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Book review

Anna Tramontano, Protein Structure Prediction, Wiley-VCH, Weinheim, Germany, 2006, ISBN: 3-527-31167-X, 205 pp. Softcover.

The prediction of proteins structures represents one of the most challenging field in molecular sciences but as structural biology is gaining year after year a key role in the understanding of the biological processes on molecular level and it has become also crucial step in pharmaceutical application and drug discovery, all the efforts made toward this direction permitted to this scientific field and its applications to grow much faster than many others.

One of the most important factor that influences computer assisted structural biology is the enormous increase in biological data availability that the completion of various genome projects together with the development of new high throughput genomic and proteomic technologies have produced. But sequencing is still much cheaper than determining protein structure, so huge amount of sequence data do not have any structural meaning still and protein structure prediction could be the gap-filler approach.

In ''Protein Structure Prediction – Concepts and Applications'' Anna Tramontano provides a complete overview of all the current methods explaining theoretical basis, application and limits of each of them.

The first chapter discusses molecular details of protein structure from basics on sequences, aminoacid properties to experimental structure determination and classification of protein structures. It gives an overview of protein structure evolution as well as its relationship with sequence evolution describing Chothia and Lesk's studies on structural core divergence in pairs of homologous protein. In the second chapter the author offers a short description of methods used to estimate the quality of a structure prediction. The chapter starts with an overview of secondary structure prediction assessment methods and gives basic concepts about q-index and SOV score calculation providing some helpful examples, while the paragraph about the evaluation of tertiary structure prediction gives some very important warnings about the misuse of rmsd value in the evaluation of molecular models, a common source of systematic errors. The second half of the chapter illustrates some of the most used benchmarking procedures in quality assessment. The ab initio methods of protein structure chapter focus on energy content calculation. It provides a short but complete summary of all the principal methods for conformer selection and energy driven structure optimization. The fourth chapter is about comparative modelling and it goes deep into all steps of such approach from templates' identification to sequences' alignment to core's main chain building to structurally divergent regions' building and model optimization. Each step is explained with an incredibly clear didactic approach and a very little prior knowledge is required to understand the concepts. Chapters five and six face the problem of having no known structure as template describing, respectively, fold-recognition methods and fragment based methods. In the chapter on fragment based methods the author basically describes the philosophy of Rosetta and Fragfold's tools explaining the scientific basis behind them to help the user to know when to use them, how to use them and how to evaluate the quality of the results. Chapter seven focuses on low-dimensionality prediction problems such as secondary structure and contact prediction. Chapter eight is about the determination of membrane protein structure and the author describes it as one of the most difficult but crucial task in computational biology as these proteins represent quite often the most interesting targets for drug discovery problems according to their key role in cells' signalling. As their experimental structure determination is still very difficult the problem is wide open at the moment and the evaluation of predicted models is still uneasy. The last chapter of the book provides examples and applications' description. The chapter goes over the history of protein structure determination with precious examples and pictures of every milestone in this scientific field providing both the proofs of technological, scientific, philosophical applicability and the inspiration for new questions and ideas in structural biology and its applications.

The author has the ability to summarize the concepts without any loss in contents. The book is an incredibly slim concentrate of molecular knowledge in which each word seems to be worth three or four as the author has a taste for going straight to the point. She often uses a question–answer approach to clarify the key point of each paragraph and this colloquial technique has the undeniable advantage to make everything much more immediate and easy. The reading is pleasant and the reader can get a lot of information with a little effort.

The book provides a good overview of every topic in protein structure prediction with a good level of details and can be very useful for beginners as its didactic approach with clear examples does require only a little knowledge on biology and biochemistry. The expert reader can also have benefits from the reading as the very high level of details provided can represent interesting information to

improve and update researcher's knowledge and as chapter organization is very practical it permits to retrieve information in a very simple and fast way.

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