

An Executive summary of the final report of the work done on the Minor Research Project of **Dr. Vinola Zeena Rodrigues** entitled "**SYNTHESIS, CHARACTERIZATION AND BIOLOGICAL ACTIVITY OF SOME AMIDES AND SULFONAMIDES**" sanctioned by UGC vide sanctioned letter no. **MRP(S)-0503/13-14/KAMA002/UGC-SWRO Dated: 28th March 2014.**

Amides are one of the important classes of organic compounds in which the hydroxy groups of carboxylic or sulfonic acids are replaced by amino groups. The versatility of the amide group in forming partial bonds with itself and many other functional groups is partly responsible for the structural subtleties of the biologically important amino acids, peptides and proteins etc., which are fundamental to all life. These can be understood in terms of delocalization of the nitrogen lone pair electron into the π -system of the carbonyl group. The latter produce partial double bond character in the $-C(O)-N$ bond and generate a 1,3-dipole, with nitrogen bearing a partial positive charge and oxygen, the partial negative charge. The donor-acceptor properties of the amide moiety manifest in acid-base and complexing interactions and a tendency to self-associate.

Sulfonamides and their analogues show distinct physical, chemical and biological properties. Sulfonamide drugs were the first among the chemotherapeutic agents to be used for the cure and prevention of bacterial infection in human beings. Sulfonamides have been known to exhibit a wide variety of biological activities such as antibacterial, insecticidal, antifungal, antihepatitis, anti-inflammatory, antitumor, anticancer, anti-HIV and antitubercular activities. Knowledge of structure of materials is essential for a proper understanding of their physical and chemical properties. Thus crystal structure studies have been extensively used to investigate the structural aspects of a variety of compounds. By considering the wide range of application of sulfonamides, we attempted the synthesis, characterisation of *N*-(4-substituted phenyl)-4-arylsulfonamides extensively by crystal structure analysis.

The following compounds were synthesized and characterized

- 1) *N*-(4-Bromophenyl)-4-methoxybenzenesulfonamide
- 2) *N*-(phenyl)-4-methoxybenzenesulfonamide
- 3) *N*-(4-methoxyphenyl)-4-methoxybenzenesulfonamide
- 4) *N*-(4-chlorophenyl)-4-methoxybenzenesulfonamide
- 5) 4-methoxy-*N*-(4-methylphenyl)benzenesulfonamide
- 6) *N*-(4-fluorophenyl)-4-methoxybenzenesulfonamide
- 7) 4-bromo-*N*-(4-nitrophenyl)benzenesulfonamide
- 8) 4-fluoro-*N*-(4-nitrophenyl)-4-benzenesulfonamide
- 9) 4-Bromo-*N*-(4-bromophenyl)benzenesulfonamide
- 10) 4-Bromo-*N*-(4-fluorophenyl)benzenesulfonamide

The compounds crystallized in orthorhombic and monoclinic crystal system. The parent compound *N*-(phenyl)-4-methoxybenzenesulfonamide, crystallizes in the orthorhombic crystal system and $P2_12_12_1$ space group. Introduction of the para substituent in the anilino ring was done to produce *N*-(4-Bromophenyl)-4-methoxybenzenesulfonamide, *N*-

(4-methoxy phenyl)-4-methoxy benzenesulfonamide, N-(4-chlorophenyl)-4-methoxybenzenesulfonamide, 4-methoxy-N-(4-methylphenyl)benzenesulfonamide, N-(4-fluorophenyl)-4-methoxybenzenesulfonamide. It is observed that the introduction of the electron withdrawing groups at the para position changed the crystal system from orthorhombic to Monoclinic in all the cases except for fluoro substituent. It retained to be orthorhombic, same as the parent N-(phenyl)-4-methoxybenzenesulfonamide. Introduction of the methyl substituent to the parent also changed the crystal system from orthorhombic to monoclinic.

An attempt was also done to synthesize para substituted phenyl-4 bromo benzene sulfonamide. The molecule of 4-Bromo-N-(4-fluoro phenyl)benzenesulfonamide is U-shaped, with the central C4—S1—N1—C7 fragment having a torsion angle of 68.4. The dihedral angle between the planes of the two benzene rings is 41.17. In comparison, the dihedral angles between the planes of the two benzene rings in the structures of 4-bromo-N-(4-bromophenyl)benzenesulfonamide and 4-bromo-N-(4-nitro phenyl) benzenesulfonamide, are slightly less than that in 4-Bromo-N-(4-fluorophenyl)benzenesulfonamide, with values of 38.5 (2) in 4-bromo-N-(4-bromophenyl)benzenesulfonamide and 32.6 (6) in 4-bromo-N-(4-nitrophenyl)benzenesulfonamide. The crystal structure of 4-Bromo-N-(4-fluorophenyl)benzenesulfonamide features strong N1—H1—O2 hydrogen bonds between the molecules, forming infinite one-dimensional C(4) chains. These chains are interconnected forming a one-dimensional ribbon-like architecture. In contrast, in 4-bromo-N-(4-bromophenyl)benzenesulfonamide and 4-bromo-N-(4-nitrophenyl)benzenesulfonamide, three-dimensional supramolecular architectures are present as a result of N—H—O chains, structure-directing C—H—O interactions and other weak interactions of the types Br—Br and Br—O.

The above discussion reveals that the site and nature of the substituent in the benzene group significantly alters the structural studies and thus facilitates the biological behavior in these class of compounds.

The data of the work done has been published as research articles in various international journals.

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