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Solvents are substances that are capable of dissolving or dispersing one or more substances. They may be used as a separation agent, a cleaning agent, a reaction medium, a carrier and many more purposes. Today solvents are intensively used in many industries, such as, chemical, fine chemical, pharmaceutical, food, and agrochemical industries within a wide range of applications including extraction and cleaning, separation processes, organic synthesis, and product delivery.

Since solvents must satisfy cost, processing, environmental, safety and health related specifications, solvent selection is a complex problem, which requires decision making in several levels. Furthermore, since used solvents are potential hazardous wastes, it becomes very important to minimize and optimize the use of organic solvents as much as possible, to satisfy the "Green Chemistry Principles".

In general, the search for and selection of appropriate solvents is based on a combination of heuristics and experimental studies that may be time-consuming and expensive. Hence computer-aided molecular design techniques are being increasingly used to identify promising candidates from an enormous range of potential alternatives. Such techniques are intended to develop molecules directly according to property and performance specifications, most commonly by employing a reverse engineering approach in which various sets of structural groups (building blocks) is systematically combined to form chemically feasible molecules.

The purpose of this contribution is to present a systematic general framework and its implementation in a general purpose software for selection and design of solvents for most of the common solvent applications, including organic synthesis, complex reaction systems and solvent-based separations. In this paper, three of the modules of the framework will be highlighted through appropriate case studies. Other modules in the framework include selection/design of solvents for separation, such as, extractive distillation, liquid-liquid extraction, crystallization and gas absorption, for use in product delivery and for cleaning.

The first module of the framework is dedicated to the solvent selection and design for organic synthesis. The solvent selection methodology handles single as well as multi-step chemical synthesis problems. Also, a solvent substitution feature replaces solvents for specific reaction steps in existing processes with better substitutes. The second module of the framework includes a model-based method for solvent screening and solvent mixtures design for pharmaceutical applications. The method is based on the theory of the conceptual segments (hydrophobic, polar and hydrophilic), the so-called NRTL-SAC method. In order to make the method completely independent from the availability of experimental data, a group contribution model for the prediction of the conceptual segment parameters has been developed. With the extended method, the API molecule can be described in terms of the conceptual segments and its solubility in different solvents can be evaluated. Combining it with the solvent design method, good solvents and solvent mixtures can also be identified. The third module of the framework identified ionic liquids as suitable solvents. Based on objective for the given system this module finds the best ionic liquids. In recent years, ionic liquids have attracted considerable attention for their potential as "designer solvents". This means that their properties can be adjusted to suit the requirements of a particular process. Properties such as melting point, viscosity, density, and hydrophobicity can be varied by simple changes to the structure of the ions.