

Slow ligand migration dynamics in sperm whale carbonmonoxy myoglobin at cryogenic temperature

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Myoglobin (Mb) is a small globular heme protein in muscle, which reversibly binds gas ligands at the heme iron site buried inside the protein matrix. This ligand dissociation can be triggered by photo irradiation [1]. The ligand binding reaction in carbonmonoxy myoglobin (MbCO) has been extensively studied by X-ray diffraction experiments (e.g. Laue diffraction experiments at room temperature [2, 3] or monochromatic X-ray diffraction experiments at cryogenic temperature [4]). In spite of lots of known details regarding the gas ligand molecules trapped in internal cavities of Mb, there exists no direct evidence to show the migration pathways connecting these cavities. In order to explore the ligand migration pathways in myoglobin induced by ligand dissociation, we have carried out cryogenic X-ray crystallographic investigations of native sperm whale MbCO crystals illuminated by a laser. Slow ligand migration in Mb was observed at the cryogenic temperatures.

Reference

- [1] Q. H. Gibson, *J. Physiol.*, **134** (1956) 112-122.
- [2] F. Schotte *et al.*, *Science*, **300** (2003) 1944-1947.
- [3] V. Šrajer *et al.*, *Biochemistry*, **40** (2001) 13802-13815.
- [4] T.-Y. Teng *et al.*, *Nature Struct. Biol.*, **1** (1994) 701-705.