

SAAMBE-3D

Running predictions of $\Delta\Delta G$ due to single mutation (1)

User Input Mutations

Prediction of $\Delta\Delta G$ over Single Mutation (1)

PDB Selection: 1a22.pdb (3)

Mutation Details:

Position: 182 (5)	Chain: A (6)
Original Amino Acid: C (8)	Mutated Amino Acid: A (9)

Prediction of Disruptive/Non-Disruptive Mutations (2)

PDB Selection: (4)

Mutation Details:

(7)

Upload a plain text file with one mutation per line, [click here](#) to view an example for reference

Results will be displayed here

Structure: 1a22.pdb
Chain: A
Position: 182
Original Amino Acid: C
Mutated Amino Acid: A
ΔΔG Prediction: 0.80 kcal/mol, Destabilizing

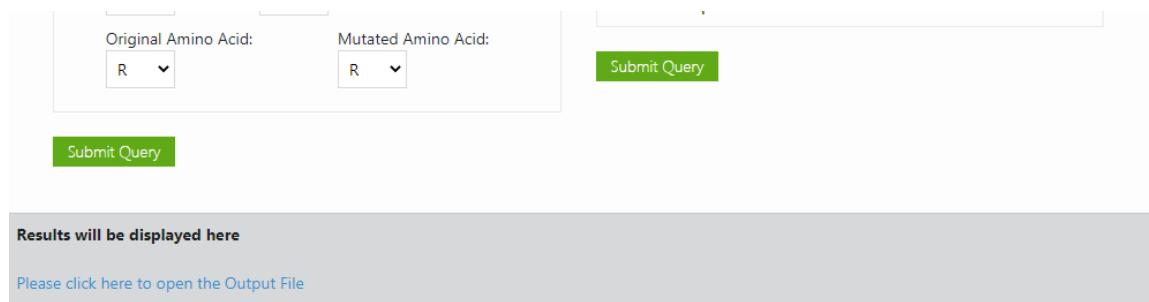
- The *Single Mutation* option allows the user to submit one single mutation for prediction.
 - Users are required to provide a wild-type structure by uploading (3) a file in pdb format.
 - Details on the single mutation should be provided: (5) *residue position*, (6) *mutated chain*, (8) *wild type amino acid* and (9) *mutant amino acid* (using the one letter amino acid code). The residue position must be consistent with the PDB file.
- The *Mutation List* option allows the user to submit a list of single mutations to be analyzed in batch.
 - Similar to the *Single Mutation* option, a wild-type sequence is required and can be input by uploading (4) a file in pdb format.
 - The list of single-point mutations must be input (7) by uploading a file containing the mutation information (*chain identifier, residue position, wild-type residue code and mutant residue code*). The file format requires one mutation per line (split by space). A sample file is also provided.

Results

Single Mutation

- The predicted $\Delta\Delta G$ for a single-point mutation will be displayed on the bottom of the same page.

Multiple single mutations



Original Amino Acid: R

Mutated Amino Acid: R

Submit Query

Results will be displayed here

Please click here to open the Output File

- The predicted $\Delta\Delta G$ for the multiple single mutations will be showed on the bottom of the same page. Users can download the output file.

Predict whether the given mutation is disruptive or non-disruptive (2)

The input is exactly the same as the predictions of $\Delta\Delta G$, and the result is displayed in the same position (bottom).