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Applications of Structure Based Drug Design Approaches towards Design and Development of Calcium Channel Blockers

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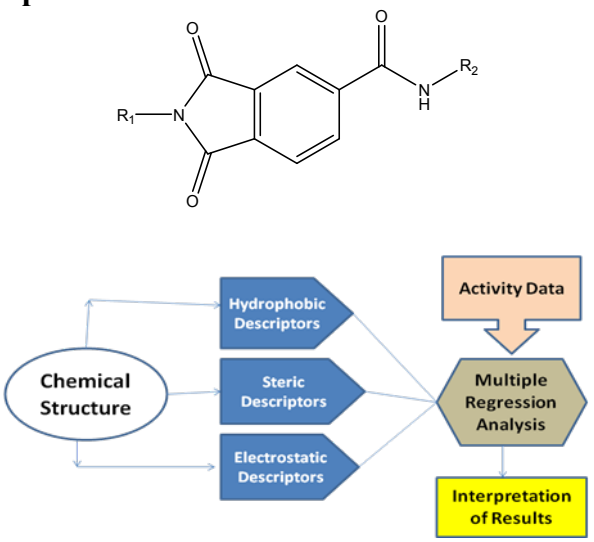
Graphical Abstract



Abstract.

Structure-Based Drug Discovery approaches facilitate the efforts towards drug discovery and in this communication these are applied towards development of Calcium Channel Blockers (CCBs). Quantitative structure-activity relationship (QSAR) studies were carried out on a series of 1,3-dioxoisoindoline-5-carboxamide derivatives and the contributing descriptors were identified as hydrophobicity, electronic constant (σ_{RI}) and some indicator parameter (I). The data set designed based on QSAR conclusions was screened against Voltage gated CCB receptor and the binding profile was predicted.

References

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