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QSAR AND MOLECULAR MODELING STUDIES ON CALCIUM CHANNEL BLOCKERS: A COMPREHENSIVE NOTE

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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, asthma, dysmenorrhea, premature labor, cancer, epilepsy, glaucoma etc. The three principal 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 Ca^{2+} influx into heart muscles by blocking slow inward channels for Ca^{2+} or inhibit Ca^{2+} influx into vascular smooth muscles. The result is negative inotropism of smooth muscle relaxation, which is translated into hypotension. Author intend to present a comprehensive review, including the most recent studies, on quantitative structure-activity relationship (QSAR) and molecular modeling 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. These studies provide the ways to find new more potent calcium channel blockers to be therapeutically more useful.