signalling networks. Identification of disordered regions in protein sequences can help identify such proteins and to reduce bias in sequence similarity analysis. A practical spin-off for structural biology work is to delineate boundaries of protein domains to guide structural and functional studies (Ferron, et al., 2006). Several state-of-the-art approaches have been proposed for prediction of ordered and disordered residues, such as neural networks, NNs, and Support Vector Machines, SVMs. We introduce Conditional Random Fields, CRFs (Lafferty, et al., 2001), as a new method for accurately predicting the transition between structured and highly flexible or disordered regions in proteins. Our Order and Disorder predictor, OnD-CRF, relies only on features which are generated from the amino acids sequence and from the predicted secondary structure. Benchmarking results rank the OnD-CRF model highest among the fully automatic server group (Wang and Sauer, 2008). Availability: http://babel.ucmp.umu.se/ond-crf/

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Keywords: protein disorder, flexibility, domain boundary

P08.10.94

Acta Cryst. (2008). A**64**, C447

The remarkable “polymorphism” of aspirin

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The crystal structure of aspirin, *ortho*-acetylsalicylic acid, has been established since 1964. A second polymorph was reported in 2005. The new crystal structure (“form II”) is closely related to the long-established structure (“form I”). Both structures contain identical layers of centrosymmetric dimers, linked by O-H···O hydrogen bonds between their carboxyl groups. In the form I structure, adjacent layers are arranged so that their acetyl groups meet to form a centrosymmetric arrangement of C-H···O contacts. In the form II structure, adjacent layers are translated relative to each other so that C-H···O contacts link the acetyl groups into catemeric motifs. The two arrangements have been calculated to be approximately isoenergetic. Diffraction patterns reveal that aspirin crystals can exhibit one-dimensional stacking disorder, incorporating both interlayer arrangements. Two sets of Bragg reflections demonstrate extended domains with the form I and form II structures, while diffuse features reveal less ordered regions. The relative proportions of the two interlayer arrangements are variable. Pure form I crystals are commonplace but pure form II crystals have not so far been realised. This disordered system raises interesting questions with regard to the definition of polymorphism in molecular crystals: is aspirin polymorphic, and if so, how many polymorphs exist? The question is especially relevant given the pharmaceutical prominence of aspirin, and may prove to be significant in the context of the patentability of crystalline forms.

Keywords: pharmaceuticals, polymorphism, disordered solids

P08.10.95

Acta Cryst. (2008). A**64**, C447

Polymorphism and structural mechanism of the phase transformation of phenyl carbamate (PC)

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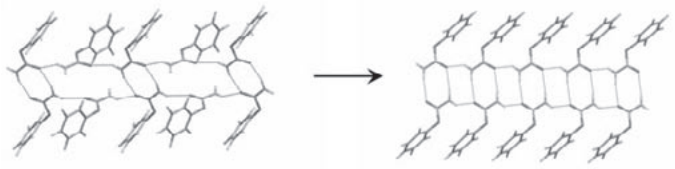
Co-crystallization experiments with phenyl carbamate (PC) as a hydrogen bond donor with crown ethers have led to the serendipitous discovery of three crystal forms of PC. These newly discovered polymorphs have been characterized by a variety of methods including variable temperature powder X-ray diffraction (PXRD), vibrational spectroscopy (Infrared and Raman), calorimetry (DSC) and optical hot stage microscopy (HSM). Forms I and II have been obtained from a number of solvents while Form III was obtained only by heating Form II and was observed only transiently in the DSC, HSM and PXRD. Form I transformed to Form II both through solution-mediated phase transformation and solid state transformation. A comparison of the two structures of Form I and Form II provides a qualitative model for the structural mechanism of the transformation. The relatively small changes in IR and Raman peak positions imply that the major differences between the two structures are associated with changes in the environment of the phenyl ring as revealed in the single crystal structure analysis.



Keywords: polymorphism, hydrogen bonds, structurally dependent related phase transformatio

P08.10.96

Acta Cryst. (2008). A**64**, C447-448

Polymorphic study of the model system hexamidine diisethionate

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Polymorphism in drug substances may cause severe problems during manufacturing processes. Hexamidine diisethionate (HDI) is an aromatic diamidine linked by a flexible eight-membered chain and resembles the type of molecules which form liquid crystals. Since HDI is used as a preservative mainly in solution, no polymorphism has been described to date. The drug is closely related to the polymorphic pentamidine diisethionate [1], which has a seven-membered connecting chain, so that the existence of multiple crystal forms of HDI was anticipated. By applying multiple analytical techniques, ten anhydrous crystal forms were discovered. In particular, thermal-analytical techniques and temperature controlled X-ray diffraction turned out to be superior analytical tools to identify and characterize the various polymorphic transitions. Additionally, two enantiotropically related triclinic dihydrates were