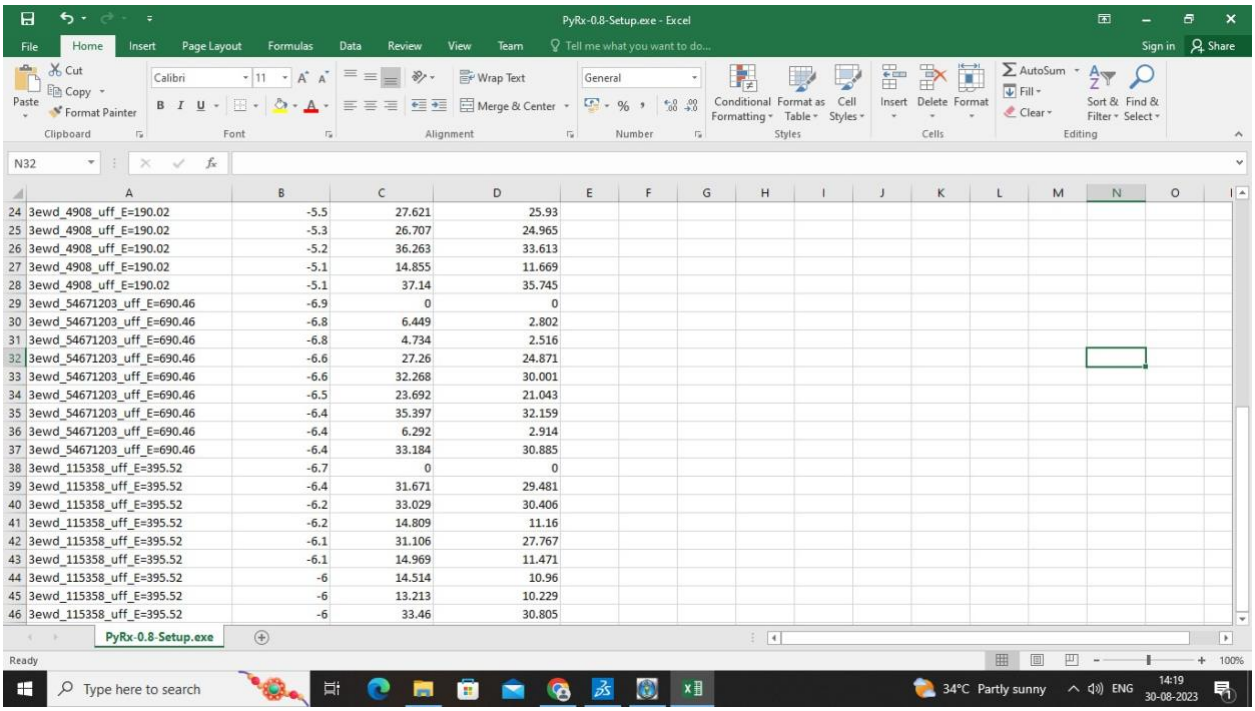




3ewd

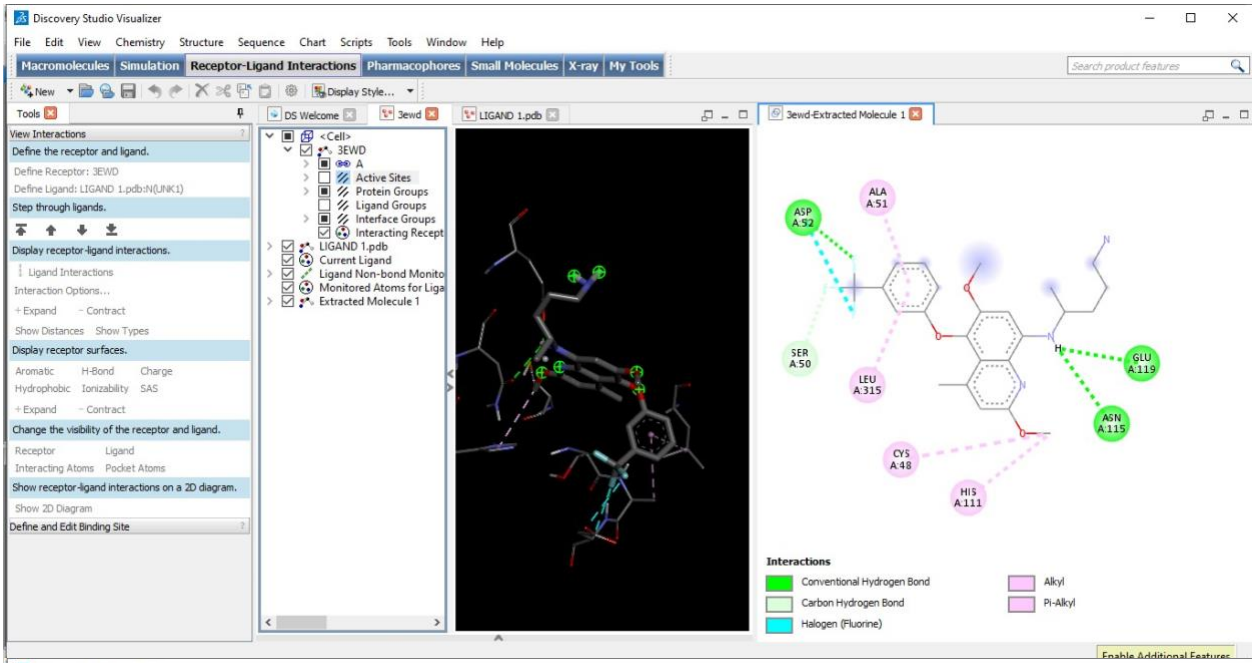


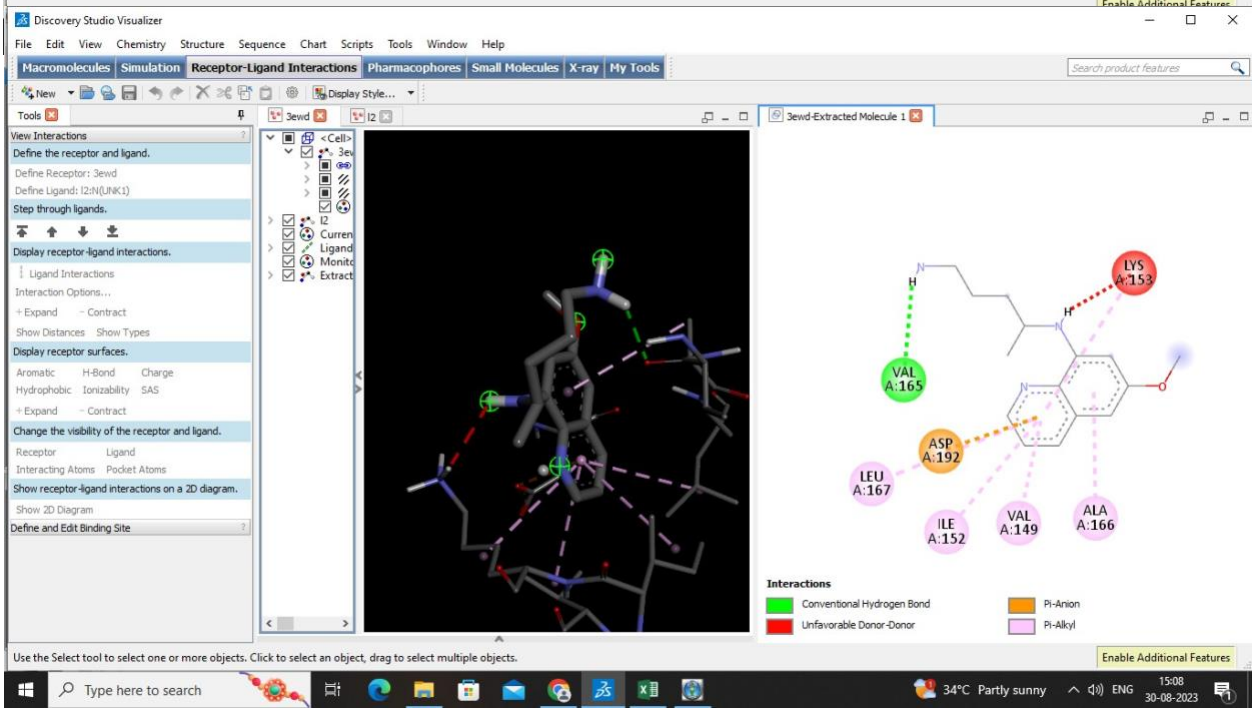
	A	B	C	D
1	Ligand	Binding Affinity	rmsd/ub	rmsd/lb
2	3ewd_2719_uff_E=262.55	-4.6	0	0
3	3ewd_2719_uff_E=262.55	-4.4	35.564	33.686
4	3ewd_2719_uff_E=262.55	-4.4	15.959	13.011
5	3ewd_2719_uff_E=262.55	-4.4	31.121	28.693
6	3ewd_2719_uff_E=262.55	-4.4	31.044	27.87
7	3ewd_2719_uff_E=262.55	-4.3	30.672	28.327
8	3ewd_2719_uff_E=262.55	-4.2	28.869	27.549
9	3ewd_2719_uff_E=262.55	-4.2	29.634	27.722
10	3ewd_2719_uff_E=262.55	-4.2	28.585	27.522
11	3ewd_4046_uff_E=250.59	-7.8	0	0
12	3ewd_4046_uff_E=250.59	-7.4	3.784	1.518
