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PARAMETRIC CONTRIBUTION IN PHARMACOPHORE MODELING OF BENZODIAZEPINE DERIVATIVES: A CHEM BIOINFORMATIC APPROACH

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Present study is aimed to describe the pharmacophoric requirements in reference to anti-hypertensive activity of the benzodiazepine derivatives. A set of seventy benzodiazepine derivatives with inhibitory concentration (logIC50) and verity of structural features, electronic properties, dimensional features and quantum chemical parameters are subjected to the studies using *in silico* drug design approach.

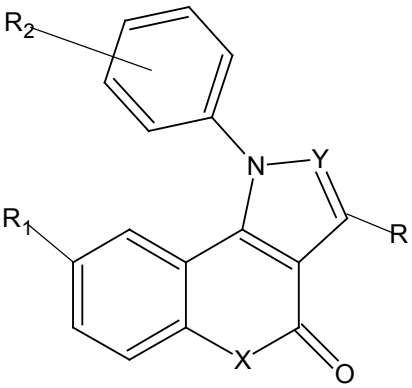

Fig.1. Parent structures of Benzodiazepine derivatives

In the process of analysis, role of structural, quantum chemical and dimensional features have been studied in respect to the pharmacophoric behavior of the benzodiazepine derivatives and their biological activity. To see more inside out about the role of electronic and energy parameters in modeling of pharmacophore for the anti-hypertensive activity of benzodiazepine derivatives, conformational study is performed using Huckel molecular orbital theory and quantum molecular mechanics method applying MM+ force field, to find out the suitable confirmer with respect to the energy and electronic features for desired biological function. Energy and other modeling parameters like electron density, net charge and stabilization factor are tested in multiple linear regression analysis helped in finding out the combination of parameters emphasizing the pharmacophoric features and can be used for the modeling of pharmacophors in benzodiazepine derivatives. Pharmacophoric features are also verified by performing docking studies using receptor ligand docking process.

Note: