02. STRUCTURAL MOLECULAR BIOLOGY

02.1-12 CRYSTALLOGRAPHIC STUDIES OF Mb:Cu(II)

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Three-dimensional diffractometric data of sperm-whale Mb and Mb:Cu(II) were collected to 2.0 Å resolution using Cu Kα radiation. Difference synthesis with Fourier coefficients R Donetsk using phases calculated from Takano’s 2.0 Å resolution model (J.Mol.Biol. (1997). 110, 59-77), were calculated during the localization of the Cu(II) ions in the complex. Although a similar two-dimensional determination was already done by Banaszak et al. Three-dimensional diffractometric data of sperm-whale Mb have the following unit cell dimensions: a = 64.72, b = 105.72, c = 34.82 Å, β = 110.57°; the space group is P2₁. The diffraction data were obtained from two different crystals not affected by the distance shift; other residues affected include Val E₁₁, Arg 45 and Asp 60. Minor modifications are observed also in the stereochemistry of the porphyrin system and in the position of the iron atom.

02.1-14 X-RAY CRYSTAL STRUCTURE ANALYSES OF MYOGLOBINS RECONSTITUTED WITH SYNTHETIC HEMES.


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Three-dimensional structures of myoglobins reconstituted with synthetic hemes have been determined by means of X-ray diffraction in order to elucidate the functions of heme-proteins. The following four synthetic hemes were used:

(a) R₁ = H, R₂ = -CH₂CH₃
(2-vinyldeuteroheme)

(b) R₁ = H, R₂ = -CH=CH₂
(isopemptoheme)

(c) R₁ = H, R₂ = -CH₂CH₃
(4-vinyldeuteroheme)

(d) R₁ = H, R₂ = -CH=CH₂
(4-ethyldeuteroheme)

(c) of (d) R₁ = R₂ = -CH₂CH₃
(native)

Crystals of four reconstituted myoglobins, all of which belong to the monoclinic system (space group P2₁), are isomorphous with the native metmyoglobin. Intensity data of (a), (b) and (d) to 2.2 Å resolution (as 7000 independent reflections) were collected on a Rigaku four-circle diffractometer. Data collection of (c) is in progress. In Fourier syntheses, phase angles were calculated from atomic coordinates of metMb except for the porphyrin ring (Takano, J. Mol. Biol. (1977) 110, 597). Electron density map on the heme plane of (a) and (d) are presented in the Figure. In isopemptoheme-Mb(a), the modified heme is inserted into apo-Mb in the same position and orientation as that in the native Mb. On the other hand, the heme group is recombined inversely with apo-Mb in 4-ethyldeuteroheme-Mb (d). In pemptoheme-Mb(b), most of hemes in crystal locate similarly as those in the native Mb and the rest inversely.

The difference Fourier syntheses (|F(modified) − |F(native)|) do not give any significant peaks except for residues of hemes, which show no large change in the main chains and residues in these reconstituted myoglobins.

Figure. left: (a), right: (d)