International Conference on Engineering, Trends in Engineering, Science, Humanities and Management (ICETESHM – 2024)
31st March, 2024, Karol Bagh, New Delhi, India.

CERTIFICATE NO: ICETESHM /2024/ C0324319

Analysing Conformational Isomers and Tautomers of Isatin-3-Thiosemicarbazone

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ABSTRACT

Isatin-3-Thiosemicarbazone (I3TSC) is a bioactive compound known for its antimicrobial, anticancer, and antiviral properties. Its structural flexibility allows it to exist in different conformational isomers and tautomeric forms, which can significantly influence its chemical reactivity, stability, and pharmacological behavior. Conformational isomerism in I3TSC arises due to the rotation around single bonds, particularly in the thiosemicarbazone (-NH-C(=S)-NH-) moiety. Different conformers may exist based on intramolecular hydrogen bonding, steric hindrance, and electronic effects, impacting molecular interactions and biological activity. Tautomerism in I3TSC primarily involves keto-thione and imine-thiol equilibria. The presence of a thiosemicarbazone group allows for keto-thione tautomerization, where the sulfur-bound proton can shift between nitrogen and sulfur atoms. Similarly, imine-thiol tautomerism leads to variations in electronic density and hydrogen bonding patterns, affecting ligand-binding properties and stability in biological systems. Spectroscopic techniques such as NMR, IR, and UV-Vis spectroscopy, along with computational modeling, help in characterizing these isomers and tautomers. Understanding these structural variations is crucial for optimizing the pharmacological potential of I3TSC, aiding in drug design and development for various therapeutic applications.