13	3ewd_4046_uff_E=250.59	-7.3	26.722	24.114
14	3ewd_4046_uff_E=250.59	-7.2	26.782	25.414
15	3ewd_4046_uff_E=250.59	-7.1	26.738	25.54
16	3ewd_4046_uff_E=250.59	-7	26.892	24.939
17	3ewd_4046_uff_E=250.59	-7	26.775	25.199
18	3ewd_4046_uff_E=250.59	-6.7	5.652	3.393
19	3ewd_4046_uff_E=250.59	-6.7	6.898	3.77
20	3ewd_4908_uff_E=190.02	-5.7	0	0
21	3ewd_4908_uff_E=190.02	-5.6	27.116	25.174
22	3ewd_4908_uff_E=190.02	-5.5	4.104	2.115
23	3ewd_4908_uff_E=190.02	-5.5	36.582	35.438

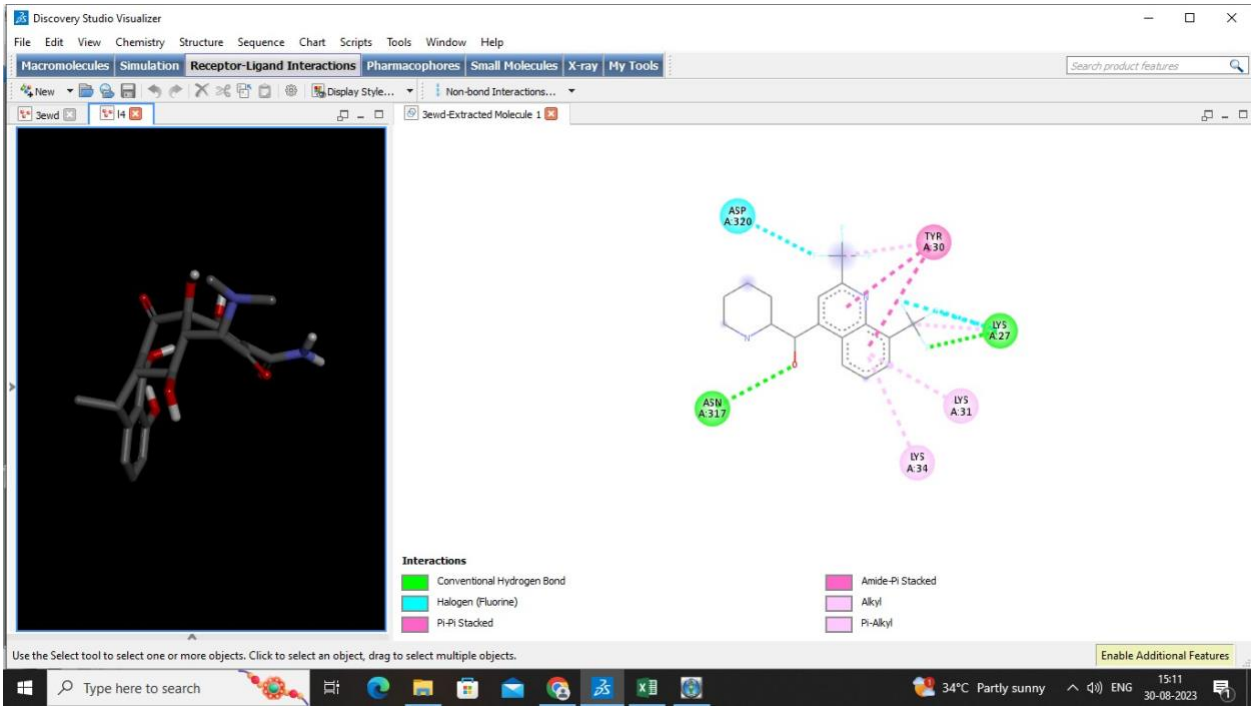


	A	B	C	D
24	3ewd_4908_uff_E=190.02	-5.5	27.621	25.93
25	3ewd_4908_uff_E=190.02	-5.3	26.707	24.965
