Carlo simulated annealing [3, 4]. The prediction has been performed for nitrobenzenes with a following second substituent: hydroxyl, amino, nitro or methyl group or chlor, brom, iod atom. The calculations have been carried out for a standard choice of space groups. The *Polymorph Predictor*, module of *Cerius*^{2} program was used [5].

The predicted structures are compared with our experimental results or with crystal structures retrieved from CSD [6]. The polymorph structures are analysed in terms of molecular interactions that influence nucleation, crystallisation and stability of polymorphs.

[1] Gavezzotti A., *Cryst. Eng. Comm.*, 2002, **4**, 343-347. [2] Price S.L., *Advanced Drug Delivery Reviews*, 2004, **56**, 301-319. [3] Leusen F.J.J., *J. Cryst. Growth*, 1996, **166**, 900-903. [4] Gdanitz R.J., *Chem Phys. Letters*, 1992, **190**, 391. [5] *Cerius*^{2}®, Accelrys, 9685 Scranton Road, San Diego, CA 92121-3752. [6] Allen F.A., Kennard O., *Chem.Des.Autom. News*, 1993, **1**, 31.
Keywords: crystal structure prediction, nitrobenzene derivatives, polymorphs

P.02.10.3
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Structural Modeling of Sterol Carrier Protein-2 from Plants
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Sterol carrier protein-2 (SCP-2) is a small, cytoplasmic protein that was originally described as a cholesterol transfer protein. Later it has been shown that SCP-2 binds a variety of lipids but its actual biological function remains unclear. SCP-2-like proteins have been found in various organisms from vertebrates to bacteria, and recently also in plants. In order to characterize SCP-2 from the plants *Arabidopsis thaliana* (AtSCP-2) and *Euphorbia lagascae* (ElSCP-2) we have built structural models of the two proteins in apo and ligand-bound conformation [1] based on the known crystal structures of rabbit SCP-2 [2], the SCP-2 like domain of human D-bifunctional enzyme [3] and the yellow fever mosquito SCP-2 [4]. Although the sequence identity between AtSCP-2 and ElSCP-2 is high (67.5%), they preferably bind different lipids. We have examined the ligand-binding cavities of the AtSCP-2 and ElSCP-2 structural models in apo and ligand-bound conformations in order to find out structural properties, which would explain the differences in ligand binding.

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Keywords: protein modelling, protein-lipid complexes, protein structure comparison

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Powder Diffraction and Crystal Structure Prediction: A Two-Way Relationship?
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The most common complementary use of theoretical and experimental methods is structural rationalization from crystal structure prediction and X-ray powder diffraction techniques[1]. This aids both the rationalization of crystal structures generated in a prediction, and the characterization of solids from powder data that precludes indexing or structure solution.

Powder data from the prediction is often compared visually or purely on a fingerprinting basis with the experimental, and there are only a few cases of organic materials in which the predicted structures have been used as a starting point for Rietveld refinement[1,2]. One possible reason for this is that even though the variation in lattice parameters between the experimental and calculated structures is relatively small, the difference in the respective patterns often makes automated quantitative comparison difficult and attempts at refinement unsuccessful. As prediction calculations search for the energetically optimal packing at 0 K, use of low temperature powder data would enable a more meaningful comparison of the two profiles.

We will present our results from the study of several organic materials at low temperatures and their subsequent comparison to the predicted structures using a number of quantitative guides.

[1] Tremayne M., Grice L., Pyatt J.C., Seaton C.C., Kariuki B.M., Tsui H.H.Y., Price S.L., Cherryman J.C., *J. Am. Chem. Soc.*, 2004, **126**, 7071. [2] Payne R.S, Roberts R.I., Rowe R.C., Docherty R., *J. Comput. Chem.* , **19**, 1.
Keywords: structure prediction, powder diffraction, low-temperature structures

P.02.10.5
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Can a Computational Search Predict Complications in Single Crystal Growth?
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To study the variation in possible crystal packing of structures with respect to the relative positions of functional groups, five dichloronitrobenzenes have been studied both experimentally and computationally. A manual polymorph screen has been carried out for each compound using a variety of solvent methods and sublimation to grow crystals.

