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THE APPLICATION OF BIOINFORMATIC METHODS FOR THE ANALYSIS OF PROTEIN TARGETS OF MICROORGANISMS PRODUCING BIOSURFACTANTS

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Aim. The objective of this study is to identify key protein targets involved in the metabolism, regulation, and transport of biosurfactants. Target selection was based on a comprehensive analysis of biological databases and scientific literature. The identified proteins are essential for biosurfactant biosynthesis and will serve as the foundation for subsequent investigations using reverse molecular docking.

Methods. Protein targets were identified through open-access biological databases, including RCSB PDB and UniProt, with a focus on microorganisms recognized as biosurfactant producers. Relevant literature was analyzed to validate the functional roles of specific proteins in biosurfactant metabolism. Selection criteria encompassed proteins directly involved in enzymatic synthesis, transport pathways, and gene expression regulation associated with biosurfactant production.

Results. Eight protein targets were identified as being associated with biosurfactant synthesis. Functional annotation and literature validation confirmed their relevance to microbial biosurfactant metabolism.

Conclusion. These findings provide a solid basis for further research, including computational modeling and experimental validation, to clarify the roles of the identified proteins in biosurfactant production. The study underscores the importance of integrating electronic databases with literature analysis to identify potential biomolecular targets for future biotechnological applications.

Key words: biosurfactants, databases, protein targets, molecular docking, microbial metabolism.

Biosurfactants produced by microorganisms have a variety of industrial and environmental applications [1]. Identification of key proteins involved in the metabolic pathways of biosurfactant synthesis and regulation is of practical importance, as it provides the basis for studying their molecular mechanisms of action. In this study, biological databases and scientific literature were searched to identify proteins, based on their

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functional role, and annotated as enzymes, transporters, or regulatory factors in these pathways. Based on their functional role, key target proteins were selected.

The objective of this study was to identify and select key protein targets, including enzymes, transporters, and regulatory proteins, that responsible for the metabolism, regulation, and transport processes underlying biosurfactant biosynthesis. The selection was based on an extensive review of biological databases and scientific literature. The selected targets will form the basis for further studies using reverse molecular docking.

Methods

We searched for proteins related to the synthesis of biosurfactants within the open databases RCSB PDB and UniProt, focusing on microorganisms such as *Pseudomonas aeruginosa*, *Escherichia coli*, *Bacillus subtilis*, *Staphylococcus aureus*, and *Brevibacillus parabrevis*, all known for producing surface-active substances. We analyzed literature data to confirm the role of specific proteins in metabolism.

The proteins were selected based on their role in the biosynthesis of biosurfactants, including enzymes, transporters that facilitate biosurfactants secretion, and regulatory proteins that control gene expression.

Results and Discussion

The selection process led to the identification of several proteins that are directly related to surfactant biosynthesis. A diverse set of targets associated with various aspects of biosurfactant metabolism, including the biosynthetic enzymes involved, their regulation, and biosurfactant transport, have been obtained. A list of eight protein targets was compiled by integrating data from different sources. PDB ID: 1ABE, 1JMK, 2B4Q, 2CBG, 3RKY, 4MRT, 8F7F, 8IK2 [2–9]. Fig. 1 shows the resolution of the protein structure of each of the eight targets.

The analysis of functional annotations and literature data provided a solid basis for the choice of proteins that play a key role in the synthesis of biosurfactants. Although the approach used in this study ensures a thorough selection process, certain limitations remain. Using existing annotations and literature data means that some potentially key but less characterized proteins may have been missed. Nevertheless, the selected targets represent a well-founded basis for future research and experimental validation, including mathematical modeling, to confirm their functional role and potential applications.

