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## Chemoinformatics in understanding the SAR's in substituted octahydropyrazinopyridoindoles class of antihistamine H

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Drug discovery and development is highly challenging, expensive and time consuming process. For the identification of drug candidates having potential role in human therapeutics, it involves two major steps; viz. the identification of the lead in terms of both target and the design of novel prototypes and the second rate limiting step for finding the candidate drug for development through optimization of the lead molecule. The chemoinformatics including ligand based and structure based approaches help in accelerating the drug discovery and design process through better understanding of the structure and activity relationships. The 2-substituted octahydropyrazinopyridoindoles have shown potent histamine H1 receptor antagonism and the ligand based 2D & 3D QSARs explained well the SARs except for some outliers. The absence of human H1 crystal structure at that time prompted us to construct a homology model of H1 using the bovine rhodopsin as template which also could not explain the outlier behavior of these compounds. The structure based studies carried out on the crystal structure of human H1 receptor have been used to explain the behavior of these outliers.

### Biography

Mridula Saxena is the Head of Department of Chemistry, Amity University, Lucknow, India and is dynamically involved in teaching and drug discovery research. She worked for her PhD degree at Central Drug Research Institute, Lucknow and received her degree from the Meerut University in 1986. She had worked on different positions like Research Associate ships of ICMR/CSIR and Research Pool Scientist till 1999. There after she got herself associated with both teaching and research and got DST sponsored project in 2004 as well as faculty position at Amity University, Lucknow. All through her 39 years of teaching and research experience she has >30 papers and review/book articles in national and international journals, >30 conference papers and has 4 patents in her credit. She has visited many countries like, Germany, Hong Kong, China, Turkey, Slovenia, Russia, Greece, Egypt, South Korea and Montenegro for presenting her work.

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