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New developments in the BayMEM Suite

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The program suite BayMEM consists of the programs PRIOR, BayMEM and EDMA. It is intended to apply the Maximum Entropy Method (MEM) to ordinary and modulated structures[1]. The PRIOR program is intended to calculate the prior density for the MEM calculation, but it has been recently shown that it can be used to calculate the dynamic charge density from multipolar refinements[2] as well. As a new functionality it is now also possible to calculate the electrostatic potential from the dynamic deformation density by the method described by Steward and Spackman[3]. We will present a new MapConverter program which allows to convert electron density stored in different file formats into an other. It is also possible to rearrange and cut the density in such a way, that it is possible, to have clear view of one molecule, not obscured by its symmetry mates, in a molecular viewer like MoleCoolQt for example.

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