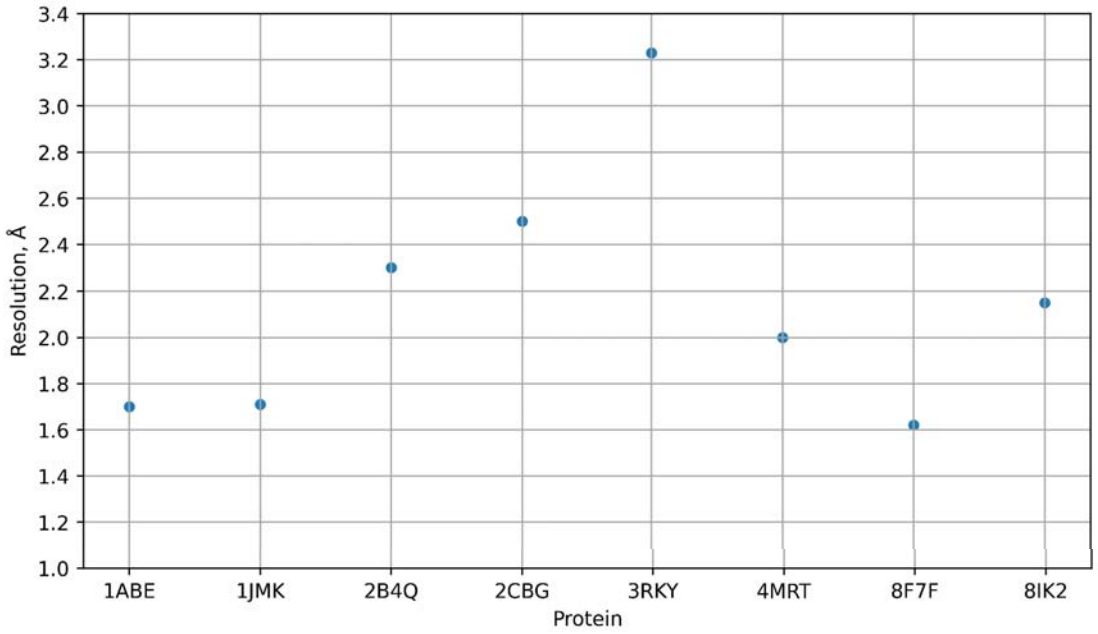

Fig. 1. **Resolution (Å) of PDB structures of target proteins from the RCSB electronic database**

Conclusions

Eight protein targets involved in the metabolism, transport, and regulation of biosurfactant production were identified. The selection was based on an extensive review of biological databases and scientific literature to ensure the relevance of biosurfactant-related processes. The results provide a basis for future biomolecular studies to elucidate the role of these proteins in the synthesis of microbial biosurfactants. The work demonstrates the importance of electronic databases and preliminary identification of protein targets, highlighting key proteins that can be further investigated by reverse molecular docking.

Authors' contribution

Ye.B. Yanvarov — developed the concept and collected relevant sources; V.V. Havryliak — project administration, conceptualization, data curation; H.V. Melnik — collected relevant sources; V.O. Stepanenko — review & editing.

