

Publication

3D-Beacons: decreasing the gap between protein sequences and structures through a federated network of protein structure data resources

JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)**ID** 4660376**Author(s)** Varadi, Mihaly; Nair, Sreenath; Sillitoe, Ian; Tauriello, Gerardo; Anyango, Stephen; Bienert, Stefan; Borges, Clemente; Deshpande, Mandar; Green, Tim; Hassabis, Demis; Hatos, Andras; Hegedus, Tamas; Hekkelman, Maarten L.; Joosten, Robbie; Jumper, John; Laydon, Agata; Molodenskiy, Dmitry; Piovesan, Damiano; Salladini, Edoardo; Salzberg, Steven L.; Sommer, Markus J.; Steinegger, Martin; Suhajda, Erzsebet; Svergun, Dmitri; Tenorio-Ku, Luigi; Tosatto, Silvio; Tunyasuvunakool, Kathryn; Waterhouse, Andrew Mark; Schwede, Torsten; Orengo, Christine; Velankar, Sameer**Author(s) at UniBasel** [Schwede, Torsten](#) ; [Tauriello, Gerardo](#) ; [Bienert, Stefan](#) ; [Waterhouse, Andrew](#) ;**Year** 2022**Title** 3D-Beacons: decreasing the gap between protein sequences and structures through a federated network of protein structure data resources**Journal** GigaScience**Volume** 11**Pages / Article-Number** giac118**Keywords** bioinformatics; experimentally determined structures computationally predicted structures; federated data network; structural biology**Mesh terms** Amino Acid Sequence; Databases, Protein; Computer Simulation; Metadata; Records

While scientists can often infer the biological function of proteins from their 3-dimensional quaternary structures, the gap between the number of known protein sequences and their experimentally determined structures keeps increasing. A potential solution to this problem is presented by ever more sophisticated computational protein modeling approaches. While often powerful on their own, most methods have strengths and weaknesses. Therefore, it benefits researchers to examine models from various model providers and perform comparative analysis to identify what models can best address their specific use cases. To make data from a large array of model providers more easily accessible to the broader scientific community, we established 3D-Beacons, a collaborative initiative to create a federated network with unified data access mechanisms. The 3D-Beacons Network allows researchers to collate coordinate files and metadata for experimentally determined and theoretical protein models from state-of-the-art and specialist model providers and also from the Protein Data Bank.

ISSN/ISBN 2047-217X**edoc-URL** <https://edoc.unibas.ch/93047/>**Full Text on edoc** Available;**Digital Object Identifier DOI** 10.1093/gigascience/giac118**PubMed ID** <http://www.ncbi.nlm.nih.gov/pubmed/36448847>**ISI-Number** MEDLINE:36448847**Document type (ISI)** Journal Article