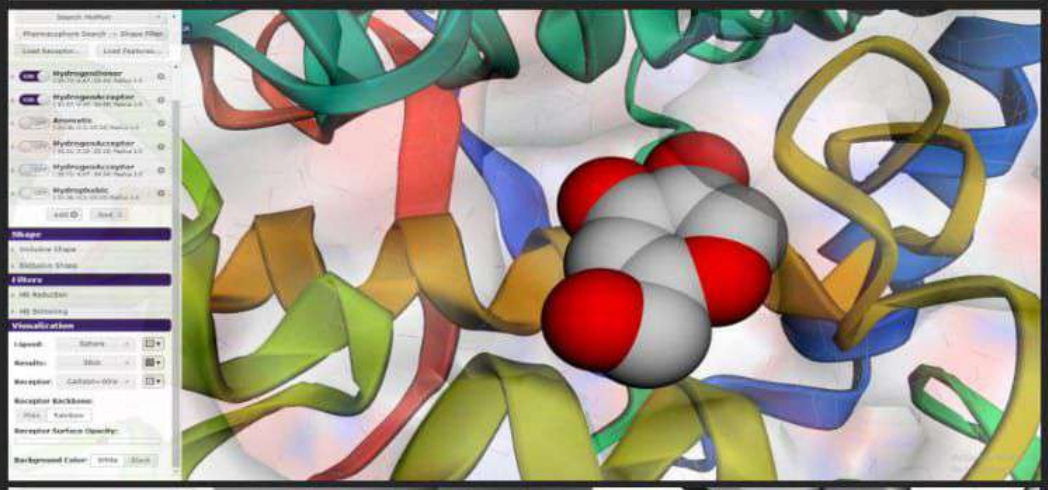
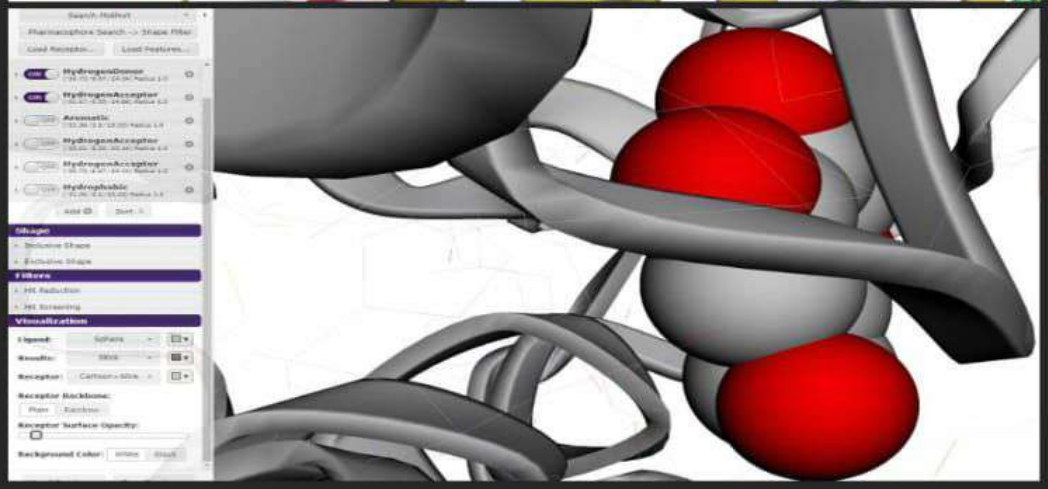
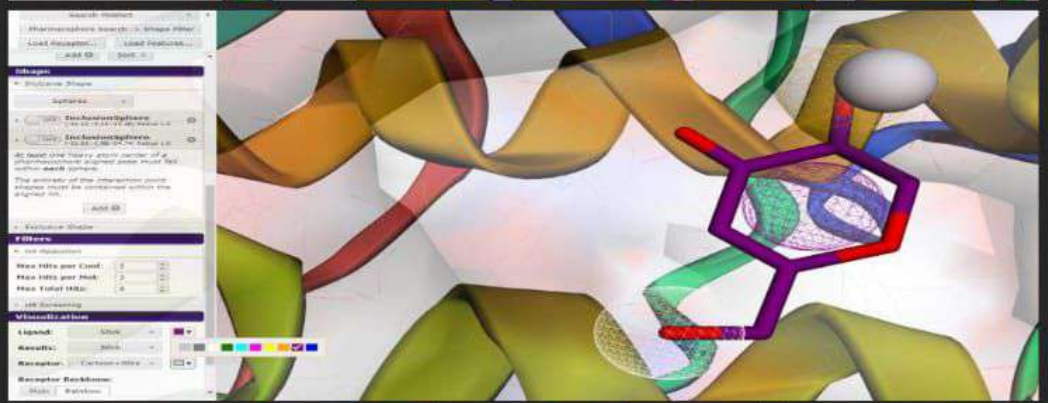
