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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 Á 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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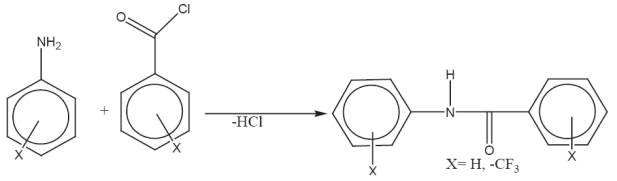
The importance of the C-F bond is now recognized with a large number of compounds (~20% of all pharmaceuticals and ~30% of all agrochemicals) containing organic fluorine. Inspite of its very high electronegativity, the involvement of organic fluorine in weak interactions has been extensively debated 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^3)-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^2)-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_3 group. Investigation of their crystal structure shows presence of C-H…F-C(sp^3), 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.



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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 $P2_1/c$ 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.

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Keywords: semicarbazone, single-crystal X-ray diffraction, DFT.

MS17.P03

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Crystal engineering of hydroxybenzoic acids. Influence of solvent in the synthon diversity and crystal packing

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Systematic analysis of intermolecular interactions formed between various molecular building units is an interesting topic in the area of crystal engineering. [1] Although the acid-pyridine interactions are well known in literature, the studies pertaining to triazines are relatively rare. Melamine is an interesting candidate due to its symmetry and the availability of several hydrogen bond donor and acceptor functionalities. Further, it is an important compound from the industrial and economical perspective. The recognition patterns of melamine with a series of substituted hydroxybenzoic acids have been studied with the assumption that the OH and COOH groups can make a cooperative influence in the recognition process and results in diverse synthons and supramolecular architectures. All these complexes form solvated assemblies and the solvent of crystallization plays an important role in the structure stability. The molecular adducts exhibit a salt-cocrystal continuum and the formation of the salts cannot be predicted on the basis of ΔpK_a values, as most of the molecular candidates have similar pKa values.[2] The synthon diversity and the crystal packing in terms of intermolecular interactions provide useful inputs for crystal design.

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Keywords: crystal engineering, supramolecular synthon, salt-cocrystal continuum

MS17.P04

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Synthesis and structures of binuclear dioxomolybdenum schiff base complexes

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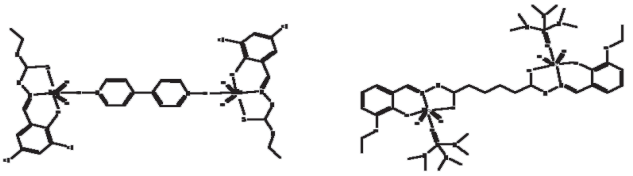
Two types of binuclear dioxomolybdenum Schiff base complexes were synthesized and their X-ray crystal structures were determined. In the first instant, the reaction of bis(acetyacetonato)dioxomolybden um with 3,4-dichlorosalicylaldehyde 4-ethylthiosemicarbazide in the presence of 4,4'-bipyridine or 4,4'-bipyridine *N*-oxide gave a binuclear *cis*-dioxomolybdenum complex in which the bidentate ligand, 4,4'-bipyridine or 4,4'-bipyridine *N*-oxide formed a bridge between the two molybdenum atoms. The overall geometry at each molybdenum site can be regarded as a distorted octahedron, with the equatorial plane formed by the imino nitrogen, phenoxyl oxygen, hydroxyl oxygen of the Schiff base and one of the terminal oxygen atoms of the dioxomolybdenum cation. The other terminal oxygen and the donor atom from the 4,4'-bipyridine or 4,4'-bipyridine *N*-oxide ligand occupy the apical position. In the case of the binuclear dioxomolybdenum complex containing the 4,4'-bipyridine *N*-oxide ligand, the molecules are linked by N-H·····O hydrogen bonds into a polymeric chain.



The second type of binuclear dioxomolybdenum(VI) Schiff base complexes was formed by the reaction of bis(acetyacetonato)dioxomolyb denum with 1,4-bis(3-ethoxy-salicylaldehyde carbohydrazonato)butane in the presence of ethanol or hexamethylphosphoramide. In this case, the two molybdenum atoms are not bridged directly by a bidentate ligand, but coordinated at each end to the O,N,O donor atoms of the symmetrical hexadentate Schiff base ligand. Each of the molybdenum atoms also adopts the distorted octahedral configuration with the equatorial plane formed by the imino nitrogen, phenoxyl oxygen, hydroxyl oxygen of the Schiff base and one of the terminal oxygen atoms of the dioxomolybdenum cation. The other terminal oxygen and the donor atom from either ethanol or hexamethylphosphoramide molecule occupy the apical position. In the case of the complex containing the ethanol molecule, adjacent molecules are linked by O-H·····N hydrogen bonds into a polymeric chain that runs along the a-axis of the monoclinic unit cell.

Keywords: Schiff base, dioxomolybdenum

MS17.P05

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Is molecular adduct formation predictable?

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The purpose of our study was to check the predictability of the formation of molecular adducts using the recently developed hydrogen bond propensity method[1,2]. Six new drug forms **1a-1f** of the anti-malarial drug pyrimethamine, **1** were synthesized with trans-cinnamic acid, **a**; ibuprofen, **b**; aspirin, **c**; glycolic acid, **d**; 4-methylbenzenesulfonic acid, **e** and carbamazepine, **f** respectively. Their crystal structures will be described. Salt formation (by the transfer of the proton from the coformer to the most basic heteroaromatic nitrogen of pyrimethamine) was observed in all the complexes except **1f**. The attempted cocrystallization reactions (**1g-1h**), of pyrimethamine, with hexachlorobenzene; **g**, and 1,4-diiodobenzene; **h**, respectively were unsuccessful in yielding adducts. Hydrogen bond propensity calculations [1], [2] were carried out to check the predictability of formation/non-formation of these molecular adducts. For **1a-1f**, the bonds of highest propensity were calculated between **1** and the corresponding coformers rather than self-association, predicting the formation of adducts. In contrast the bonds of highest propensity were calculated for self-association of molecules of **1**, for **1g-1h**, in agreement with the unsuccessful reactions.