s10.m1.p9 **Structure solution from powder pattern for a derivative of ascomycin using Cerius[2] software.** L. Motta-Viola, S. Pfeffer-Hennig and D. Giron. *Novartis-Pharma AG, Klybeckstrasse, 4002 Basel (Switzerland)*
Keywords: powder diffraction, advanced methods, structure determination.

This poster presents the evaluation of the Powder Solve module of Cerius[2] software[1] for an ascomycin derivative monohydrate. This drug substance has been choosen because synchrotron XRPD data and the correct conformation of the molecule known from the single crystal structure (hydrate form) were available. The procedure has been applied with synchrotron data and lab data to investigate the influence of correct intensities for 12 degrees of freedom.

From the experimental synchrotron XRPD pattern, the cell dimension and lattice symmetry has been easily found by the program.

The molecule in its known conformation, and the water molecule as a second independent molecule were introduced. Then the program was able to find the correct position in the unit cell for both, drug substance and water molecules.

The same procedure was performed with laboratory data measured in reflection mode. In this case, again the cell dimensions and lattice symmetry could be found by the program (using mainly the peak positions of the experimental pattern). But for the second step, totally different positions for molecules were found due to the different peak intensities of the experimental X-ray pattern.

It can be concluded that structure solution from XRPD data depends strongly on their quality, determined by the correct peak position and peak intensities. Using synchrotron data and the correct conformation, it was possible for 12 degrees of freedom to get straightforward the solution. Furthermore, intensities for lab data were not suitable enough.

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[1] Engel G.E., Wilke S., König O., Harris K.D.M. and Leusen F.J.J.;"Powder Solve – a complete package for crystal structure solution from powder diffraction patterns", J. appl. cryst., (1999), 32, 6, 1169-1179.

s10.m1.p10 **X-Ray Powder Diffraction experiments with a 32-channel Si microstrip detector.** V. Psycharis, A. Gantis and C.P.Raptopoulou *Institute of Materials Science, N.C.S.R. "Demokritos",15310 Ag.Paraskevi, Athens, GREECE.* V. Perdikatsis, *Institute of Geology and Mineral Exploration, Messogion 70, 115 27 Athens, Greece.* A. Pavlidis and D. Loukas *Institute of Nuclear Physics, N.C.S.R. "Demokritos",15310 Ag.Paraskevi, Athens, GREECE.*
Keywords: powder diffraction, advanced methods, structure determination.

A 32-channel Si microstrip detector has been installed in a X-Ray powder diffractometer which has a Debye Scherrer geometry and is equipped with an elliptic Goebel mirror and a fine focus tube. The samples are mounted in capillaries at a distance of 250mm from the focusing line produced by the mirror. On the same system a conventional NaI scintillation detector is also used and the 2T range that is accessible (120^o) can be scanned in any desired step (0.001^o minimum) . The distance between two successive readout channels of the silicon detector is ?S= 200 μm. The 2T range covered by the 32-channel microstrip Si detector is $\approx 1.5^o$ for a measuring circle radius of 250mm. Calibration curves, the process for instrument alignment and a series of measurements of standard samples will be presented. The single channel NaI detector is used for calibration purposes of the diffractometer. Models for absorption corrections for spectra recorded from capillary mounted samples (with μr> 1) for an effective Rietveld refinement will also be presented.