

Lab Worksheet 15

SDS348/385

All enzymes contain a cluster of functional amino acids called catalytic residues. We are interested in visualizing those residues. Write a python PyMOL script that:

- Downloads an enzyme structure of your choice
- Shows the catalytic residues as white spheres
- Shows the rest of the structure as a cartoon
- Colors the structure (except catalytic residues) according to b-factors

HINTS:

- Find an enzyme in the RCSB database. Enzymes typically end in “-ase.”
RCSB database: <http://www.rcsb.org/pdb/home/home.do>
- After you have selected a structure and have its PDB ID, you can find catalytic residue information in the Catalytic Site Atlas:
<http://www.ebi.ac.uk/thornton-srv/databases/CSA/>