Calculation of Biological Units from Protein Crystallography Data

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Solution of protein structures by means of X-ray diffraction delivers crystal structure and protein coordinates that form an asymmetric unit of the crystal. These coordinates do not necessarily identify the biological unit, or protein assembly that performs a certain physiological function. However, it is reasonable to expect that biological units last out to the crystallization and therefore it may be possible to find their structure and composition from the crystal data.

We propose a method for the calculation of protein assemblies from crystal structures, which is different from previously published [1,2] in that it is based on general principles of chemical thermodynamics. Our method employs graph techniques for the identification of all potential assemblies in a crystal, represented as a periodic graph, and each assembly is then analyzed for chemical stability on the basis of protein affinity and entropy change upon dissociation. As found for structures with experimental evidence of their oligomeric states, our method achieves 89% of correct predictions, which is higher then previously reported [1,2].

The developed software has been made available to public by setting up a web service that can take uploaded PDB and mmCIF coordinate files for analysis. The service also provides protein interfaces and protein assemblies precalculated for all PDB entries of structures solved by X-ray diffraction.

[1] Henrick K., Thornton J., *Thrends Biochem. Sci.*, 1998, **23**, 358. [2] Ponstingl H., Kabir T., Thornton J., *J. Appl. Cryst.,* 2003, **36**, 1116.

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