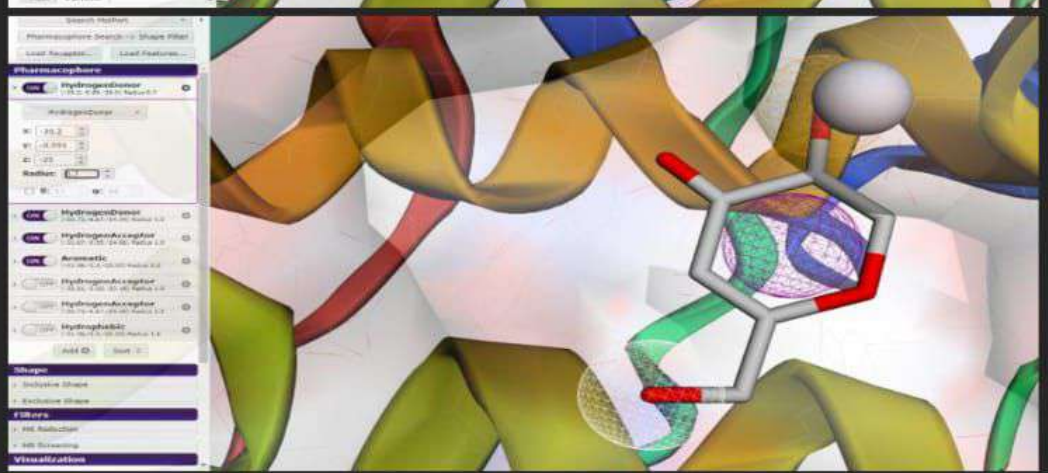
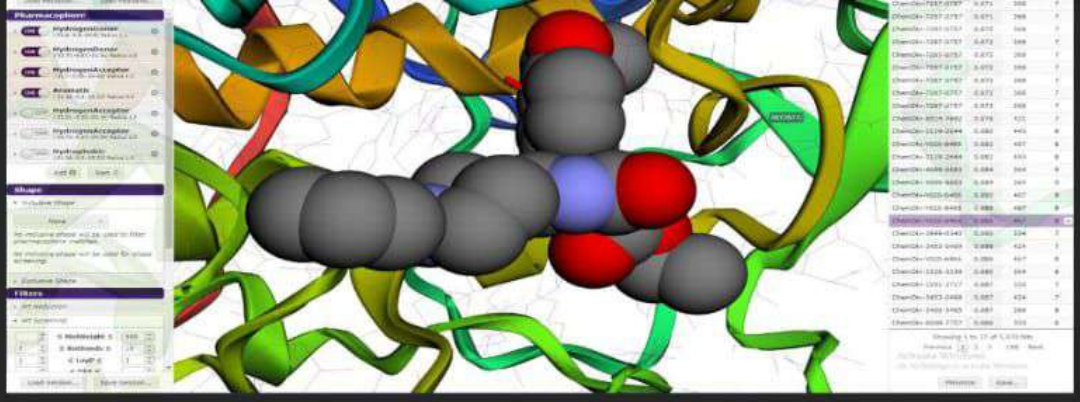


