ESRF	**Experiment title:** XANES and EXAFS studies of substitutes of malarial pigments	**Experiment number:** MD-317
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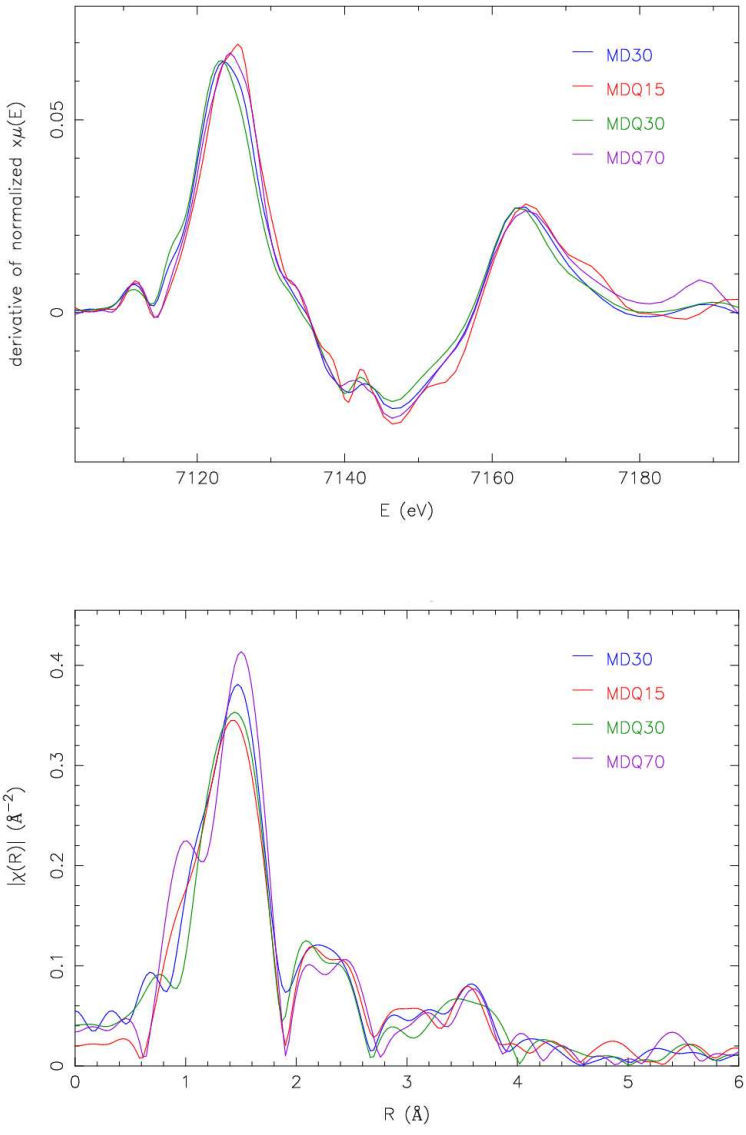
Report:

It is now well established that malaria pigment, hemozoin, is chemically and structurally identical to the synthetic product known as β-hematin. The crystal structure of hemozoin and its synthetic analogue, β-hematin, has been solved by X-ray powder diffraction (S.Pagola et al., Nature 404(2000) 307-310). The structure of both is built of chains of dimers. These dimers are formed by the FeIII protoporphyrin-IX molecules through reciprocal iron-carboxylate bonds to one of the propionic side chains of each porphyrin. Newly-synthesized soluble β-hematin-like compound, mesoporphyrin-IX anhydride (MD) has been studied by extended X-ray absorption fine structure (EXAFS) and X-ray absorption near edge structure (XANES) techniques to determine the ionic state and distribution of atoms around Fe atom in solution with and without presence of antimalarial drug. Spectra were acquired on iron edge using fluorescence detection mode. EXAFS spectra of MD in acetic acid with addition of water with ratio 1:30 (MD30) differ from spectra of exactly this solution after adding chloroquine drug (MDQ30) already in first shells, four plane nitrogens and axial oxygen. However this difference is not so significant as between spectra of MDQ30 solution and acetic-water(ratio 70:1) or acetic-water (ratio 15:1) mesoporphyrin-IX with chloroquine solution, MDQ70 and MDQ15 respectively.

The same conclusion one can get from XANES spectra where MDQ70 and MDQ15 edge is slightly shifted towards higher energies. The pattern of changes for solutions with antimalarial drug is not consistent so the conclusion is that the MD molecules' atoms displacement can be caused by the interaction with solvent particles as well as chloroquine drug itself. Proposed in the literature models of ferriprotoporphyrin IX interaction with chloroquine drug will be checked in comparison to ferriprotoporphyrin IX bonding with acetic acid molecule.



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