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Advances in QSAR Studies on Calcium channel blockers

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Calcium channel blockers (CCBs) have got potential therapeutic uses against several cardiovascular and non-cardiovascular diseases, such as angina, hypertension, arrhythmias, sthma, dysmenorrhea, premature labor, cancer, epilepsy, glaucoma, etc. The three principia structural classes of compounds have been found to act as potent calcium channel blockers and they are phenylalkylamines, 1,4-dihydropyridines (DHPs), and benzodiazepines. Recently, a few more classes of CCBs have been studied. All these classes of CCBs have been found to be the most effective drugs against vasospastic angina. These drugs selectively inhibit Ca2+ influx into heart muscles by blocking slow inward channels for Ca2+ or inhibit Ca2+ influx into vascular smooth muscles. The result is negative inotropism of smooth muscle relaxation, which is translated into hypotension. We intend to present a comprehensive review, including the most recent studies, on quantitative structure-activity relationship (QSAR) and molecular modelling studies on all kinds of CCBs. These studies lead to highlight the essential structural features and physicochemical properties that the compounds should possess to act as potential CCBs. These studies also describe vividly the mechanism of interaction of CCBs with the calcium channel.

Biography

After his doctorate, in 1973 from the University of Allahabad, Dr. Gupta spent a couple of years at Tata Institute of Fundamental Research (TIFR), Mumbai, working on the structure and functions of bio membranes. In 1973, he joined Birla Institute of Technology and Science (BITS), Pilani, from where he recently moved to Meerut Institute of Engineering and Technology (MIET), Meerut. Since long he has been working on the theoretical aspects of drug design. He has made notable contributions in this area, for which he has been bestowed upon, in 1990, the Ranbaxy Research Foundation Award, a coveted national award, and made, in 1985, the Fellow of the National Academy of Sciences, India (F.N. A. Sc.). He has been an advisory member of the Technical Resource Group on Research and Development on HIV/AIDS, constituted by Ministry of Health and Welfare, Government of India. Dr. Gupta is has been the Editor-in- Chief of four international journals, namely Cardiovascular and Haematological Agents in Medicinal Chemistry, Current Computer-Aided Drug Design, Current Enzyme Inhibition, and Current Bioinformatics, all published by the Bentham Science Publishers BV, The Netherlands and U.S.A. He has also acted as a guest editor of a few prestigious international journals and recently guest-edited two volumes of Topics in Heterocyclic Drugs.