MR using CCP4i:TOXD

From Phaserwiki

Data for this tutorial are found here (http://www.phaser.cimr.cam.ac.uk/index.php/Tutorials)

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Reflection data: toxd.mtz
Structure files: 1BIK.pdb, 1D0D_B.pdb
Sequence file: toxd.seq
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This tutorial demonstrates the ensembling procedure in Phaser.

α-Dendrotoxin (TOXD, 7139Da) is a small neurotoxin from green mamba venom. You have two models for the structure. One is in the file 1BIK.pdb, which contains the protein chain from PDB entry 1BIK, and the other is in the file 1D0D_B.pdb, which contains chain B from PDB entry 1D0D. 1BIK is the structure of Bikunin, a serine protease inhibitor from the human inter-α-inhibitor complex, with sequence identity 37.7% to TOXD. 1DOD is the complex between tick anticoagulant protein (chain A) and bovine pancreatic trypsin inhibitor (BPTI, chain B). BPTI has a sequence identity of 36.4% to TOXD. Note that models making up an ensemble must be superimposed on each other, which has not yet been done with these two structures.

1. Use the SSM superpose option in coot to superimpose 1BIK on 1D0D_B, saving the resulting coordinates in 1BIK_on_1D0D.pdb.
2. Start the ccp4 GUI by typing ccp4i at the command line.
3. Make a new project called "phaser_tute" using the Directories&ProjectDir button on the RHS of the GUI. Set the "Project" to phaser_tute and "uses directory" to the directory where the files for this tutorial are located, and make this the "Project for this session of the CCP4Interface". You will then be able to go directly to this directory in the GUI using the pull-down menu that appears before every file selection.
4. Go to the Molecular Replacement module, in the yellow pull-down on the LHS of the GUI
5. Bring up the GUI for Phaser
6. All the yellow boxes need to be filled in.
    - It is a good idea to change the Ensemble id from the default.
    - It is also a good idea to fill in the TITLE.
7. When you have entered all the information, run Phaser.
8. Has Phaser solved the structure? What was the LLG of the best solution? What was the Z-score of the best translation function solution?
    - The meaning of the Z-score is given in the documentation
9. Look though the log file and identify the anisotropy correction, rotation function, translation function, packing, and refinement modes. Draw a flow diagram of the search strategy.
10. How many potential solutions did Phaser find or reject at each stage? What were the selection criteria for carrying potential solutions forward to the next step in the rotation and translation functions? How many other selection criteria could have been used, and what are they?
    - Use the documentation
11. Run Phaser again without using ensembling i.e. run two jobs, one using 1BIK only and the other using 1D0D only as models. What are the LLGs of the final solutions? What are the Z-scores of the translation functions? Was ensembling a good idea?

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