The experimental search found considerable difficulty in growing crystals suitable for single crystal X-ray diffraction with many exhibiting multiple domains and plate-like morphologies. Redeterminations have been carried out at low temperature but have not shown a marked improvement on the published refinements.

The computational searches found the known structures as the global minimum in a few cases. For each compound, though, there were many hypothetical structures within a small energy range of that minimum with many of these being variants on the experimentally observed sheet structures.

The predicted low energy structures illustrate variations in the sheet packing which could be indicative of, for example, slippage between the layers or disorder in the stacking. A possible link between this phenomenon and the problems associated with crystal growth and structure determination will be discussed.

Figure 1. Two variations on the stacking of sheets related by slippage along c.
Keywords: prediction, crystal growth, organic compounds

P.02.10.6
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Binding Pocket Shape Analysis for Protein Function Prediction
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We present a novel method for the comparison of protein binding pockets and ligands. An increasing number of protein structures are being determined for which no biochemical characterisation is available. The analysis of protein structure and function assignment is becoming an unexpected challenge and major bottleneck towards the goal of well-annotated genomes. As shape plays a crucial role in biomolecular recognition and function, shape techniques are likely to be of prime importance for understanding protein structure-function relationships.

A highly efficient shape comparison technique based on a real spherical harmonics expansion is presented for protein function prediction from structure. Our approach identifies the active site by a geometrical surface analysis method combined with an evolutionary trace technique. The binding pocket is then placed into a standard frame of reference using a heuristic that employs the first three moments of the spatial extent of the shape to find the orientation. The method uses the coefficients of a real spherical harmonics expansion to describe the shape of a protein's binding pocket. Shape similarity is computed as the Euclidean distance in coefficient space and is

therefore extremely fast, enabling thousands of comparisons to the carried out per second on a standard PC.

[1] Morris R.J., Najmanovich R.J., Kahraman A., Thornton J.M., *Bioinformatics*, 2005, *in press*.

Keywords: bioinformatics, function prediction, active-site recognition

P.02.11.1

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Powder Struture Resolution of 1,7-Dioxaspiro[4.4]nonane

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Different attempts to crystallise compound 1,7-dioxaspiro[4.4]nonane, led to very small and irregular crystals which were not good enough to be analysed by the single-crystal X-ray diffraction technique. Moreover, the data collected with powder diffraction technique, was very poor to work with conventional direct methods for the structure solution.

The powder pattern was indexed using the program suite Crysfire. We have modeled different configurations in agreement with the other experimental analyses in order to test them with the powder diffraction data. We have located the different modeled solutions into the refined unit cell with the F.O.X. program. The Rietveld method was used for the refinement of the positions of non H atoms using the Bruker AXS Topas program.

Based on the results of the above mentioned method, it is possible to conclude that the technique of structural resolution by powder diffraction data is sensitive to changes of the atomic positions, or on the nature of atoms of the modeled molecule, and that this technique has allowed the confirmation of the structure of mentioned compound as it was suggested by means of spectroscopic techniques.

Keywords: powder structure resolution, organic structure determination, 1,7-dioxaspiro[4.4]nonanes

P.02.11.2

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The Structure Determination of Single-component Molecular-metal

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The single-component molecular metals, $Ni(tmdt)_2$ [1] and related materials, have attracted much interests due to their characteristic properties. Many other related materials have been produced by changing the metal atom and extended-TTF ligands. The crystal structure determination of newly produced materials is often very difficult due to only small amount of powder sample being available.

