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Monitoring flavin X-ray radiation damage using single crystal spectroscopy

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Considering that more than one thousand structures in the Protein Data Bank contain flavin cofactors (1), it is of interest to verify the flavin geometry and electronic state when using these structures for deducing reaction mechanisms and when analyzing the conformational interplay between the cofactor and its protein scaffold. Inspecting flavin structure with QM/MM methods and monitoring of flavin vibrational modes with single-crystal spectroscopic methods during X-ray data collection provide important information regarding the actual flavin state. Here we present data collected from crystals of the flavoprotein NrdI, comparing high resolution crystal structures, geometry optimized models, and single crystal Raman spectra, showing that flavin geometry and state indeed are changed when exposed to X-ray radiation (2).

References

- 1) Senda, T., Senda, M., Kimura, S., Ishida, T. (2009) *Antioxid.Redox Signal.* 11, 1741-1766.
- 2) Røhr, A.K., Hersleth, H.-P., Andersson, K.K. (2010), *Angew. Chem. Int. Ed. Engl.* 49, 2324-2327.

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