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## Selective X-ray induced NO-photodissociation in hemoglobin crystals: evidences from a crystallography-assisted Raman microscopy study

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Despite the high physiological relevance, hemoglobin crystal structures with NO bound to heme are less than 1% of the total ligated hemoglobins (Hbs) deposited in the Protein Data Bank. One of the major difficulties in obtaining nitrosyl-ligated Hbs is probably related to oxidative denitrosylation, being nitrosylated species very reactive toward O<sub>2</sub>. Raman-assisted crystallography can be a valuable tool to follow derivative crystal preparation[1,2], metal coordination states[3,4], and X-ray photodamage[5,6]. Here, using X-ray crystallography-assisted Raman microscopy, we show that upon X-ray exposure (SLS, X10SA beamline), crystals of nitrosylated hemoglobin from *Trematodus bernacchii*[7] undergo a selective photodissociation of the Fe-NO bond at the  $\beta$  chains generating penta-coordinate species. These data provide a physical explanation of the small amount of nitrosylated Hbs structures available in the literature, suggesting that X-ray induced photodissociation is a frequent and underestimated phenomenon[8,9].

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