CFEL SCIENCE

SEMINAR

06th December 2017 - 2:00 p.m.

CFEL-bldg. 99, seminar room IV

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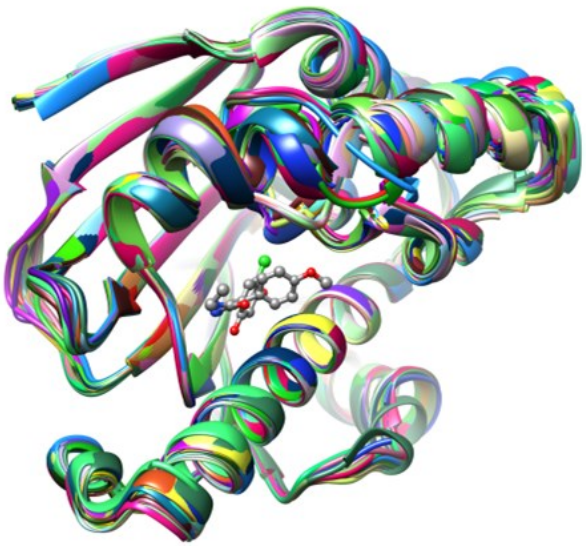
Computational methods to deal with large protein structure collections

Due to technological advances in x-ray crystallography and cryo-electron microscopy, the amount of available protein structures is substantially increasing. Novel technologies will most likely steepen the growth rate even further. While protein structures are used as individual data elements in biotechnology and pharmacology research for decades, our computational methods for performing statistical analysis on large structure collections are still rather limited. The international Protein Databank (PDB) offers a wealth of options to analyze protein structures, however, search for the intrinsic information, namely the geometry of atomic arrangements, remains a challenging problem. Several data preparation steps to use protein structures in modeling approaches require manual intervention making it difficult to use large structure sets in a fully automated fashion. For over five years now we address these issues by new algorithmic approaches for automatic, reliable, large-scale processing of experimentally determined protein structures with a focus on protein-ligand interactions. In this talk, an overview of the developed methods ranging from automatic estimation of electron density support for modeled structures via preprocessing steps like prediction of tautomeric and protonation states up to flexible geometric searching will be presented.



Active-site centric, fully-automated extracted and superimposed structures of Heat Shock Protein 90 (HSP90)

Recent overview article: Bietz et al. (2017), Journal of Biotechnology, 261:207-214

Host: Robin Santra – CFEL-DESY Theory Division