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Crystallographic and molecular packing interaction analysis of cholest-based steroids: A CSD study

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Biological activity of steroids is one of the most important reasons for their synthesis and structural characterization. Cholestane ($C_{27}H_{48}$), the parent compound of all steroids, is obtained by the removal of hydroxyl group (from C3 position) and reduction of double bond (between C5 and C6 atoms) from the basic cholesterol nucleus. A total number of twenty-three structures of cholestane derivatives were obtained from the CSD for a comparative analysis of their crystallographic structures, computation of their possible biological activities and molecular packing interaction analysis. Intermolecular interactions of the type X-H…A [X=C,O, N; A=O, Cl, N, Br, F] have been analysed for a better understanding of molecular packing in cholestane class of steroids and discussed on the basis of distance-angle scatter plots. A careful examination of the entire interaction data reveals that the C-H…O hydrogen bonding is quite predominant in cholestane derivatives. The nature of the substituent at C3 position of the cholestane nucleus makes these molecules very interesting candidates for hydrogen bonding analysis. In most of the cases, the substituent at C3 position is primarily responsible for the occurrence of intermolecular hydrogen bonding in cholestanes. These substitutions are linked by intermolecular hydrogen bonding which in turn help to understand the dynamics of stacking interactions in supramolecular structures. Similar studies have also been carried out on various other classes of Cholest-based steroids, viz. Cholane, Pregnane, etc., to look for a possible solution to some of the following queries: (i) Could structural diversity in steroids be explored for a generalized crystallographic co-relations? (ii) Which of the X-H...A interactions (intra- or intermolecular) are dominant in various classes of steroids? (iii) Is there any preference of linearity for different hydrogen bonded interactions? Results of the emperical analysis of various kinds of cholest-based steroids as picked up from the CSD shall be presented.

Biography

Rajni Kant completed his PhD from University of Jammu (India) in 1989 and Post-PhD from Oxford University (UK) during 1994-95. Presently, he is Professor of Physics at University of Jammu and also the Editor-in-Chief for *Open Journal of Inorganic Chemistry* (Scirp, USA). He has guided 21 PhD students, 48 MPhil students and has published over 350 research papers in journals of international repute. He has authored a book titled "*Applied Solid State Physics*", published by Wiley-India Ltd.

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