BITS :: Call for Abstracts 2019 - Oral communication

Type	Oral communication
Session	Big Data: Storage, Analysis and Visualization Biological Databases
Title	ModiDB 3.0: intrinsic disorder annotation and integration in UniProtKB
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Motivation

Many proteins play their biological function as ensemble of conformations rather than assuming a well-defined structure. Intrinsically disordered proteins (IDPs) or regions (IDRs) are devoid of order in their native unbound state. Intrinsic disorder is prevalent in the human proteome, appears to play important signaling and regulatory roles and is frequently involved in disease. As intrinsic disorder is emerging as a general phenomenon, databases are collecting and presenting disorder related data in a systematic manner. MobiDB has been a major contributor by providing consensus predictions and functional annotations for all UniProt proteins, driving the field ahead. For these reasons the MobiDB upgrade and integration of its annotations in UniProt are essential to the field development.

Methods

MobiDB 3.0 is intended to be a central resource for large-scale intrinsic disorder sequence annotation. It is organized by both type of disorder annotation and quality of disorder evidence. Disorder information is grouped in three different sections: disorder, linear interacting peptides (LIPs) and secondary structure populations. The latter represents the conformational heterogeneity of IDPs and IDRs as the ability to populate different secondary structure populations in solution. LIPs are structure fragments that interact with other molecules preserving an elongated structure or folding upon binding. The data in MobiDB is organized hierarchically. The top tier is formed by manually curated data from external databases and represents the highest quality annotations. Annotations derived from experimental data such as X-ray and NMR chemical shifts are indirect but far more abundant. At the bottom, predictions provide disorder annotation at lower confidence than experimental evidence. The main disorder definition in MobiDB is provided by a consensus combining all available sources prioritizing curated and indirect evidences over predictions in analogy to the previous version. In the following, we will describe the main recent improvements since the previous release. The database schema, web interface and server have been completely redesigned and the underlying technology updated. A complete and documented suite of RESTful APIs allow public data retrieval from external resources. Through this feature, MobiDB data will be integrated and natively displayed in UniProt entry pages.

Results

The MobiDB (URL: mobidb.bio.unipd.it) database of protein disorder and mobility annotations has been significantly updated and upgraded since its last major renewal in 2014. Several curated datasets for intrinsic disorder and folding upon binding have been integrated from specialized databases. The indirect evidence has also been expanded to better capture information available in the PDB, such as high temperature residues in X-ray structures and overall conformational diversity. Novel NMR chemical shift data provides an additional experimental information layer on conformational dynamics. Predictions have been expanded to provide new types of annotation on backbone rigidity, secondary structure preference and disordered binding regions. MobiDB 3.0 contains information for the complete UniProt protein set and synchronization has been improved by covering all UniParc sequences. An advanced search function allows the creation of a wide array of custom-made datasets for download and further analysis. A large amount of information and cross-links to more specialized databases are intended to make MobiDB the central resource for the scientific community working on protein intrinsic disorder and mobility. Part of MobiDB annotation, namely intrinsic disorder prediction from MobiDB-lite are already integrated in InterPro and MobiDB is cross-linked from UniProt entry pages. In the near future, position specific disorder annotation from MobiDB will be displayed in the Function section of UniProt entry pages, widely increasing its visibility and usability.

Info

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Figure

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Availability	http://mobidb.bio.unipd.it/

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