s6.m22.o5 **Conformational Chirality of Sulfonylpyrimidine Derivatives.** Aleksandar Visnjevac,[a] Marija Luic,[a] Mladen Zinic[b] and Biserka Zinic[b], [a]*"Ruder Boskovic" Institute - ZFK, P.O.B. 180, HR-10002 Zagreb, Croatia, and* [b]*"Ruder Boskovic" Institute - OKB, P.O.B. 180, HR-10002 Zagreb, Croatia. E-mail: aleksandar.visnjevac@irb.hr*

Keywords: Conformational Chirality; Racemic Twinning; Pyrimidine Nucleobases

The title compounds belong to a novel series of pyrimidine nucleobase derivatives possessing a sulfonamide pharmacophore. Some of them exhibit significant anticancer activity *in vitro*.[1] As the part of the overall structural examination, the crystal structures of 1-tosylthymine (**1**) and 1-tosyluracil (**2**) are presented. Both compounds crystallise in orthorhombic system (**1** in *Pbca* and **2** in $P2_12_12_1$), whereby the cell volume of **1** is twice as large as the one of **2** (doubling of one axis). The axial conformational chirality was encountered in both compounds, as the consequence of the S1-N1 single bond free rotation hindrance in solid state *(atropisomerism)*. [2]

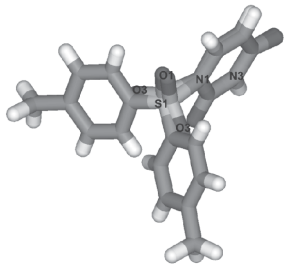

*Fig. 1. Overlap of two atropisomers of **2**.*

The spontaneous resolution of R_a and S_a enantiomers occured only during the crystallisation of **2**, whereas **1** crystallised as a racemate. Formation of chiral crystals of a compound without any stereogenic element is rare and of great interest in the field of absolute asymmetric synthesis in the solid state as well as in connection with the origin of homochirality of life. [3] The SHELXL merohedral twin refinement was applied in the case of the racemically twinned species (**2**), and the resulting Flack parameter was discussed. The interdependence of the crystal packing and the occurence of the spontaneous resolution was discussed, bearing in mind tiny chemical differences between **1** and **2**.

[1] Ruder Boskoviæ Institute (B. Zinic, M. Zinic, I. Krizmaniæ) EP 0 877 022, 2003.
[2] I.D. Cunningham, S.J. Cooles, M.B. Hursthouse, *Chem. Comm*. (2000) 61-62.
[3] I. Azumaya, T. Kato, I. Okamoto, R. Yamasaki, A. Tanatani, K. Yamaguchi, H. Kagechika, H. Takayanagi, *Org. Lett*. (2003) **5**, 3939-3942.

s7.m23.o1 **A Third Blind Test of Crystal Structure Prediction.** James A Chisholm *Cambridge Crystallographic Data Centre, 12 Union road, Cambridge CB2 1EZ, UK and Pfizer Institute for Pharmaceutical Materials Science, University of Cambridge, Department of Materials Science and Metallurgy, Pembroke Street, Cambridge CB2 3QZ, UK. E-mail:chisholm@ccdc.cam.ac.uk*

Keywords: Crystal Structure Prediction; Polymorph; Structure Comparison

In May 2004 the CCDC hosted a meeting to discuss the results of the third blind test of Crystal Structure Prediction (CSP). The challenge of the competition was to predict the experimentally observed crystal structure of the 4 small organic molecules shown in figure 1 given information only on the molecular diagram, the crystallisation conditions and the fact that Z' would be no greater than 2. The results of the competition are presented including an analysis of each participants extended list of candidate structures. A computer program COMPACK has been developed to identify crystal structure similarity. This program is used to identify at what positions the observed structures appear in the extended lists. Also, predicted structures obtained from the various participants are compared to determine whether the different approaches and methodologies attempted produce similar lists of structures. The hydrogen bond motifs predicted for molecule I are also analysed and an assessment made as to the most commonly predicted motifs and a comparison made to common motifs observed for similar molecules found in the Cambridge Structural Database.

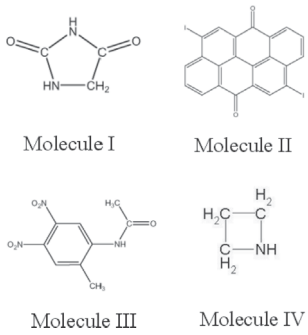

Figure 1. The four molecules selected for the third blind test.