MS19 P11

Hydrogen bonded rings as supramolecular motifs Catharine Esterhuysen, Martin W. Bredenkamp, Leonard J. Barbour *Dept. of Chemistry and Polymer Science, University of Stellenbosch, Private Bag X1, Matieland, 7602, SouthAfrica.* E-mail: ce@sun.ac.za

Keywords: hydrogen bonding, computational analysis of crystallographic data, DFT

Four and six-membered hydrogen bonded rings are common motifs in supramolecular architectures. Their influence on the formation of certain clathrate structures has been investigated and is described herein. This study includes a computational part at the B3LYP/6-31G(d) level of theory, where the hydrogen bond stabilisation involved when such a hydrogen bonded ring is formed is analysed, and an examination of the Cambridge Structural Database (CSD) [1]. In particular, the presence of the six-membered hydrogen bonded ring in the solid state structure of racemic Dianin's compound (4-*p*-hydroxyphenyl-2,2,4-trimethylchroman) [2] appears to play the most crucial role in the crystallisation of the clathrate, with the formation of the large clathrate void (240 $Å^3$). The hydrogen bond stabilisation for a series of model compounds containing four and six-membered hydrogen bonded rings is shown to be substantially greater than that of four or six equivalent individual hydrogen bonds. The effect of cooperativity of hydrogen bonds is further explored.

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MS19 P12

Crystal Structures and Interactions in Packing of Novel Thiadiazolyl - and Triazolyl-benzimidazole Derivatives F. Betül Kaynak[a], Süheyla Özbey[a], Gülgün Ayhan Kılcıgil[b], Canan Kuş[b] [a]*Department of Physics Engineering, Hacettepe University, 06800 Beytepe, Ankara, Turkey.* [b]*Deparment of Pharmaceutical Chemistry, Pharmacy Phaculty, Ankara University, 06100 Tandoğan, Ankara, Turkey.*
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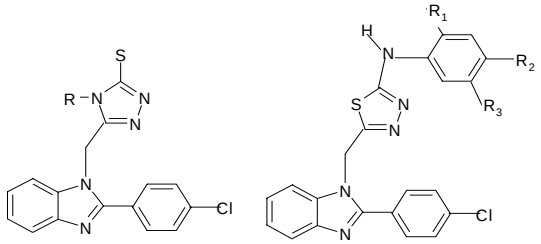
The development of resistance to current antibacterial therapy
continues to derive the search for more effective agents. In addition, primary and opportunistic fungal infections continue to increase the number of immunocompromised patients, those suffering from such as AIDS or cancer or who have undergone organ transplantation. It is well known that benzimidazoles exhibit antimicrobial [1], [2], antitubercular, anticancer, anthelmintic, antiallergic, antioxidant [3], anticonvulsant [4] and analgesic activities. It is also well known that thiadiazoles possess anti-inflamatory [5] and antimicrobial [6,7] activities.
In this paper our attention was directed toward the examination of crystal structures, hydrogen bonding characteristics and crystal packings of thiadiazolyl- and triazolyl-benzimidazole derivatives. The crystal and molecular structures of some novel benzimidazole derivatives were determined by single crystal X-ray diffracrion. In the crystal structures there are intra- and intermolecular hydrogen bonds. The crystal packing of all compounds are stabilized by hydrogen bonding and N – H···F / Cl, C – H···N and C – H··· π interactions.



R=CH_3, $C_6H_4OCH_3$; R_1=F, H; R_2=CH_3, H; R_3=Cl, H

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MS19 P13

3-(methoxyanilino)phthalides Mustafa Odabaşoğlu[a] and Orhan Büyükgüngör[b], [a]Department of Chemistry, Ondokuz Mayis University, TR-55139, Samsun, Turkey, [b]Department of Physics, Ondokuz Mayis University, TR-55139, Samsun, Turkey. E-mail: muodabas@omu.edu.tr

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Benzolactones (phthalides) are found in plants and are known to show diverse biological activities as hormones, pheromones and antibiotics. These compounds possess several important properties, such as fungicidal, ctericidal and herbicidal, analgesic and hypotensive and vasorelaxant activities. In addition, phthalidederivatives are useful in the treatment of circulatory and heart-related diseases. They are also found to be associated with pesticidal activities. In addition, phthalide is a versatile synthetic building block, particularly for the synthesis of carbocyclic and heterocyclic compounds. We decided to investigate the solid-state structures of 3-substituted phthalides by X-ray diffraction methods and present here the3-(methoxyanilino)phthalides of the title compounds (I-III).