*Data article*

# Molecular docking of *Sulfobacillus acidophilus* barbiturase with s-triazine compounds

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**Abstract**

Barbiturases have scarce structural information available and do not fit in the conventional group of proteins. It is contemplated that they play a role in catabolism of s-triazine herbicide compounds. Structure as well as interaction data information of barbiturase with s-triazine compounds is missing. Sequence data is a goldmine of biological information and acts as raw material for structure and docking analysis. De novo structure prediction of the *Sulfobacillus acidophilus* DSM 10332 barbiturase has been attempted in this data article. Molecular docking analysis was carried out with atrazine, simazine and hexazinone belonging to s-triazine class of herbicides. The analysis revealed key residues necessary for these interactions. The generated data could be used by environmental scientists working on the enzyme assisted herbicide degradation.

**Keywords:** barbiturase, s-triazine compounds, homology modeling, molecular docking, *in silico*.

**Specifications Table**

| | |
|---|---|
| Subject area | *Biology, Chemistry, Environmental Sciences, Bioinformatics, Computational Biology, Enzymology* |
| More specific subject area | *Bioremediation* |
| Type of data | *Table, figures* |
| How data was acquired | *Database, Software, Webserver* |
| Data format | *Raw, analyzed* |
| Experimental factors | *Energy minimization and Clustering RMSD 4Å for docking* |
| Experimental features | *Homology modeling of barbiturase using I-TASSER. Visualization in Pymol. Molecular docking using Patchdock. 2D plot analysis of docked complex for inferring interactions using LigPlot*$^{+}$. |
| Data accessibility | *Sequence data for barbiturase can be accessed at NCBI database using accession no. AEW05774.1. Chemical structuresof s-triazine compounds are available at PubChem database.* |

**Value of the data**

- Data could be used for generating better mutants of barbiturase for improved s-triazine compound degradation.
- Data could be used as baseline for expanded analysis of barbiturase with other triazine compounds.
- Comparison of conserved active site residues essential for degradation of class of these compounds could provide useful insights to environmental scientists working on bioremediation.

**Summary**

Binding geometries and interactions are mandatory to aid bioremediation catalyst design using combination of docking and visualization. Visual examination of predicted binding geometries (docking poses), contributes crucially to the further development of a better mutant either towards enhanced binding affinity leading towards efficient activity or towards increased tolerance to extreme environmental conditions.

Structure of the barbiturase enzyme and interaction parameters with three triazine compounds is reported in this data article. Molecular docking sheds light on putative binding and non-binding sites of barbiturase with s-triazine compounds. Experimental testing is recommended for validation of this information.

**Experimental Design, Materials and Methods**

Sequence data of barbiturase with Accession no: AEW05774.1 was obtained from NCBI database (http://ncbi.nlm.nih.gov). 2D structure of three s-triazine compounds atrazine, simazine and hexazinone was obtained from Pubchem (http://pubchem.ncbi.nlm.nih.gov). They were converted to PDB format using OpenBabel software (OLBoyle et al. 2011). Structure modeling of barbiturase was attempted using I-TASSER as previously described (Zhang, 2008; Roy et al. 2010; Basharat and Yasmin, 2015; Basharat and Yasmin, 2016). Model with best confidence score of 2, estimated TM-score of 0.99±0.04 and estimated RMSD of 2.5±1.9Å was selected for further analysis (Fig. 1, Supplementary File 1).

Model was rendered in Pymol. After energy minimization with MOE software, docking was carried out using Patchdock server (http://bioinfo3d.cs.tau.ac.il/PatchDock) (Table 1). 2D plot was visualized using LigPlot$^{+}$ to infer interactions involving hydrogen bonds and hydrophobic interactions in barbiturase-atrazine complex (Fig. 2, Supplementary File 2), barbiturase-simazine complex (Fig. 3, Supplementary File 3) and barbiturase-hexazinone complex (Fig. 4, Supplementary File 4).

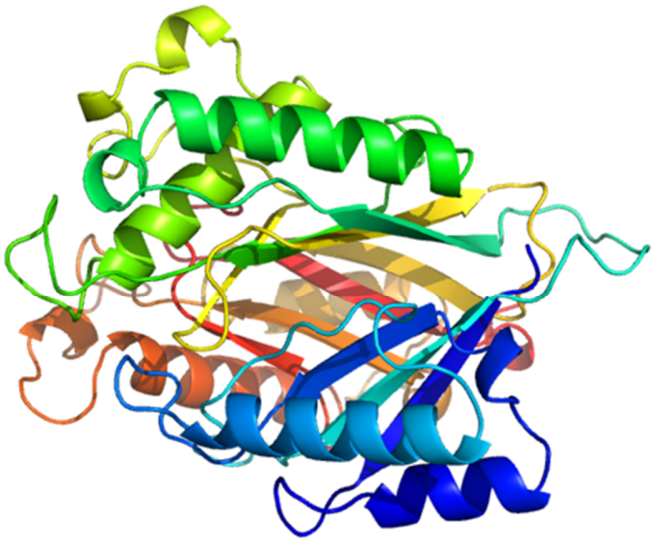

Fig. 1. 3D structure of the *Sulfobacillus acidophilus* DSM 10332 barbiturase enzyme.

