

Spontaneous Resolution of *N*-sulfonylpyrimidine Compounds Induced by Chemical Modifications

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The title compounds belong to a novel series of pyrimidine nucleobase derivatives, some of which exhibit significant anticancer activity *in vitro*. [1] The crystal structures of 1-tosylthymine (**1**), 1-tosyluracil (**2**), α -naphthyl derivatives of thymine (**3**) and uracil (**4**) are presented. The conformational chirality was encountered in all compounds, as the consequence of the S-N single bond free rotation hindrance in solid state (*atropisomerism*). [2]

The spontaneous resolution (*à la Pasteur*) of *P* and *M* conformational enantiomers occurred during the crystallization of **2** and **4**, whereas their 5-methyl analogues, **1** and **3**, crystallized as racemic mixtures. Moreover, spontaneous resolution in the case of **2** was accompanied by a formation of racemically twinned crystals regardless of the solvent used. Obviously, substituents at C-5 position of pyrimidine base as well as in -SO₂-R group dictate the occurrence (or absence) of spontaneous resolution.

[1] Žinić B., Žinić M., Krizmanić I., *Ruđer Bošković Institute*, EP 0 877 022, 2003. [2] Cunningham I.D., Cooles S.J., Hursthouse M.B., *Chem. Comm.*, 2000, 61-62.

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