Active Site Determination of an Enzyme

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Computational Biology Project

I am presenting a computational biology tool that helps in the determination of the presence of active sites in peptide molecules. Active sites are the resides of a peptide molecule that form temporary bonds with substate molecules.
The probable active sites of the peptide being probed are noted from another tool available online. The PDB file of the protein and the residue numbers of the probable active sites are given as input.
This tool confirms if the suspected active sites are present and gives out the PDB files of the active sites as outputs.
The output PDB files can be visualised with the help of already existing softwares like PyMol.
For the purpose of demonstration on how to use this tool, 8tim.pdb are 5ire.pdb have been taken as examples.

How to use it:

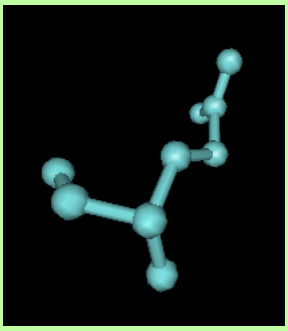
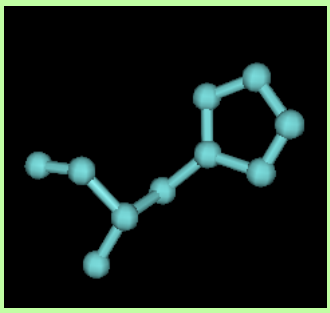
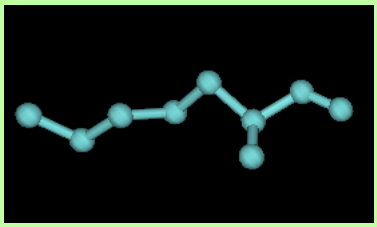
Step-1: You have to rename your .pdb file with the name “filename.pdb” and save it in the program folder.
Step-1: Then, you have to run the “Tool” named .exe file present in the “Program folder”.
Step-2: You will be prompted to enter the residue numbers of the probable active sites which you can find out from this online portal: http://sts.bioe.uic.edu/castp/index.html?1ycs
Step-3: Follow other commands given on the console window.

Output:

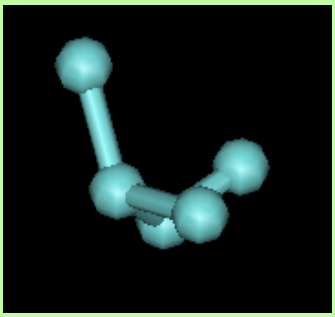
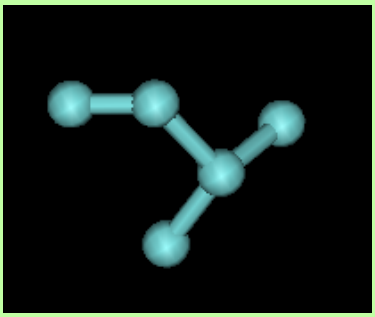
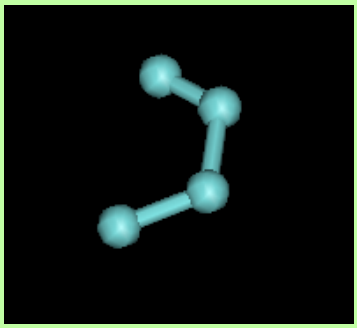
The pdb files of the residues of the active sites will be written on the already existing pdb files in the program folder which have names, ActiveSiteA, ActiveSiteB, ActiveSiteC and ActiveSiteD. If there are only two three residues then, ActiveSireD will be empty. If there are only 2 active sites then, ActiveSiteC and ActiveSiteD will be empty, and so on.

Examples:
The output pdb files were visualised using other existing tools, here are the images of the structures outputted.

1) 8tim.pdb

1) 5ire.pdb

Applications:
It can be useful in screeening proteins that contain a particular active site. Thus it can be a helpful tool in drug discovery.
Its modified versions might be used to determine active sites from pdb files without any prior hint.