26	3ewd_4908_uff_E=190.02	-5.2	36.263	33.613
27	3ewd_4908_uff_E=190.02	-5.1	14.855	11.669
28	3ewd_4908_uff_E=190.02	-5.1	37.14	35.745
29	3ewd_54671203_uff_E=690.46	-6.9	0	0
30	3ewd_54671203_uff_E=690.46	-6.8	6.449	2.802
31	3ewd_54671203_uff_E=690.46	-6.8	4.734	2.516
32	3ewd_54671203_uff_E=690.46	-6.6	27.26	24.871
33	3ewd_54671203_uff_E=690.46	-6.6	32.268	30.001
34	3ewd_54671203_uff_E=690.46	-6.5	23.692	21.043
35	3ewd_54671203_uff_E=690.46	-6.4	35.397	32.159
36	3ewd_54671203_uff_E=690.46	-6.4	6.292	2.914
37	3ewd_54671203_uff_E=690.46	-6.4	33.184	30.885
38	3ewd_115358_uff_E=395.52	-6.7	0	0
39	3ewd_115358_uff_E=395.52	-6.4	31.671	29.481
40	3ewd_115358_uff_E=395.52	-6.2	33.029	30.406
41	3ewd_115358_uff_E=395.52	-6.2	14.809	11.16
42	3ewd_115358_uff_E=395.52	-6.1	31.106	27.767
43	3ewd_115358_uff_E=395.52	-6.1	14.969	11.471
44	3ewd_115358_uff_E=395.52	-6	14.514	10.96
45	3ewd_115358_uff_E=395.52	-6	13.213	10.229
46	3ewd_115358_uff_E=395.52	-6	33.46	30.805

Protein – 3ewd ; Drugs : Chloroquine, primaquine,mefloquine, doxycycline, tafenoquine






Discovery Studio Visualizer
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Macromolecules Simulation Receptor-Ligand Interactions Pharmacophores Small Molecules X-ray My Tools
Search product features
New
Display Style...
