enz

February 12, 2021

enz

enz is a python package for enzyme deisgn

enz is an interface to protein structure-prediction and molecular docking algorithms

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enz uses *pyrosetta* for structure predictions and *autodock vina* for molecular docking

enz commands

- `enz.protein(...` - initialize a protein object from a `.pdb` file

- `enz.protein.mutate(` - mutate a residue

- `enz.protein.refold()` - predict the structure of the mutant

- `enz.protein.dock(` - dock a ligand to a site in the protein

other **enz** objects

- `results` - returned by the `dock()` function
- `mol` - a generic molecule object, used to represent poses in `results`