MM009- APPLICATION OF UNSUPERVISED CHEMOMETRICS METHODS TO A SET OF INHIBITORS OF *ESCHERICHIA COLI* ENOYL-ACP REDUCTASE, FABI

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Introduction: The important structural element of diazaborines is a heterocyclic 1,2-diazine ring containing a boron as a third hetero atom. Purpose: Selection of the descriptors calculated from a set of fifty-one diazaborines based on their relationship with the biological activity data. Methodology: Three-dimensional models of diazaborines in their neutral forms were built using two crystallographic structures as geometry reference. Partial atomic charges were computed employing the AM1 semipempirical method. Energy minimization and molecular dynamic simulations (MDSs) were carried out (MOLSIM 3.2). The lowest energy conformer for each of ligand from MDSs was used to obtain the descriptors. Principal component analysis (PCA) and hierarchical cluster analysis (HCA) were used to treat the calculated descriptors. Results: Three sample groups are shown in the HCA. According the PCA, the partial atomic charges of the 1,2-diazine ring are seemingly important contributions to the biological activity. Perspectives: Apply the receptor-independent (*RI*) 4D-QSAR formalism to this set of diazaborines for predicting the interaction pharmacophoric elements (IPEs) as well as the alignment in the FabI active site.

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