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Low resolution *ab initio* phasing of *Sarcocystis muris* lectin SML-2

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The structure analysis of the lectin SML-2 [1] faced difficulties when applying standard crystallographic phasing methods. The crystal with dimensions of 0.2x0.2x0.2 mm^3 belongs to the primitive orthorhombic space group $P2_12_12_1$ with a unit cell of a=53.23 Å, b=130.12 Å, and c=160.05 Å and diffracts to about 5-6 Å resolution at 100 K at the HASYLAB PETRA I undulator beamline at the PETRA storage ring, DESY, Hamburg. Co-crystallization of the lectin SML-2 with a modified galactose [1] resulted in a second crystal form, $C222_1$ with a unit cell of a=74.70 Å, b=81.97 Å, and c=131.00 Å. In an N_2 cryostream, after annealing this crystal switched to space group $P2_12_12_1$ yielding a crystal isomorphous to that of the native apo-protein. For the Matthews coefficient to be in the range of 2.3-3.0 $Å^3$/Da, the asymmetric part of the unit cell of the $P2_12_12_1$ space group crystals could contain 6-8 monomers.

The connectivity-based *ab initio* phasing method [2] allowed to compute a 16-Å resolution Fourier synthesis and derive primary structural information. Random phases sets were generated and selected following the features of corresponding Fourier syntheses. At the first three steps of phasing the selection rule was simply '3 blobs per asymmetric unit' for Fourier syntheses in several resolution zones (resolution varied from 27 to 17 Å). No symmetry conditions were imposed on the images analyzed. At every step 100 selected phase sets were aligned and averaged producing approximate phases and their individual figures of merit as the output. Other rules were checked as well but the Fourier maps obtained were inconsistent with the rules and therefore rejected. At the following phasing steps the selection rule was completed by a condition that the three connected blobs at the Fourier maps should have approximately the same volume.

It was found that SML-2 crystals have three dimers in the asymmetric part of the unit cell. These dimers are linked by a non-crystallographic symmetry close to the translation by (0,0,⅓). Patterson maps and analysis of the distribution of structure factor intensities confirmed experimentally a non-crystallographic character of this pseudo translation. An identification of the position of the non-crystallographic two-fold axis in the crystal explains a space group transformation from the primitive $P2_12_12_1$ to C-centered $C222_1$ observed during annealing procedures within an N_2 cryostream for co-crystals of SML-2 and galactose. Related packing considerations predict a possible arrangement of SML-2 molecules in a tetragonal unit cell. Multiple non-crystallographic symmetries and crystal forms provide a basis for further image improvements.

[1] Müller J.J., Müller E.-Ch., Montag Th., Zyto N., Löschner B., Klein H., Heinemann U., Otto, A., *Acta Cryst.*, 2001, D57, 1042.
[2] Lunin V.Y., Lunina N.L., Urzhumtsev A., *Acta Cryst.*, 2000, A56, 375.

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Investıgatıng the molecular formatıon propertıes of ethyl 4-(2-oxobenzothıazolın-3-yl) butanoate usıng pm3, am1, mndo methods

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In this study in order to apply the geometry optimization to the ethyl 4-(2-oxobenzothiazolin-3-yl) butanoate crystal, which is used for forming analgesic and antienflamatuar medicine and of which crystal structure was determined using x-ray diffraction method, PM3 (Parametric Model 3), AM1 (Austin Model 1) and MNDO (Modified Neglect of Diatomic Overlap) semi emprical molecular orbital methods found in the HyperChem program were used. By the geometry optimization geometric parameters of the molecules having the minimum energy were found. These values which were theoretically obtained were compared with the emprical values obtained by x-ray diffraction method. These results showed that for the $C_{13}H_{15}NO_3S$ crystal, both in bond lengths and angles AM1 method was found to be consistent with the emprical x-ray diffraction data. By geometry optimization using PM3, AM1 and MNDO methods relevant energy values of the molecular structure were calculated.