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A STUDY OF TAUTOMERIZATION AND E-Z ISOMERIZATION IN ISATIN-β-SEMICARBAZONE (IBS)

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ABSTRACT

Isatin-β-Semicabazone (IBS) is a biologically significant compound known for its pharmacological properties, including antimicrobial and anticonvulsant activities. The molecular structure of IBS allows it to exhibit both tautomerization and E-Z isomerization, which can significantly influence its stability, reactivity, and biological efficacy. Tautomerization in IBS primarily occurs due to the presence of the semicarbazone (-NH-N=CH-) functional group, which can undergo keto-enol tautomerization. This equilibrium shift between different tautomeric forms affects the electronic distribution and hydrogen bonding capabilities, impacting the compound's chemical behavior. E-Z isomerization in IBS arises from the restricted rotation around the C=N bond in the semicarbazone moiety. The E (trans) and Z (cis) isomers differ in their spatial arrangement, leading to variations in steric hindrance and intermolecular interactions. These isomers can interconvert under thermal, photochemical, or catalytic conditions, influencing IBS's biological activity and pharmaceutical applications. Understanding these structural transformations is crucial for designing IBS-based drugs with optimized properties. Computational studies, spectroscopy (such as NMR and IR), and crystallographic analysis provide insights into the preferred tautomeric and isomeric forms under different conditions, aiding in the development of more stable and effective pharmaceutical compounds.