Poster Presentation

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Optimization in S-SAD phasing - difference between solved and unsolved structure

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Development of X-ray diffraction technologies have made de novo phasing of protein structures by single-wavelength anomalous dispersion by sulphur (S-SAD) more common. As anomalous differences in the sulphur atomic factors are in the order of errors of measurement, careful intensity reading and data processing are crucial. S-SAD was used for de novo phasing of a small 12 kDa protein with 4 sulphur atoms per molecule at 2.3 Å, where the data did not enable a straightforward structure solution. Data processing was performed using XDS [1] and scaling using XSCALE. The sulphur substructure was determined by SHELXD [2] and phases were obtained from SHELXE [2]. Both algorithms strongly depend on input parameters and default values did not lead to the correct phases. Therefore a systematic search of optimal values of several parameters was used to find a solution. This method helped to confirm sulphur substructure and to differentiate the handedness of the solutions. Moreover, a script for comfortable conversion of SHELX outputs to MTZ format was developed, using programmes included in the CCP4 package [3]. The previously unsolvable protein structure was successfully resolved with the described procedure. This work was supported by the Grant Agency of the Czech Technical University in Prague, (SGS13/219/OHK4/3T/14), the Czech Science Foundation (P302/11/0855), project BIOCEV CZ.1.05/1.1.00/02.0109 from the ERDF.

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