

Modeling of streptokinase protein

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ABSTRACT

Modeling of streptokinase protein was done using SWISS-MODEL software and valuable structural details were studied. The reacting sites in the protein could be visualised.

Key words: Modeling, streptokinase, protein

INTRODUCTION

Streptokinase protein derived from *Streptococcus pyogenes* plays an important role in dissolving clots/blockages in the blood vessels and thus is very useful from medicinal point of view. Study of its structures could help in understanding it fully.

MATERIALS AND METHODS

Protein

Streptococcus pyogenes sk gene for streptokinase, isolate Indian was downloaded GenBank: AM903378.1 linear 1353 bp DNA and amino acid sequence was used for modelling.

Modelling software

<https://swissmodel.expasy.org> was reached to model the protein.

RESULTS AND DISCUSSION

Project summary

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MKNYLSFGMFFALFTFGTVKPVQAIAGPEWLLDRPSVNNSQLVVSVAGTVEGTNQEISLKF FEIDLTSQPAHGGKTEQGLSPKSKP 12
FATNSSAMPHKLEKADLLKAIQEQLIANVHSN 0

DGYFEVIDFASDATITDRNGKVYFADRDDSVTLPTQPVQEFLLSGHVRVRPYQPKAVHNSAERVN VNVEVSFVSETGNLDFTPSLKER 24
YHLTTLAVGDSLSSQELAAIAQF ILSKEHPDY 0

IITKRDSSIVTHDNDIFRTILPMDQEFTYHIKDRQAYKANSKTGIVEKTNNTDLISEKYYVLKKGKPYDPFDRSHLKLFTINYVDV 36
NTKALLKSEQLLTASERNLDFRDLYDPRDKAK 0

