the presence of the two heavy atoms on the benzene ring, which make the compound potentially favourable for further liquid scattering studies to examine the crystal growth from the nucleation point. The physical form has been characterised at low temperature due to sublimation occurring at room temperature – this makes the full characterisation of the crystallisation conditions for this material challenging. The solubility profile, as a function of temperature, and metastable zone-width experiments, that have been studied using in situ measurements from ATR-UV spectroscopy and FBRM measurements, have been determined for this compound. We present our findings to date and comment on the suitability of this compound for further examination using scattering techniques.

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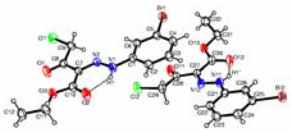
MS20 P13

(*Z*)-Ethyl 2-[2-(3-bromophenyl)hydrazono]-4-chloro-3-oxobutanoate Gökhan Alpaslan[a], Özgür Özdamar[b], Mustafa Odabaşoğlu[b], Nazan Ocak İskeleli[a], Ahmet Erdönmez[a] [a]*Ondokuz Mayıs Univ., Department of Physics, Samsun-Turkey.* [b]*Ondokuz Mayıs Univ., Department of Chemistry, Samsun-Turkey.* E-mail: gokhana@omu.edu.tr

Keywords: Single-crystal X-ray study; Keto-hydrozo tautomeric form, aliphatic chain

(*Z*)-Ethyl 2-[2-(3-bromophenyl)hydrazono]-4-chloro-3-oxobutanoate ($C_{12}H_{12}ClBrN_2O_3$) was synthesized and its crystal structure determined. It crystallizes in the monoclinic space group, $P2_1/n$, with a = 7.4266(3), b = 14.1636(7), c = 26.6760(10) Å, $R(F^2)$ = 0.032 for 5479 independent reflections.



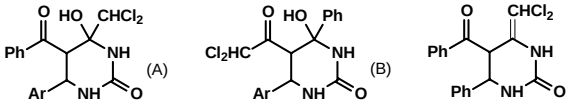
There are two crystallographically independent molecules in the asymmetric unit of the title compound, $C_{12}H_{12}ClBrN_2O_3$. The molecules adopt a keto-hydrazo tautomeric form, stabilized by an intramolecular hydrogen bond.

MS20 P14

Crystal and molecular structure of 4,5,6-trisubstituted perhydropyrimidin-2-one derivatives. Ekaterina V. Mironova, Aidar T. Gubaidullin, Igor A. Litvinov, Svetlana V. Vdovina, Vakhid A. Mamedov. *A.E. Arbuzov Institute of Organic and Physical Chemistry, Russian Academy of Sciences, Kazan, Russia.* E-mail: katy@iopc.knc.ru.

Keywords: 2(1*H*)-pyrimidones, X-ray structure, tautomerism.

2(1*H*)-Pyrimidones represent a heterocyclic system of remarkable pharmacological activity. In recent years functionalized derivatives have emerged as calcium channel modulators, α_1-adrenoreceptor selective antagonists and antiviral agents. Here we report the structures of four novel compounds of this range (**I-IV**), which were analysed in order to make the definite choice between two possible isomeric products of the reaction in the system containing urea, aromatic aldehydes and dichloromethylacetylbenzoylmethanes. The compounds **I**, **II**, **IV** crystallize in centrosymmetric space groups, **III** – in noncentrosymmetric space group (conglomerate). The molecules **I, II** form the solvates with DMSO and acetonitrile respectively. The heterocycle of molecule **I** has "envelope" conformation, and **II**, **III**, **IV** – "half-chair" conformation.



Ar = 2-IC_6H_4 (**I**); 3-IC_6H_4 (**II**); 4-$Me_2NC_6H_4$ (**III**)

The hydrogen bonds system (intra- and intermolecular ones), the packing coefficient and solvent accessible potential area in crystal were also analyzed. The authors greatly acknowledge the Russian Foundation for Basic Recearch (grant N. 04-03-32156 and 05-03-33008) and Russian Science Support Foundation for the financial support.

MS20 P15

Structural Diversity of Synthetic Estrogen Solvates Jan Smits, Carmen Guguta, Ineke Eeuwijk, René de Gelder, *Molecular Materials, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands.*
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Keywords: single crystal structure determination, solvates, drug packing

The success rate of discovering new polymorphs by crystallization from solution may be increased if solvents with diverse properties are used during initial polymorph screening. Over the last years, several solvent classifications were made to provide guidelines for the judicious choice of solvents with diverse properties for polymorph screening. Often solvates are found instead of new polymorphs. At the moment the formation of solvates is little understood and systematic studies on the formation and crystal structure determination of solvates are important for obtaining insight into the factors that determine the formation of these multicomponent crystals [1-2]. We have been engaged in such a study, focusing on ethinyl estradiol and related estrogen analogues. Estrogens are the essential hormones for the development of primary and secondary female sex characteristics and have a common steroid ring skeleton. Steroids in general have been studied intensively with respect to their molecular and crystal structures. Thousands of crystal structures of steroids are present in the Cambridge Structural Database and for certain steroids large series of solvates are found.

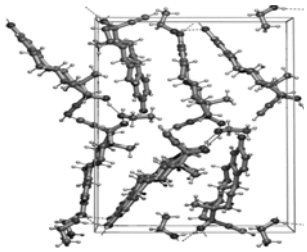

Figure 1. Crystal structure of ethinyl estradiol ethanolate

For ethinyl estradiol we determined crystal structures of several unknown solvates by single-crystal X-ray diffraction.
Ethinyl estradiol shows a remarkable flexibility in forming distinctly different hydrogen bonding patterns, resulting in a diverse set of solvate structures. The structural aspects and scope of solvate formation of ethinyl estradion is discussed and compared to other related estrogens.

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[2] Nangia, A.; Desiraju, G.R., *Chemm. Commun.* 1999, 605

MS20 P16

Crystal structure of penicillin binding protein 4 (dacB) from *Escherichia coli*. S-Y. Park, J.R.H. Tame, *Protein Design Laboratory, Yokohama City University, Suehiro 1-7-29, Tsurumi-ku, Yokohama 230-0045, Japan*
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Keywords: antibiotics, crystallography, protein crystals

The bacterial cell wall is a single molecule of peptidoglycan, which is essential for cell growth and survival under normal conditions. Since the enzymes involved in peptidoglycan synthesis have no counterpart in mammalian biochemistry, they present a variety of attractive targets for antibiotic design. Many natural bacteriocidal compounds, including the penicillin family, also exploit the dependence of bacterial survival on the integrity of the cell wall.
The crystal structure is presented of penicillin binding protein 4 (PBP4) from *Escherichia coli*, a bifunctional enzyme with both DD-endopeptidase and DD-carboxypeptidase activity. PBP4 is one of 12 penicillin binding proteins in *E.coli* involved in the synthesis and maintenance of the cell wall. The model contains a penicillin binding domain similar to known structures, but includes a large insertion which folds into domains with unique folds. The structures of the protein covalently attached to five different antibiotics presented here show the active site residues are unmoved compared to the apo protein, but nearby surface loops and helices are displaced in some cases. Movement of conserved residues suggests a possible cause for the slow deacylation rate of PBP4[1].

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