s8a.m4.p9 Recognition of Haem by Proteins. Insight from Structural Data Bases (CSD and PDB) Analysis.

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A variety of *haem* proteins display diverse biological fonctions, such as oxygen carrier or storage, electron transfer and redox catalysis, though they employ a simple porphyrin as a common cofactor. Each specific function of *haem* proteins is regulated by the environment around the porphyrin core. In each case, *haem* recognition is guided by electrostatic attraction to the metal ion and/or interactions with the hydrophobic functionality. Another common feature is the binding of small axial ligands (O-O, C-O, N-O, C-N...) to the sixth coordination site of the iron which can be expected to influence the aromatic side chain-porphyrin interactions. In turn, the small-molecule ligands are recognised by the protein. Thus, the binding of *haem* is a result of three cooperative effects: metal-ligand coordination, ligand-side chain interactions, *haem*-hydrophobic interactions. Now little is known about the exact nature of the synergy between these diverse interactions.

An enormous amount of publicly available high resolution crystal structures of proteins (the Brookhaven Data Base, PDB)1 and small molecules (the Cambridge DataBase, CSD)2 provides an efficient tool to study the *haem* interactions. With both Data Bases the following topics were explored: (i) metal-porphyrin binding; (ii) metal-axial igand binding; (iii) *haem*-hydrophobic interactions; (iv) axial ligand-protein interactions.

The environment of *haem* in proteins and synthetic mimics was characterised in a systematic manner in order to understand the structural role of the different partners (axial ligands and aromatics...) and to elaborate different concepts concerning fixation, recognition and coordination.

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s8a.m4.p10 Crystal structure of β-cinnamomin, a protein elicitor produced by a phytopathogenic fungus,

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Fungi of the genus *Phytophtora* (*P.*) are a major cause of crop devastation, like the late blight disease of potatos, soybean, black shank of tobacco plants. In particular, the disease called "cork oak decline" has been linked to *P. Cinnamomi*[1]. Most species of *Phytophtora* produce 10 kDa extracellular protein elicitors, called elicitins, which induce leaf necrosis in infected plants and elicit an incompatible hypersensivitive-like reaction, leading to a systemic acquired resistance against a range of fungal and bacterial plant pathogens[2]. In order to study the role of cinnamomin (CIN) in the pathogenesis of *P. cinnamomi* and *Quercus suber* (cork oak), a synthetic gene was constructed and expressed in *Pichia pastoris* in a biologically active form.

Good quality crystals of CIN were obtained by the vapour diffusion method from either 2.2 M ammonium sulphate, 5% MPD, 0.1 M HEPES at pH 7.0, or from 30% PEG 4K, 10% butanol, 0.2 M ammonium sulphate, 0.1 M Tris-HCl at pH 7.5. These crystals are isomorphous and belong to the triclinic space group, with cell dimensions a = 31.69 Å, b = 36.99 Å, c = 44.09 Å, α = 76.86°, β = 84.41° and γ = 80.26°. A complete diffraction data set was collected to 1.45 Å resolution on a synchrotron radiation source at ESRF[3]. The structure of CIN was solved by molecular replacement using the X-ray structure of β-cryptogein (PDB entry 1BEO), an elicitin secreted by *P. cryptogea*. The overall structure reveals a novel fold, consisting of six α helices and a two-stranded β-sheet facing an Ω loop, with a hydrophobic pocket and three disulfide bridges. Recently, elictins were proposed to constitute a new class of sterol carrier proteins[4]. Since fungi of the *Phytophtora* genus do not synthetize sterols, elicitins would allow them to sequester sterols from the invaded plant cell membrane. The crystal structure of an elicitin-ergosterol complex was determined (PDB entry 1BXM), which is consistent with this hypothesis.

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