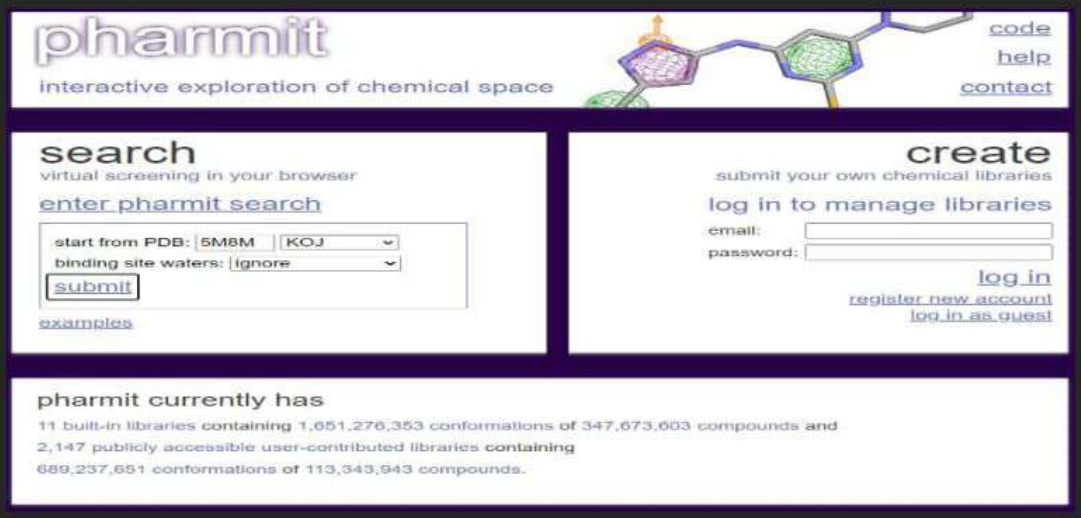


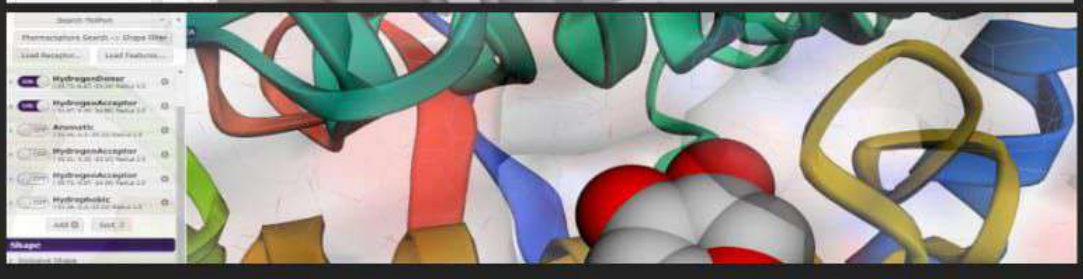







RCSB PDB
5M8M
Crystal structure of human tyrosinase related protein 1 in complex with kojic acid


pharmit
interactive exploration of chemical space
code
help
contact
search
virtual screening in your browser
enter pharmit search
start from PDB: 5M8M KOJ
binding site waters: ignore
submit
examples
create
submit your own chemical libraries
log in to manage libraries
email:
password:
log in
register new account
log in as guest
pharmit currently has
11 built-in libraries containing 1,651,276,353 conformations of 347,673,603 compounds and
2,147 publicly accessible user-contributed libraries containing
689,237,651 conformations of 113,343,943 compounds.



Rules:-

1) No more than 5 hydrogen bond donors.
2) No more than 10 hydrogen bond acceptors
3) Molecular mass less than 500 daltons
4) Octanol water partition coefficient (log P) Should be less than =5
5) Rotatable bond (<=10)

* After setting all parameters & constraints press the arrow next to first button on left side bar to search database.
* The option will open select the desired databases & press search button to initiate search.
* Right side bar opens display search result.
* For saving & loading session two buttons at the bottom left side bar can be used.
* The results are saved, by clicking on save page.

Result & Discussion:-

* Result are plotted in increasing or decreasing order based RMSD, mass, number of rotatable bonds.
* The sorting was done based on RMSD & obtain results were recorded.
* The query allined pose was visualised by clicking the corresponding row in results panels.
* A selected compound was option initiating a new query using compound as query ligands. can further used docking studies.

Name of Experiment.....
Experiment No. 11
Date 21/2/24
Experiment Result.....
Page No. 35

URL: https://pharmit.csb.pitt.edu/index
www.rcsb.org.

Query:- 2054/4BB2/5M80/5M8M/4PPS.

Procedure:-

* Login using the URL https://pharmIT.csb.pitt/edu.index.php to initiates a search using PDB accusion code.
* Structure can be obtained directly from entering four character PDB identifier in first text box.
* A list of possible small molecules will be generated automatically in second box. Select ligand of interest
* Binding site waters may be excluded entirely or otherwise as it is optional pharmaco-features.
* Click on Submit to proceed.
* Click on optionally, Click on enter format search to upload structural files.
* After being redirected to search page choose load features to upload ligand SDS/PDB/mol-2 formats.
* A receptors file in any of the same format may optionally provided as well.
* Visualization of molecule can be done after the desired structure are provided.
* All possible Pharmaco features will be identified next it will enter the features & use set of default visualization option to displayed provided structure.

* Scroll down to visualization menu in left sidebarn & toggle the option as desired.
* To obscure the pharmacofeature, reduce the surface receptor opicity at lowest setting.
* Click on spears of both pharmacophore & Shape Constors & toryal between solid & wire display
* Pharmacophore used to define molecular similarity & perform structural alignment. This feature is also available in site bar menu & Can be toggled ON/OFF to include them or remove them.
* Press arrow on left of given pharmacophore & vary tie, radius & location of pharmacophore
* Restrict the atom number associated of required.
* Shape constrains are introduced by choosing spear option in dropdown menu & press ADD.
* Set position & Size of sphere.
* press add again to continue adding sphere.
* Defined both inclusive & exclusive shape constrains using legends & receptor surfaces.
* Click on the filters option to screen for Lits & Flexibility.
* Here Lipinskin parameters are set to generate the best pattern also set maximum hits per Conf" per molecules (Lipinskin rule).

Experiment No. ..... Experiment Result .....

Derivation of Pharmacophore pattern for selecting ligands.

Aim:- To design a pharmacophore pattern for relative ligand using pharma IT online software tool.