Non-bond Interactions...
3ewd
I4
3ewd-Extracted Molecule 1
ASP A:320
TYR A:30
LYS A:27
ASN A:317
LYS A:31
LYS A:34
Interactions
Conventional Hydrogen Bond
Halogen (Fluorine)
Pi-Pi Stacked
Amide-Pi Stacked
Alkyl
Pi-Alkyl
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34°C Partly sunny
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15:11
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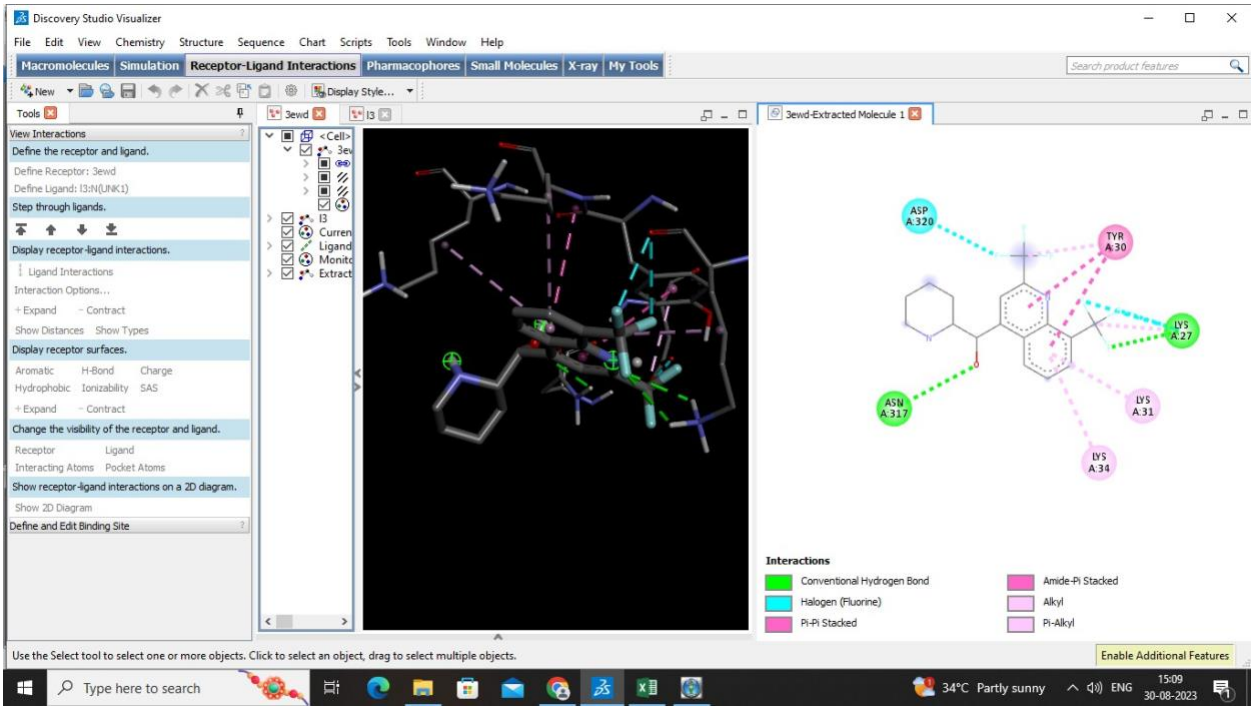
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View Interactions
Define the receptor and ligand.
Define Receptor: 3ewd
Define Ligand: I3:N(UNK1)
Step through ligands.
Display receptor-ligand interactions.
Ligand Interactions
Interaction Options...
+ Expand - Contract
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Display receptor surfaces.
Aromatic H-Bond Charge
Hydrophobic Ionizability SAS
+ Expand - Contract
Change the visibility of the receptor and ligand.
Receptor Ligand
Interacting Atoms Pocket Atoms
Show receptor-ligand interactions on a 2D diagram.
