

## Microsymposium

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*MoProViewer: a tool to study proteins from a charge density science perspective*

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Applying the charge density science methods to the structural biology field remains a considerable challenge. Several approaches were followed in the past years, focusing either on multipolar refinement of the rare available subatomic resolution protein structures or on the application of the transferability principle for the evaluation of electrostatic and energetic properties in protein-ligand complexes. However, the usually large size of macromolecules and the consequently large number of multipolar parameters in the Hansen & Coppens formalism [1] obviously complicates the feasibility of such kind of studies. In this presentation, we introduce the tools implemented in the MoProViewer software, part of the MoPro Suite for charge density refinement, especially designed to ease the analysis of a protein structure from a charge density perspective. These tools focus on helping the user in the computation of properties deriving from a refined or transferred [2] protein charge distribution and to manage a large number of atoms described in the multipole formalism in terms for instance of atomic local axis, symmetry or chemical equivalences constraints definitions. Moreover we will present new methods based on the topological analysis of the electrostatic potential [3]. They are designed to allow an original use of the electrostatic properties of a protein-ligand complex structure and rely on the computation and the representation of electrophilic and nucleophilic influence zones of atoms involved in protein-ligand interactions or in a biochemical process. The computational details of these methods as well as application examples on selected protein-ligand complexes will be given.

[1] N. K. Hansen, P. Coppens, *Acta Cryst A*, 1978, 34, 909-921, [2] S. Domagala, B. Fournier, D. Liebschner et al., *Acta Cryst B*, 2012, 67, 250-262, [3] I. Mata, E. Mollins, E. Espinosa, *J. Phys. Chem. A*, 2007, 111, 9859-9870

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