Comparative Study of the Binding of Different Gd Complexes in Protein Crystals

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A series of Gd complexes was used for obtaining high-phasing power heavy-atom derivatives. Ease of use of the complexes and high success rate in obtaining good derivatives were demonstrated by a large number of tests [1]. Here we present a comparative study of the different complexes and data analysis of about 50 derivatives obtained with 8 different proteins.

For highly occupied binding sites a model of the corresponding complex was built and refined. This allowed identification of the binding mode of the complexes. For less occupied binding sites the binding site locations and occupancies were determined. Combining these different kinds of information may allow the identification of systematic patterns and thus to predict the behavior of the different complexes with proteins of unknown structure, depending on the nature of residues at the protein surface, and possibly on other factors such as the precipitating agent.

In addition to working on derivative crystals of several test proteins (urate oxidase from Aspergillus flavus, hypothetical protein Yggv from E. coli, glucose isomerase from Streptomyces rubiginosus, thaumatin from Thaumatococcus daniellii) several new protein structures were solved de novo using the complexes.

[1] Girard É., Stelter M., Vicat J., Kahn R., *Acta Cryst.*, 2003, **D59**, 1914-1922.

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