

restricted to react from one side only, i.e. if bound to molecular oxygen on one side.

[1] D.J. Sullivan, I.Y. Gluzman, D.G. Russell, D.E. Goldberg, *P Natl Acad Sci USA* **1996**, *93*, 11865. [2] S. Pagola, P.W. Stephens, D.S. Bohle, A.D. Kosar, S.K. Madsen, *Nature* **2000**, *404*, 307. [3] R. Buller, M.L. Peterson, O. Almarsson, L. Leiserowitz, *Cryst Growth Des* **2002**, *2*, 553. [4] N. Marom, A. Tkatchenko, S. Kapischnikov, L. Kronik, L. Leiserowitz, *submitted* **2011**.

**Keywords:** hemozoin, bio-mineralization, x-ray diffraction

## MS16.P71

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### Crystal structure of human RNase H2

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Human RNase H2 is a heterotrimeric enzyme involved in DNA replication and maintenance of genome stability. Mutations in any of the three subunits result in the development of Aicardi-Goutières Syndrome (AGS). Here, we report the crystal structure of human RNase H2 ABC complex at 3.1 Å resolution. Conformation of the catalytic subunit A resembles known structures of monomeric RNases H2 from archaea and bacteria, while the overall structure and arrangement of individual subunits in the complex is similar to the mouse RNase H2 structure. The B and C subunits form an intertwined dimer which makes contacts with two loops and the C-terminus of the A subunit. Human RNase H2 exhibits different substrate specificity and activity than bacterial RNases H2. Finally, we were able to map all 29 AGS-related mutations onto the structure thus providing insight into the molecular mechanisms underlying pathogenesis of this disease.

**Keywords:** RNase H2, crystal structure, disease

## MS17.P01

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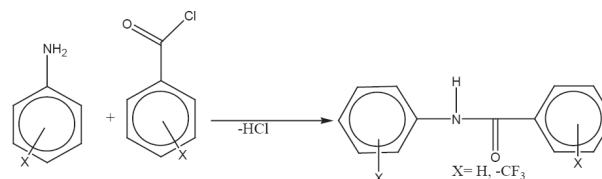
### Investigation of interactions involving organic fluorine in trifluoromethylated benzanilides

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The importance of the C-F bond is now recognized with a large number of compounds (~20% of all pharmaceuticals and ~30% of all agrochemicals) containing organic fluorine. In spite of its very high electronegativity, the involvement of organic fluorine in weak interactions has been extensively debated over a period of time. This feature has been ascribed due to its small size and very low polarizability [1]. Since the presence of organic fluorine in an organic molecule results in a modification in the chemical reactivity and biological activity, compared to its non-fluorinated analogue [2], it is imperative to understand interactions involving the fluorine atom. The formation of intermolecular O-H...F-C and N-H...F-C hydrogen bond were assumed important in the binding of the fluorinated compound to enzyme active sites [3]. In the last few years, the primary focus amongst the structural chemists has shifted towards the determination of crystal

and molecular structures of drugs and pharmaceuticals containing organic fluorine [3].

In this regard, a library of *mono*- and *bis*-trifluoromethyl substituted benzanilides, have been synthesized and their crystal structures studied to investigate the nature of weak interactions involving the C(sp<sup>2</sup>)-F bond. Benzanilides have been selected for this purpose due to the presence of -CO-NH- moiety which is an integral part of many drugs, biological molecules like amino acids, proteins etc. Crystallographic studies performed on a series of *mono*- and *di*- substituted fluoro benzanilide, containing C(sp<sup>2</sup>)-F bond, shows mainly isosteric replacement of H-atom by F-atom along with the presence of C-H...F, F...F and C-F...π contact which dictate packing of molecules in the crystal lattice [4]. In comparison with fluoro substituted benzanilides, trifluoromethyl substituted compounds shows a wide range of crystal structures, crystallizing in triclinic, monoclinic, orthorhombic and the rare and unique tetragonal system. These crystallographic determinations are characterized by the presence of rotational disorder associated with the -CF<sub>3</sub> group. Investigation of their crystal structure shows presence of C-H...F-C(sp<sup>3</sup>), lone pair...π, involving the fluorine atom along with the presence of strong N-H...O=C, weak C-H...O=C hydrogen bond and C-H...π interactions.



[1] D. O'Hagan, *Chem. Soc. Rev.* **2008**, *37*, 308-319. [2] H. Roesky, *Nature Chemistry* **2010**, *2*, 240. [3] D. Chopra, T.N. Guru Row, *CrystEngComm (Highlight)* **2010**, DOI: 10.1039/C0CE00538J. [4] D. Chopra T.N. Guru Row, *CrystEngComm* **2008**, *10*, 54-67.

**Keywords:** fluorine, intermolecular, conformation

## MS17.P02

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### Synthesis, crystal structure and theoretical calculations of Isonicotinaldehyde-N-phenylsemicarbazone and Biphenyl-4-carbaldehyde-N-phenylsemicarbazone

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Semicarbazones and their metal complexes are important classes of compounds which have long attracted attention, owing to their remarkable biological and pharmacological properties, such as antibacterial, antiviral, antineoplastic and anti-*Mycobacterium tuberculosis* activity [1]. Using the semicarbazone template was demonstrated, through a series of successive works, the significant anticonvulsant potential in epilepsy models for *aryl* semicarbazones [2].

In view of the importance of these compounds, two new semicarbazones (I) and (II) has been synthesized, and their crystal structures are reported here. Both semicarbazones molecules crystallize in a P2<sub>1</sub>/c space group. In the crystal packing the molecules are connected through N-H...O and N-H...N hydrogen bonds to form a centrosymmetric *synthon*. Other interactions like C-H...π and π...π stacking helps to stabilized the crystals.

The experimental geometries of the two compounds obtained from single-crystal X-ray diffraction were compared with those obtained from quantum-mechanical calculations. Theoretical calculations were performed by Gaussian03.