Poster Presentation

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ARP/wARP for crystallographic model building and drug discovery

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The ARP/wARP software project combines automated model building and refinement into an unified approach for macromolecular crystal structure determination. The project is based on two decades of extensive research and development in the areas of macromolecular X-ray crystallography, informatics, data mining and statistical pattern recognition. ARP/wARP collects a vast amount of computationally efficient methods and provides easy-to-use pipelines for building models of proteins, nucleotides, ligands, as well as their complexes. All methods are intuitively accessible from the ArpNavigator [1], which grants direct visualisation and real-time interaction with model building results. Structures determined using ARP/wARP include histones, hsp70, viral proteases, an insect antifreeze protein, transferases, deadenylases, synthases, kinases, photolyases and the spliceosome. The novel release of ARP/wARP, version 7.4, comes with notable innovations for determining structures at medium-to-low resolution such as exploitation of non-crystallographic symmetry, improved protocols for model update and estimation of validity of built models. Joint releases with the CCP4 suite improve software development and integration, and make the installation and updates fast and convenient for the user. A novel procedure for the automatic identification of ligands in electron density maps is introduced. It is based on the sparse parameterisation of density clusters and the matching of the pseudo-atomic grids thus created to conformationally variant ligands using mathematical descriptors of molecular shape, size and topology. The integration of the ViCi web-server for in-silico ligand-based drug design and updated stereo-chemical restraints for ligand fitting make ARP/wARP an asset for crystallographic drug discovery pipelines.

[1] *Langer G.G., Hazledine S., Wiegels T., Carolan C., Lamzin V.S. (2013), Acta Crystallogr D Biol Crystallogr., 69, 635-641*

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