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Analysis of common buffer molecules' conformations in ligand-protein complexes

J. Macnar [1], D. Brzezinski [2], D. Gront [3]

[1]College of Inter-Faculty Individual Studies in Mathematics and Natural Sciences, University of Warsaw - Warsaw (Poland), [2]Institute of Computing Science, Poznan University of Technology - Poznan (Poland), [3]Faculty of Chemistry, Biological and Chemical Research Center, University of Warsaw - Warsaw (Poland)

Abstract

Structural information about ligand-macromolecule complexes is key for biomedical sciences, especially for structure-based drug design and structural bioinformatics. Most of the experimental information about macromolecules complexed with ligands is coming from X-ray crystallography. The accessibility of synchrotron sources with modern appliances and software has resulted in the availability of approximately 190,000 structures deposited in the Protein Data Bank (PDB)[1]. Alas, a small number of the crystal structures available in the PDB are of suboptimal quality, including some with poorly identified and modelled ligands in protein-ligand complexes. BioShell 3.0[2] is an advanced structural bioinformatics toolkit that includes the analysis of ligand-protein complexes. By combining a graph-theoretical approach, kernel density estimators, bioinformatics methods, and chemical knowledge, we present an analysis verifying the accuracy of HEPES and MES molecules, frequent components of crystallization buffers, selected from PDB deposits. This analysis will lead to a better refinement of ligand-protein complexes.

References

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