

**P.05.08.4***Acta Cryst.* (2005). A61, C278**Synthesis and Structural Characterization of 3-(4-fluorophenyl)-2-( $\alpha$ -naphthyl)-1,3-thiazolidin-4-one**

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One of the richest sources of diversity for the medicinal chemist is small heterocyclic rings, which in addition to often exhibiting biological activity, may serve as rigid scaffolds for further display of functionalities. Thiazolidine derivatives belong to an important family of these heterocyclic compounds. Substituted thiazolidines display diverse biological activities such as tuberculostatic, fungicidal, pesticidal, herbicidal, antidiabetic, anti-inflammatory and bactericidal. The biological significance of this kind of compounds urged us to study of the synthesis and physicochemical properties of some 3-aryl-2-( $\alpha$ -naphthyl)-4-thiazolidinones due to their possible biological activities. As part of our ongoing research program aiming at the search of structural chemistry and substituted thiazolidinone synthesis from accessible aldimines, we used  $\alpha$ -naphthaldimines in the preparation of new series of 3-aryl-2-( $\alpha$ -naphthyl)-1,3-thiazolidin-4-ones.

The compound 3-(4-fluorophenyl)-2-( $\alpha$ -naphthyl)-1,3-thiazolidin-4-one crystallizes in a monoclinic cell with the cell parameters  $a = 10.6097(5)$ ,  $b = 10.8356(5)$   $c = 13.2278(6)$  Å and  $\beta = 101.0850(10)^\circ$ , Space group P2<sub>1</sub>/c [No 14],  $V = 1492.33$  Å<sup>3</sup> and  $Z = 2$ .

**Keywords:** thiazolidinone, structural characterization, single crystal

**P.05.08.5***Acta Cryst.* (2005). A61, C278**Structural Analysis of the N-terminal Domain of PriA from *E. coli***

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PriA, a DEXH-type DNA helicase, is essential for restoration of stalled replication forks and is a candidate sensor protein that recognizes arrested replication forks in bacteria [1]. The N-terminal domain binds to a free 3' terminus through the putative 3'-terminus recognition pocket [2]. We analyzed the interaction between N-terminal minimum binding domain of PriA[1-105] and oligonucleotides by using the single molecule fluorescence detection system MF20 (Olympus, Tokyo). The results indicated that PriA[1-105] recognized only the 3' terminal nucleotide portion of oligonucleotides.

We determined the crystal structure of the N-terminal domain of PriA to reveal the structural basis of the 3' terminal nucleotide recognition. Single crystals of native and SeMet PriA[1-105] were grown in hanging drops with a reservoir solution consisting of 0.1 M sodium citrate pH 3.6-3.8 and 0.15-0.35 M ammonium sulfate. Data sets were collected on BL38B1 at the SPring8 and PF-BL6A at the KEK. Native crystal diffracted to 2.8 Å and belongs to space group R32, with unit cell parameters,  $a=b=111$  Å,  $c=260$  Å.

[1] Tanaka T., et al., *J. Biol. Chem.*, 2002, **277**, 38062. [2] Mizukoshi T., et al., *J. Biol. Chem.*, 2003, **278**, 42234.

**Keywords:** DNA recognition, arrested replication fork, free 3'-terminus

**P.05.08.6***Acta Cryst.* (2005). A61, C278**Crystal Structure Determination of a Valinium Hybrid Compound**

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In recent years, organic-inorganic hybrid materials have attracted considerable attention as preferred materials in nonlinear optics (NLO), such as second harmonic generation (SHG) and optical bistability, owing to their large optical nonlinearities [1]. L-valinium hydrogenphosphite, results from our systematic investigation of organic-inorganic hybrid materials obtained by interaction between various phosphoric oxyacids and amino acids [2],[3].

As part of our continuing interest in this field, we report here the crystal structure of L-Valinium hydrogenphosphite [C<sub>5</sub>H<sub>12</sub>NO<sub>2</sub><sup>+</sup>, H<sub>2</sub>PO<sub>3</sub><sup>-</sup>], it can be described as a stacking of l-valinium and hydrogenphosphite ions. The stability of such an arrangement results from a network of hydrogen bonds, which maintain the cohesion of the organic-inorganic layers in the crystal. The asymmetric unit contains two valinium residues and two hydrogenphosphite ions, one of which is disordered.

[1] Zaccaro J., Bagieu-Beucher M., Espeso J., Ibanez A., *J Cryst. Growth*, 1998, **186**, 224-232. [2] Benali-Cherif N., Abouimrane A., Sbai K., Merazig H., Cherouana A., Bendjeddou L., *Acta Cryst.*, 2002, **E58**, o160-o161. [3] Bendheif L., Bouchouit K., Benali-Cherif N., *Acta Cryst.*, 2003, **E59**, o1407-o1409.

**Keywords:** valinium, hydrogen-bonding, disorder

**P.05.08.7***Acta Cryst.* (2005). A61, C278**SAXS Studies of Nucleation of Glycine from its Supersaturated Solution**

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The early stages of the process of crystallization, especially that of small molecules from their supersaturated solution is not yet fully understood. In an effort to understand the process of nucleation and crystallization of such molecules, small angle x-ray scattering (SAXS) has been used to study the crystallization of the amino acid glycine from its supersaturated aqueous solution. The scattering data was analyzed using the Unified Fit Model which helps in studying complex systems that may contain multiple levels of related structural features. The results suggest that glycine molecules exist as dimers in supersaturated solution. The structure factor and the form factor obey power-law behaviour that indicates the presence of fractals in the solution. A transformation from mass fractal structure to surface fractal structure is observed during the crystallization process, which could be the signature of a two-step nucleation process.

**Keywords:** SAXS, nucleation, fractals