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Protocyanin is a complex pigment extracted from flower petals of blue cornflower, *Centaurea cyanus*. The components of protocyanin were recently demonstrated to be anthocyanin (AN), flavone glycoside (FL), Fe^{3+}, Mg^{2+} and Ca^{2+} ions[1]. For X-ray structure determination, protocyanin was reconstructed from the components and crystallized in space group $P2_12_12_1$ with unit cell dimensions of a = 29.7, b = 49.2 and c = 78.3Å. Two protocyanin molecules are contained in an asymmetric unit. Data were collected on the beam line 6A at Photon Factory KEK to1.05 Å resolution.

The refined molecule has pseudo three-fold symmetry and four metals align along the pseudo three-fold axis in order of Ca^{2+}, Fe^{3+}, Mg^{2+} and Ca^{2+}. The four metals are coordinated to six AN and six FL molecules. The inner Fe^{3+} and Mg^{2+} ions are each coordinated to three AN's, respectively, while the outer two Ca^{2+} ions are each coordinated to three FL's. Both AN and FL molecules are self-associated with each other as AN-AN and FL-FL in pair and this hydrophobic association also exists between AN and FL molecules, building copigmentation stacks. Protocyanin is a tetra-metal (Fe^{3+}, Mg^{2+}, $2Ca^{2+}$) nuclear complex, a new type of supramolecular pigment.

[1] Takeda K., Osakabe A., Saito S., Furuyama D., Tomita A., Kojima Y., Yamadera M., Sakuta M., *Phytochemistry*, *submitted*.

Keywords: X-ray structure analysis, pigments, biological molecular complexes

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Crystal Structures of the Fungal Metabolite Oosporein

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Oosporein is a symmetrical red coloured 2,5-dihydroxybenzo-quinone derivative biosynthesized by a broad variety of soil borne fungi. The compound, being known for almost six decades, is the major secondary metabolite of the entomopathogenic fungi *Beauveria brongniartii* which is successfully applied as a biological control agent against the European cockchafer *Melolontha melolontha*. In the course of isolating and purifying pure oosporein from biological cultures we obtained a dioxane solvate and a non-solvated form which were characterized with different solid state analytical techniques including X-ray diffraction.

The molecular geometry of oosporein is x-shaped with a dihedral angle of 67.8 and 79.9° in the non-solvated form and the dioxane solvate respectively. Surprisingly the two forms crystallize in the same space group (monoclinic, C_2/c) showing a similar O-H...O network. The non-solvated form shows two dimensional O-H...O tetrameric layers which are off stacked leading to a densely packed structure. In the dioxane solvate one solvent molecule is involved in the O-H...O hydrogen bond network resembling the overall network of the anhydrous form. This pseudo-tetrameric arrangement results in a large channel along the c-axis which is occupied by highly disordered dioxane molecules.

[1] Frank R.L., Clark G.R., Coker J.N., *J. Am. Chem. Soc*., 1950, **72**, 1827.

Keywords: oosporein, natural organic molecules, crystal structure

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Xanthone Derivatives: Conformational Study and Development of Force Field

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Xanthone derivatives extracted from herbs are important components of homeopatic antibacterial, mycotoxic and cytotoxic medicines. Synthetic substituted xanthones tested against broad spectrum of biological activities revealed: antiinflammatory, cytostatic, antimycotic, and cardiovascular activities. In a series of newly synthesized substituted xanthones, two constitutional isomers, 2-methyl-2[2-(methyl)-6-xanthonoxy]-propionic acid, 2-methyl-2[4-(methyl)-6-xanthonoxy]-propionic acid, and racemic (RS)-2-[2-(methyl)-6-xanthonoxy]-propionic acid have shown differentiated antiinflammatory action.

The crystal structures of xanthone derivatives were solved using both single-crystal diffraction and HRPD data recorded with synchrotron radiation. In order to find the native, optimal structures of xanthone derivatives in their natural environment of lipid bilayer, additional force field parameters were obtained using X-ray diffraction data and *ab-initio* calculations.

Keywords: xanthone, *ab-initio* calculations, synchrotron radiation

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Diffraction and Computational Studies of Hydrogen Bonded Base Paired Systems

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Diffraction methods are often utilised to gain a greater insight hydrogen bonding interactions. In work to date the advantages of single crystal variable temperature x-ray and neutron diffraction, coupled with the imaging capabilities of Fourier difference maps, as complementary techniques for anomalous hydrogen bonding investigations have been highlighted [1]. In addition, recent advances in computational chemistry have enabled calculations to be carried out both on isolated molecules and in the periodic (i.e. crystalline) environment [2].

The main aim of this poster is to discuss the use of complementary methods to promote a better understanding of hydrogen bonding within carboxylic acid dimers and nucleic acid base paired systems. One particular system of interest is 3',5'-di-O-acetylthymidine and various techniques have been utilised to determine the presence of anomalous hydrogen behaviour. A crucial part of this has been a multiple temperature high resolution study carried out on station 9.8 at SRS, Daresbury. Alongside experimental work, recent computational work will highlight how these new methods can augment traditional experimental results. Overall it is hoped that the research presented will again highlight the importance of complementary techniques in crystallographic research.

[1] Parkin A., Harte S. M., Goeta A. E., Wilson C. C., *New J. Chem*., 2004, **28**, 718. [2] Wilson C. C., Morrison C. A., *Chem. Phys. Lett*., 2002, **362**, 85-89.

Keywords: hydrogen bonds, diffraction methods, computation

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Polymorphism of Crystalline Amino Acids. The Role of Non-covalent Interactions

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The crystals of amino acids are interesting from several points of view – as drugs, as molecular materials (e.g. piezo- and ferroelectrics), but also as biomimetics. Understanding the effects of pressure, temperature, and various chemicals on the crystal structures of these