In this study, we determined 5 crystal structures of $Ni(tmdt)_2$ related materials, which are $Ni(dt)_2$, $Pd(dt)_2$, $Au(tmdt)_2$, $Pd(tmdt)_2$, and $Pd(dmdt)_2$, by Genetic Algorithm combined with MEM/Rietevled method using synchrotron radiation X-ray powder diffraction data measured at SPring-8, BL02B2. The reliability factors, Rwp and RI, of Rietveld refinements are in the the range of 2~4% and 3~7%, respectively. It was found that the molecular stacking is different by the length of extended-TTF ligands. It is found that the positional relation of neighboring layers is closely related to the conductivity of materials.

[1] Tanaka H., et al., *Science*, 2001, **291**, 285-287.

Keywords: single-component molecular-metal, SR powder diffraction, genetic algorithm

P.02.11.3

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Ab-initio Structure Determination of $C_{18}H_{19}N_4S$ from Powder X-ray Diffraction

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The crystal structure of 1-(N-allythiacarbamoyl)-3-(4-methyl-phenyl)-5-(pyrol-2-yl)-2-pyrazoline, $C_{18}H_{19}N_4S$, has been solved by the method of simulated annealing from synchrotron x-ray powder diffraction data. Pyrazolines are known to display various biological functions, such as fungicidal, antibacterial activities, pharmacological properties such as anti-inflammatory agents and industrial applications. The powder sample was sealed in 1mm capillary and diffraction data was collected with curved imaging plate method using 12KeV x-rays at the BL01C2 beamline in National Synchrotron Radiation Research Center (NSRRC). The structure was determined while following these procedures: (1) determination of the unit cell parameters, (2) determination of the space group, (3) extraction process by Pawley method, (4) structure solution by simulated annealing using DASH (David et al., 1998) and (5) Rietveld refinement by GSAS (Larson &Von Dreele, 1990) programs. The title compound crystallizes in triclinic system with space group, $P\ \bar{1}$, unit cell parameters of a = 12.603(14), b = 9.094(8), c = 8.494(8)Å, α = 70.85(8)°, β = 105.26(8)°, γ = 109.10 (7)°, Volume = 855.7Å^3 and Z=2. The final reliability factors of Rietveld refinement are R_{wp} = 0.039 R_p = 0.029 R_B = 0.118 and S = 1.041.

Keywords: ab-initio structure determination, drug design, synchron powder diffraction

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Structure Determination from Powder Data of two Sub-peptides of Leu-enkephalin

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The crystal structures of two tripeptides, sub-peptides of leu-enkephalin which belongs to the opiate family of neuropeptides, have been solved from high resolution powder diffraction data using synchrotron radiation. Glycine-phenylalanine-leucine, $C_{13}N_3O_4H_{21}$, is monoclinic, space group $P2_1$, with a = 20.0024(8) Å, b = 4.8738(1) Å, c = 10.2778(2) Å, ß = 103.940(1)°, Z = 2, at room temperature. Glycine-glycine-phenylalanine, $C_{17}N_3O_4H_{24}{\cdot}2H_2O$, recrystalised from water is orthorhombic, space group $P2_12_12_1$, with a = 30.3902(2) Å, b = 10.25972(8) Å, c =4.83972(4) Å, Z = 4. The structures were solved via global optimization, programs TOPAS and FOX, and the use of maximum entropy maps.

Keywords: powder crystallography, peptides, synchrotron X-ray diffraction

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Crystal Structures of 8-Styrylxanthine Analogs from Powder Diffractin Data

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Adenosine modulates several physiological functions acting via specific G-protein-coupled receptor subtypes identified as A1, A2a, A2b and A3. Since the discovery that xanthines are the most important class of potent and selective antagonist at adenosine receptors (AR), the interest in this class of compounds has significantly increased. A novel classes of A2aAR antagonists [1] were investigated by means of X-ray powder diffractometry and the crystal structures of some analogs of 8-styrylxanthines: $C_{14}H_{13}N_6O_2Cl$, $C_{14}H_{14}N_6O_2$ (azo-analogs) and $C_{15}H_{14}N_5O_2Br$ (imine-