Poster Presentation

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"Objective" Evaluation of Macromolecular Models

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Evaluation of the accuracy and quality of molecular models from X-ray crystallography is a continuing problem. The refinement process as currently practiced is inherently biased through use of the model to provide phase information for the refinement process. To investigate the extent of model bias we are developing model-free criteria for detailed analysis of crystal structures. We present preliminary findings from comparing a set of high resolution, well-refined structures from the Joint Center for Structural Genomics repository to maps based solely on phases from selenomethionine anomalous scattering. Removal of atoms with little or no support in the "objective" map reliably improves or does not degrade the free R-factor. The selenomethionine map, or any other map produced without the assumption of a molecular model, can be used to identify features supported by diffraction data and those which come from the application of structural constraints.

Keywords: refinement