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3ewd
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3ewd-Extracted Molecule 1
ASP A:320
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Pi-Alkyl
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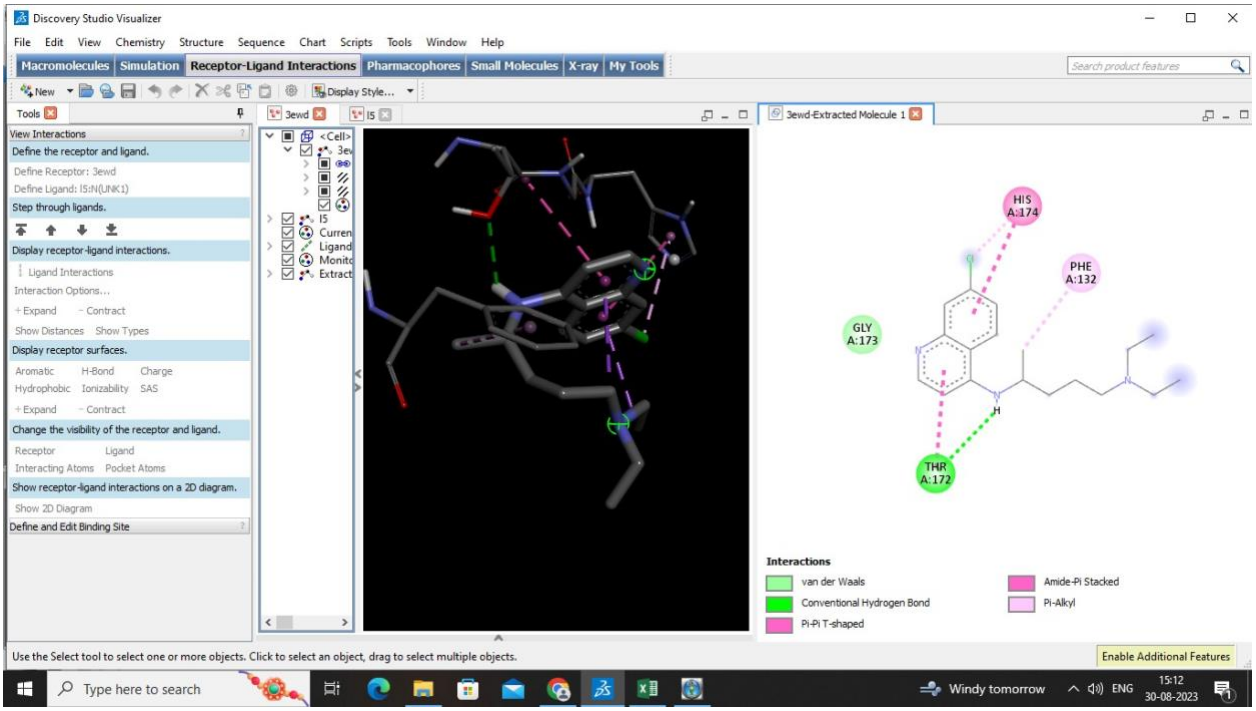
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+Expand −Contract
Show Distances Show Types
Display receptor surfaces.
Aromatic H-Bond Charge
Hydrophobic Ionizability SAS
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Change the visibility of the receptor and ligand.
Receptor Ligand
Interacting Atoms Pocket Atoms
Show receptor-ligand interactions on a 2D diagram.
