BAITOC

(Bio activity information to organic chemists)

http://www.scfbio-iitd.res.in/software/drugdesign/baitocnew.jsp

The BAITOC utility enables the user to upload his/her organic (small) molecule and informs the user about which protein from the protein data bank (PDB) repository it is likely to inhibit, the microorganism the protein belongs to along with the disease caused by the microorganism.

Step 1:

(a) Sketch the structure with **Marvin** (http://www.chemaxon.com/download/marvin/for-end-users/)/ **CHEM DRAW** or

(b) Download the molecule from a **public database** say, ZINC database (http://zinc.docking.org/); PubChem (http://pubchem.ncbi.nlm.nih.gov/); NRDBSM (http://www.scfbio-iitd.res.in/software/nrdbsm/drugsearch.jsp).

Step 2:

If the molecule is drawn by the **Marvin** then please do the following.

(a) Draw the molecule as with Chem Draw
(b) Add explicit hydrogens; Structure => Add => Add Explicit Hydrogens
(c) Convert the structure from 2D to 3D; structure => Clean 3D => Clean in 3D
(d) Save as .pdb format on your Desktop; File => Save As… => Change Files of type: Protein Data Bank/PDB (*.**pdb**)
(e) Upload the molecule in the appropriate box in BAITOC server
(f) Input formal charge of the molecule and email-id and press submit
(g) Result will be e-mailed automatically at the specified ID
(h) User can also track the job status via the Jobid.

OR

Step 2:

If the molecule is drawn by **Chem Draw** software then please do the following.

(a) Clean the structure by selecting the whole molecule and press shift+ctrl+k
(b) Save the molecule with mol file type; File => Save As… => change ChemDraw (*.cdx) to MDL Molfile (*.**mol**)
(c) Press enter to save the molecule
(d) Upload the molecule in the appropriate box at BAITOC server
(e) Input formal charge of the molecule and email-id and press submit
(f) Result will be e-mailed to you automatically at the specified Email ID
(g) User can also track the job status via the Jobid.

OR

Step 2: Molecular coordinates can be directly downloaded from ZINC database, PubChem, NRDBSM and submitted to BAITOC.

OR

Step 2: Coordinates of your own molecule (in *.pdb, *.mol, *.sdf or *.xyz formats) can be directly submitted to BAITOC.

Output

The output emailed to you will have four columns with ascending order of binding energy with the uploaded ligand (molecule) to the protein of the microorganism.

(1) First column: PDBID (www.rcsb.org) of the protein your molecule is likely to interact with;
(2) Second column: KEGG ID (say H00313); (KEGGID is the disease id of the KEGG DISEASE Database (http://www.genome.jp/kegg/disease/). This database is the collection of the human diseases caused by known genetic factor or known pathogen.
(3) Third column: Name of the Microorganism to which the above protein belongs;
(4) Fourth column: Disease caused by the pathogen (microorganism) to the human.

Some steps to remember before uploading molecules to BAITOC

For Marvin user

NB 3: Marvin is the chemical structure drawing software. It is freely available. One can directly go to the Chem Axon site (http://www.chemaxon.com/) and click for downloading Marvin software (http://www.chemaxon.com/download/marvin/for-end-users/). User has to install Windows Installer with Java for windows platform.

NB 4: Save the file at *.xyz/*.pdb format is reuired.

File => Save As… => Change Files of type: Protein Data Bank/PDB (*.**pdb**)/XYZ (***.xyz**)

For Chem Draw user

NB 1: Clean the structure by pressing shift+ctrl+k

NB 2: Save the file with extension '.mol' (as *.mol). (* refers to the name you gave to the molecule)

File => Save As… => change ChemDraw (*.cdx) to MDL Molfile (*.**mol**)