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REFERENCES

1. Sarubbo, L. A., Silva, M. da G. C., Durval, I. J. B., Bezerra, K. G. O., Ribeiro, B. G., Silva, I. A., Twigg, M. S., Banat, I. M. (2022). Biosurfactants: Production, properties, applications, trends, and general perspectives. *Biochemical Engineering Journal*, 181, 108377. https://doi.org/10.1016/j.bej.2022.108377
2. Quiocho, F. A., Vyas, N. K. (1984). Novel stereospecificity of the L-arabinose-binding protein. *Nature*, 310(5976), 381–386. https://doi.org/10.1038/310381a0
3. Bruner, S. D., Weber, T., Kohli, R. M., Schwarzer, D., Marahiel, M. A., Walsh, C. T., Stubbs, M. T. (2002). Structural Basis for the Cyclization of the Lipopeptide Antibiotic Surfactin by the Thioesterase Domain SrfTE. *Structure*, 10(3), 301–310. https://doi.org/10.1016/S0969-2126(02)00716-5
4. Miller, D. J., Zhang, Y.-M., Rock, C. O., White, S. W. (2006). Structure of RhlG, an Essential β-Ketoacyl Reductase in the Rhamnolipid Biosynthetic Pathway of *Pseudomonas aeruginosa*. *Journal of Biological Chemistry*, 281(26), 18025–18032. https://doi.org/10.1074/jbc.M601687200
5. Samel, S. A., Wagner, B., Marahiel, M. A., Essen, L.-O. (2006). The Thioesterase Domain of the Fengycin Biosynthesis Cluster: A Structural Base for the Macrocyclization of a Non-ribosomal Lipopeptide. *Journal of Molecular Biology*, 359(4), 876–889. https://doi.org/10.1016/j.jmb.2006.03.062
6. Pendini, N. R., Yap, M. Y., Polyak, S. W., Cowieson, N. P., Abell, A., Booker, G. W., Wallace, J. C., Wilce, J. A., Wilce, M. C. J. (2013). Structural characterization of *Staphylococcus aureus* biotin protein ligase and interaction partners: An antibiotic target. *Protein Science*, 22(6), 762–773. https://doi.org/10.1002/pro.2262
7. Tufar, P., Rahighi, S., Kraas, F. I., Kirchner, D. K., Löhr, F., Henrich, E., Köpke, J., Dikic, I., Güntert, P., Marahiel, M. A., Dötsch, V. (2014). Crystal Structure of a PCP/Sfp Complex Reveals the Structural Basis for Carrier Protein Posttranslational Modification. *Chemistry & Biology*, 21(4), 552–562. https://doi.org/10.1016/j.chembiol.2014.02.014
8. Folger, I. B., Frota, N. F., Pistofidis, A., Niquille, D. L., Hansen, D. A., Schmeing, T. M., Hilvert, D. (2024). High-throughput reprogramming of an NRPS condensation domain. *Nature Chemical Biology*, 20(6), 761–769. https://doi.org/10.1038/s41589-023-01532-x
9. Tang, T., Fu, L., Xie, W., Luo, Y., Zhang, Y., Zhang, J., Si, T. (2023). RhlA Exhibits Dual Thioesterase and Acyltransferase Activities during Rhamnolipid Biosynthesis. *ACS Catalysis*, 13(8), 5759–5766. https://doi.org/10.1021/acscatal.3c00046

ВИКОРИСТАННЯ БІОІНФОРМАТИЧНИХ МЕТОДІВ ДЛЯ АНАЛІЗУ ПРОТЕЇНОВИХ МІШЕНЕЙ МІКРООРГАНІЗМІВ ПРОДУЦЕНТІВ БІОСУРФАКТАНТІВ

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Мета. Метою було визначити ключові протеїнові мішені, що беруть участь у метаболізмі, регуляції та транспорті біосурфактантів. і слугуватимуть основою для подальших досліджень з використанням зворотного молекулярного докінгу.

Методи. Протеїнові мішені було ідентифіковано за допомогою біологічних баз даних з відкритим доступом, включаючи *RCSB PDB* та *UniProt*, з акцентом на мікроорганізми, визнані продуцентами біосурфактантів. Було проаналізовано відповідні джерела літератури для підтвердження функціональної ролі певних протеїнів у метаболізмі біосурфактантів. Критерії відбору охоплювали протеїни, безпосередньо залучені до ензиматичного синтезу, механізмів транспорту та регуляції експресії генів, пов'язаних із виробництвом біосурфактантів.

Результати. Було ідентифіковано вісім протеїнових мішеней, пов'язаних із синтезом біосурфактантів. Функціональна анотація та валідація літератури підтвердили їхню актуальність для метаболізму мікробних біосурфактантів.

Висновки. Ці результати забезпечують міцну основу для подальших досліджень, включаючи комп'ютерне моделювання та експериментальну валідацію, щоби з'ясувати роль ідентифікованих протеїнів біосурфактантів. Дослідження підкреслює важливість інтеграції електронних баз даних з аналізом літератури для визначення потенційних біомолекулярних мішеней для майбутніх біотехнологічних застосувань.

Ключові слова: біосурфактанти, бази даних, протеїнові мішені, молекулярний докінг, мікробіологічний метаболізм.