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STUDIES OF ANTI-HYPERTENSIVE ACTIVITY OF 1,4-DIHYDRO PYRIDINE DERIVATIVES: COMBINATIONS OF DFT-QSAR AND DOCKING APPROACHES

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1,4-Dihydropyridine (1,4-DHP) derivatives have been recognized as calcium channel blocker (CCB) agent. In this research, a series of 1,4-dihydropyridine (1,4-DHP) derivatives were theoretically examined for inhibitory activity against hypertension using density functional theory (DFT), quantitative structure activity relationship (QSAR) and docking approaches. The calculated molecular descriptors from DFT were used to develop QSAR model that related the descriptors to the bioactivity (IC_{50}). The QSAR analysis indicated that the energy of highest occupied molecular orbital (HOMO), dipole moment, solvation energy and average of electronic charges on heteroatoms are crucial parameters for the observed biological activity. The QSAR model predicted bioactivity (IC_{50}) agreed well with the experimental IC_{50}. All these compounds were docked against hypertensive cell receptors (PBD: 1IMT) and the binding free energy of ligand-receptor interactions agreed with the observed bioactivity (IC_{50}) of the 1, 4-DHPs with the receptor.

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