Show 2D Diagram
Define and Edit Binding Site
3ewd
I5
3ewd-Extracted Molecule 1
HIS A:174
PHE A:132
GLY A:173
THR A:172
Interactions
van der Waals
Conventional Hydrogen Bond
Pi-Pi T-shaped
Amide-Pi Stacked
Pi-Alkyl
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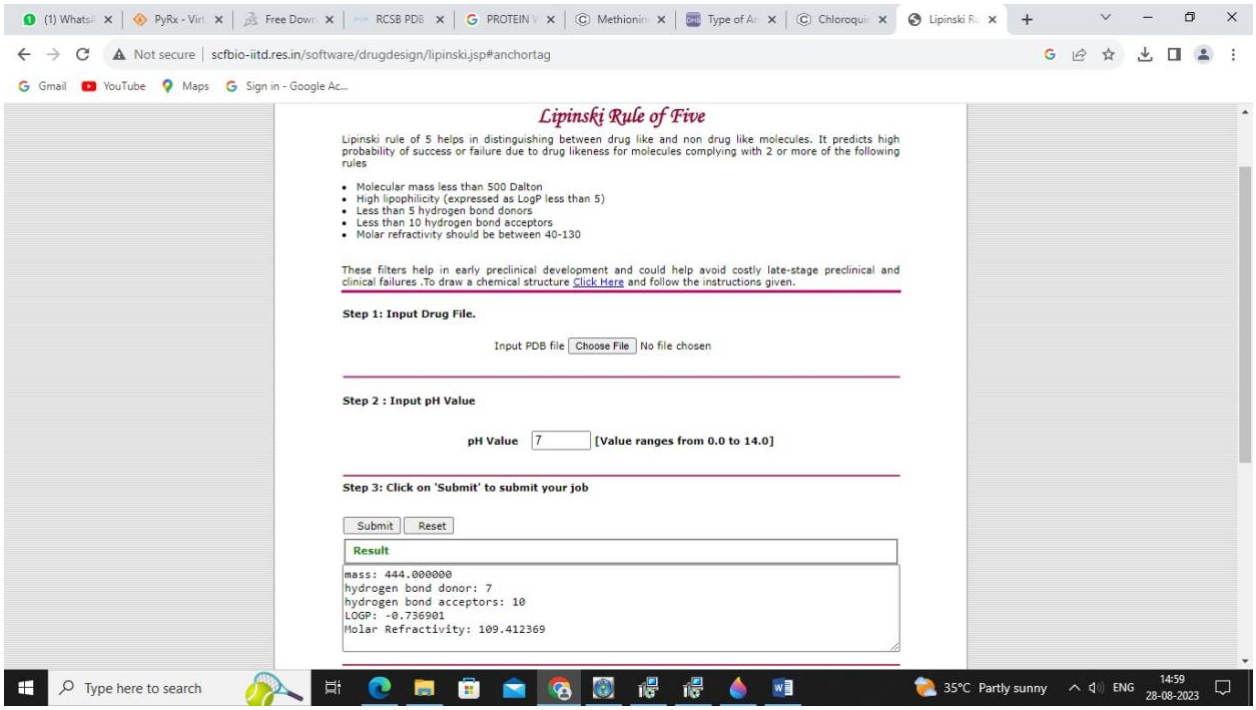
Not secure | scfbio-iitd.res.in/software/drugdesign/lipinski.jsp#anchortag
Gmail YouTube Maps Sign in - Google Ac...
Lipinski Rule of Five
Lipinski rule of 5 helps in distinguishing between drug like and non drug like molecules. It predicts high probability of success or failure due to drug likeness for molecules complying with 2 or more of the following rules
Molecular mass less than 500 Dalton
High lipophilicity (expressed as LogP less than 5)
Less than 5 hydrogen bond donors
Less than 10 hydrogen bond acceptors
Molar refractivity should be between 40-130
These filters help in early preclinical development and could help avoid costly late-stage preclinical and clinical failures .To draw a chemical structure Click Here and follow the instructions given.
Step 1: Input Drug File.
Input PDB file Choose File No file chosen
Step 2 : Input pH Value
pH Value 7 [Value ranges from 0.0 to 14.0]
Step 3: Click on 'Submit' to submit your job
Submit Reset
Result
mass: 444.000000
hydrogen bond donor: 7
hydrogen bond acceptors: 10
LOGP: -0.736901
Molar Refractivity: 109.412369
Type here to search
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ENG
14:59
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