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Azine or hydrazine? The dilemma in amidinohydrazones

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Azines belong to an important class of compounds which are found to have several applications in medicinal chemistry. Hydrazones are related and more known compounds which carry many biochemical applications. Hydrazones with appropriate substituent can show azine-hydrazone tautomerism. There are many cases in which azines are wrongly considered as hydrazones. In this article, we report the azine and hydrazone tautomeric energy differences and provide structural details of amidinohydrazones which prefer azine structure rather than the hydrazone structure, an important example being the anti-hypertensive drug–guanabenz. The importance of appropriate tautomeric representation of guanabenz has been established in terms of its molecular interactions with a known enzyme. In order to see the tautomerism in this class of molecules under experimental condition, synthesis was carried out. The experimental results are in good agreement with the DFT studies which suggest that the preferred tautomer is only azine even under experimental condition.

Biography

Sumit S Chourasiya has completed his MS (Pharm) from National Institute of Pharmaceutical Education and Research (NIPER, India), Hyderabad in the year 2011. He has a research experience of two year after MS. He worked in Albany Molecular Research Incorporation (AMRI), Hyderabad as Research Scientist Trainee from 2011-2012. He also worked as a Project Assistant in Indian Institute of Chemical Technology (IICT), Hyderabad, from 2012-2013. In 2013, he joined Indian Institute of Technology Roorkee, India, S A S Nagar and is pursuing his PhD in Medicinal Chemistry. He is currently working on the azine class of compounds, their electronic properties, tautomerism and application to the medicinal chemistry.

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