Table 1. Parameters of docked s-triazine compounds with barbiturase protein.

| Complex | Score | Area | ACE score | Transformation parameters |
|---|---|---|---|---|
| Barbiturase-atrazine | 2696 | 315.20 | -173.14 | -0.47, 0.55, 1.99, 3.93, 11.95, 8.85 |
| Barbiturase-simazine | 3172 | 363.00 | -96.82 | -1.08, 0.39, -0.59, 8.77, 0.71, -10.67 |
| Barbiturase-hexazinone | 3752 | 434.50 | -136.66 | -2.59, 0.23, -2.32, 15.49, 0.39, -8.80 |

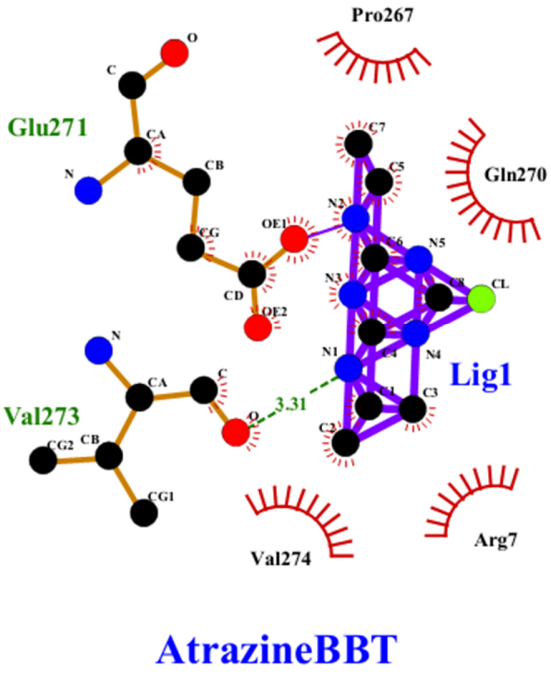


Fig. 2. Atrazine-barbiturase complex showing a hydrogen bond between nitrogen of atrazine and oxygen of barbiturase Val273. Four hydrophobic interactions of atrazine with Arg7,Val274, Pro267 and Gln270 were observed.

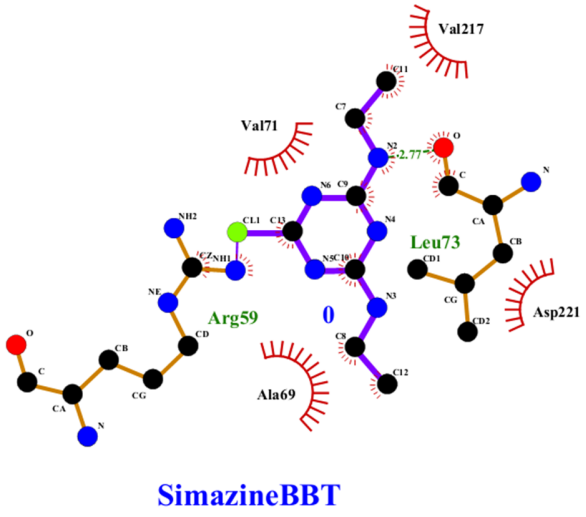


Fig. 3. Simazine-barbiturase complex showing a hydrogen bond between nitrogen of simazine and oxygen of barbiturase ALeu73. Four hydrophobic interactions of simazine with Val71, Ala69, Asp221 and Val217 were observed.

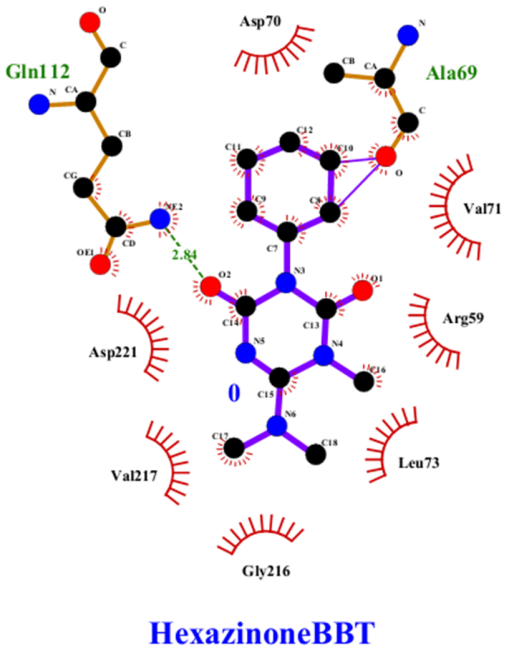


Fig. 4. Hexazinone-barbiturase complex showing a hydrogen bond between oxygen of hexazinone and nitrogen of barbiturase Gln112. Seven hydrophobic interactions of hexazinone with Val171, Arg59, Leu73,Gly216, Val217, Asp221 and Asp70 were observed.

**References**

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