Cooling Crystallization Solvent Design

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1 Brief Problem Description

Cooling crystallization is a process by which many chemicals are purified. The process works by dissolving a compound with impurities in a solvent at a high temperature where the compound should be fairly soluble. Then, the solution is allowed to cool to room temperature or below room temperature, and the solute—now less soluble in a lower temperature solution—should crystallize out, leaving behind impurities in the liquid phase. Since of course different compounds are solvated differently in different solvents, the selection of an appropriate solvent for this process is essential to good solute recovery. This specific problem involves the design of an ideal solvent for the cooling crystallization of ibuprofen. We consider five solubility properties of the compounds: the three Hansen solubility parameters (δ_h, δ_p, δ_d), the octanol-water partition coefficient (K_{ow}), and aqueous solubility (C_w). These properties will serve as the problem's degrees of freedom and are considered to be correlated with percent recovery, a metric used to quantify a solvent's goodness for this process.

2   Simulator

The executable file called MD_64 will read in inputs from in.txt, perform a molecular design problem based on the inputs given, and then return the percent recovery for the closest possible structure to the property targets. If no structure is found within a reasonable distance from the property inputs, a value of -1 is returned.
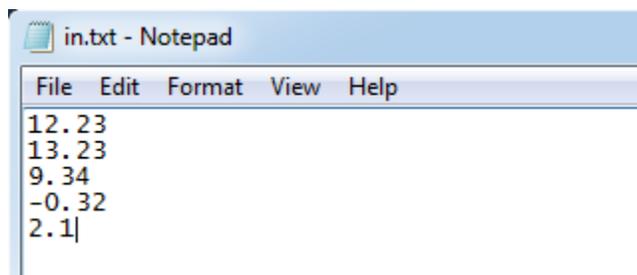
2.1   Inputs

Figure 1: Example in.txt file

The executable file reads inputs from a file called in.txt, which should appear in the current working directory. This file must be formatted as a column with one input on each line. The order of the inputs from the top is as follows: δ_d, δ_p, δ_h, K_{ow}, C_w. See the example in figure 1.

2.2   Output

The executable will run the design problem and then return the percent recovery value for a molecular candidate to a file called out.txt in the active directory. Sample output is shown in figure 2.
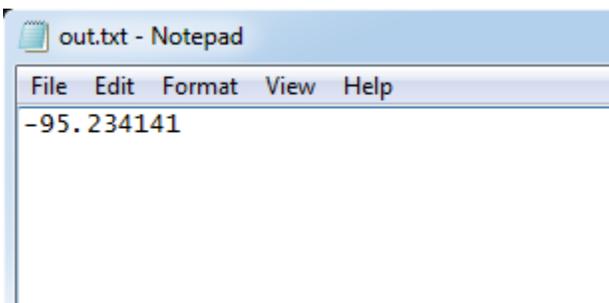

Figure 2: Example out.txt file

3   Reference

paper to come...