Oral Contributions

[MS44-02] Macromolecular Phasing with SHELXC/D/E Starting from Very Little Phase Information. Andrea Thorn.

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The initial step of expanding from very little phase information can be critical to solve a macromolecular structure. This phase information can for example be obtained from a fragment placed by molecular replacement, which comprises only a small fraction of the total scattering power, or the positions of a few Sulfur atoms in SAD phasing. The programs SHELXC/D/E [1] are designed for the phasing of macromolecules: SHELXC sets up the files and calculates phase angle shifts caused by marker atoms, SHELXD locates an initial marker atom substructure and SHELXE improves the resulting map by density modification. In the latest release SHELX_2013, this density modification can be supplemented by iterative poly-Alanine tracing. Given good-resolution native data, this is a powerful tool to get a toehold from very little phase information in order to 'climb' to a correct solution. The decisive criterion is the correlation coefficient (CC) of the poly-Alanine trace against the native data, and a CC of more than 25% appears to be a reliable indicator of success, which is already exploited in a number of pipelines. This approach was originally intended to start from experimental phase information in the form of a marker atom substructure. However, a molecular replacement solution, typically from PHASER [2], can also be used as input in order to get an improved or more complete model [3] -or for the combination with experimental phase information. The new tool ANODE [4] reads a PDB file and the anomalous data in order to estimate anomalous or heavy-atom density. Potential applications include the identification of unknown atoms, the evaluation of radiation damage on an atomic level and the validation of molecular replacement solutions. Even very weak anomalous scatterers can be located. In this talk, new features in the programs SHELXC/D/E will be explained; general guidelines and examples of the aforementioned cases will be given. SHELX_2013 is available at www.shelx.uni-ac.gwdg.de/SHELX/.

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