LLYNNLDAFGIMDYTLTGKVEDNHDDTNRIITVYMGKRPEGENASYHLAYDKDRYTEEEREVYSYLRYTGTPIPDNPDKD 44
0

```

Template Results

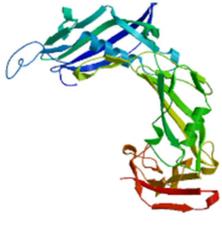
A total of 44 templates were found to match the target sequence. This list was filtered by a heuristic down to 16. The top templates are:

Sequence Identity	Biounit Oligo State	Description
1bml.1	83.70	hetero-tetramer STREPTOKINASE COMPLEX OF THE CATALYTIC DOMAIN OF HUMAN PLASMIN AND STREPTOKINASE

Sequence Identity	Biounit Oligo State	Description
1l4z.1	93.33	hetero-dimer Streptokinase X-RAY CRYSTAL STRUCTURE OF THE COMPLEX OF MICROPLASMINOGEN WITH ALPHA DOMAIN OF STREPTOKINASE IN THE PRESENCE CADMIUM IONS
1qqr.1	65.94	monomer STREPTOKINASE DOMAIN B CRYSTAL STRUCTURE OF STREPTOKINASE DOMAIN B
1qqr.3	65.94	monomer STREPTOKINASE DOMAIN B CRYSTAL STRUCTURE OF STREPTOKINASE DOMAIN B
1qqr.4	65.94	monomer STREPTOKINASE DOMAIN B CRYSTAL STRUCTURE OF STREPTOKINASE DOMAIN B

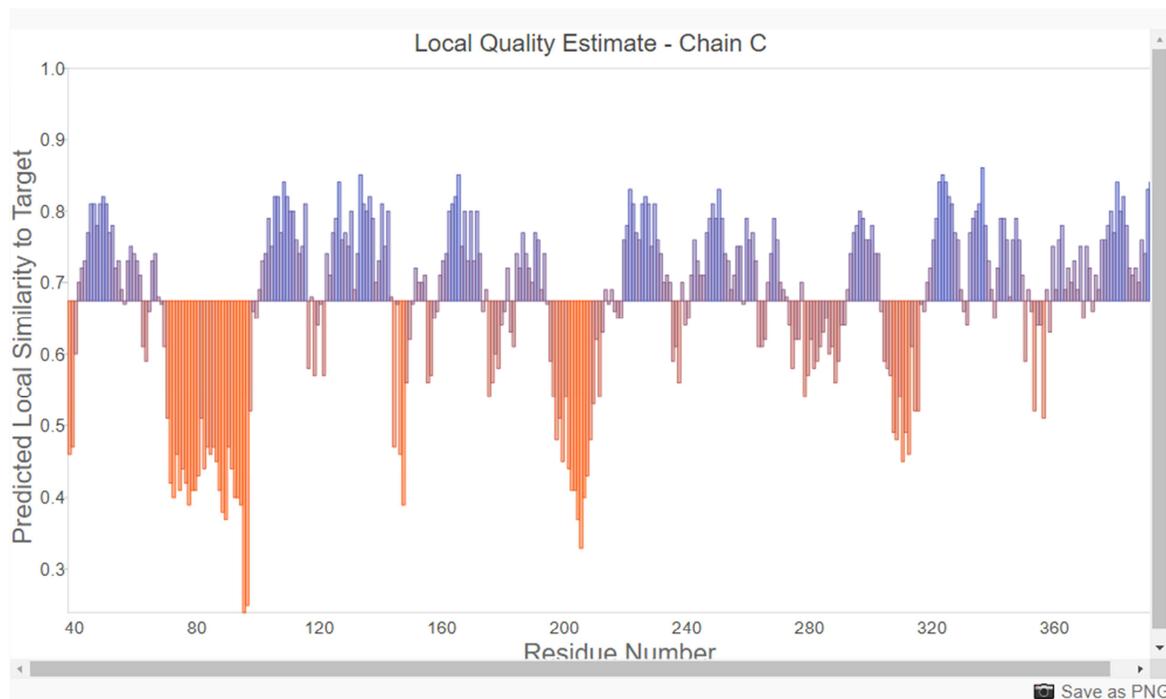
Model Results

Id Template GMQE QMEANDisCo Global Oligo State Ligands

	01	1bml.1.C	0.57	0.67 ± 0.05	monomer	-
	02	5acp.1.A	0.00	± 0.12	monomer	-



Model Results



It may be seen that valuable models were constructed and the structural details and binding sites could be visualized.

REFERENCES

Berman, H., Westbrook J., Feng Z., Gilliland G., Bhat T. N., Weissig I., Shindyalov I., Bourne P. E. 2000. The Protein Data Bank. *Nucleic Acids Res*, 28: 235-242.

Berman, H., Henrick, K., Nakamura, H. and Markley, J.L. 2007. The worldwide Protein Data Bank (wwPDB): ensuring a single, uniform archive of PDB data. *Nucleic Acids Res*, 35: D301-303.

Bienert, S., Waterhouse, A., de Beer, T.A.P., Tauriello, G., Studer, G., Bordoli, L., Schwede, T. 2017. The SWISS-MODEL Repository - new features and functionality. *Nucleic Acids Res*. 45: D313-D319

Bordoli, L., Schwede T. 2012. Automated protein structure modeling with SWISS-MODEL Workspace and the Protein Model Portal. *Methods Mol. Biol.* 857: 107-136.

Grosdidier A, Zoete V, Michielin O. 2011. SwissDock, a protein-small molecule docking web service based on EADock DSS. *Nucleic Acids Res*, 39: W270-7.

Grosdidier A, Zoete V, Michielin O. 2011. Fast docking using the CHARMM force field with EADock DSS. *J Comput Chem.* 32: 2149-2159.

Studer, G., Tauriello, G., Bienert, S., Biasini, M., Johner, N., Schwede, T. 2021. ProMod3 - A versatile homology modelling toolbox. *PLOS Comp. Biol.* 17: e1008667.

Steinegger, M., Meier, M., Mirdita, M., Vöhringer, H., Haunsberger, S. J., Söding, J. 2019. HH-suite3 for fast remote homology detection and deep protein annotation. *BMC Bioinformatics* 20: 473.



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[www. biotechnologyinternational.org](http://www.biotechnologyinternational.org)

Studer, G., Tauriello, G., Bienert, S., Waterhouse, A.M., Bertoni, M., Bordoli, L., Schwede, T., Lepore, R. 2019. Modeling of Protein Tertiary and Quaternary Structures Based on Evolutionary Information. *Methods Mol. Biol.* 1851: 301-316.

The UniProt Consortium. 2017. UniProt: the universal protein knowledgebase. *Nucleic Acids Res.* 45: D158-D169.

Waterhouse, A., Bertoni, M., Bienert, S., Studer, G., Tauriello, G., Gumienny, R., Heer, F.T., de Beer, T.A.P., Rempfer, C., Bordoli, L., Lepore, R., Schwede, T. 2018. SWISS-MODEL: homology modelling of protein structures and complexes. *Nucleic Acids Res.* 46: W296-W303.