# MEDI-Profiler: A Computational Classifier that Identifies Determinant Chemical Features and Their Influences on Pharmaceutical Drug Properties

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The pharmaceutical industry spends billions of dollars researching and developing new products; however, late in the developmental process, it is often discovered many of these seemingly hopeful drugs have unintended and undesirable consequences that render them obsolete. MEDI-Profiler is a novel computational method that classifies determinant chemical features and their influences on the biological properties of pharmaceutical drugs. Predicting side effects, biological targets and effective disease conditions to treat with small organic molecules will facilitate rapid development of drugs with dramatic cost reduction. There are several public databases available that provide rich information regarding FDA approved pharmaceutical drugs and observed side effects of the human population. Contents of such databases are increasing; therefore, an algorithm that utilizes the increasing amount of data to provide an automated classification is desired. MEDI-Profiler is designed to predict side effects, disease states/indications, targets, activities, pathways, metabolism enzymes, blood-brain barrier permeability, and taxonomical properties of conditioned small organic molecules by using only the 2D structural components fed as SMILES (Simplified Molecular-Input-Line-Entry Systems) inputted as an internal database. This algorithm utilizes independent SVM (Support Vector Machine) classifiers per biological property with optimal mathematical formulations for highest prediction accuracies. Furthermore, it can be concluded that MEDI-Profiler has the potential to become an efficient method for predicting the variables of the biological properties from the associated substructures of compounds. It is anticipated that MEDI-Profiler will aid researchers in repositioning compounds.