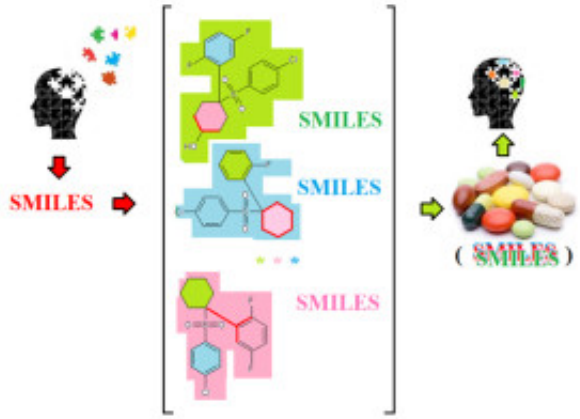
Alzheimer’s disease: SMILES to preserve wisdom

Simplified molecular input-line entry systems (SMILES) is informative representation of molecules. This representation gives possibility to compare molecules in their architecture and in their action. Molecules characterized by good pharmaceutical action can be modified in order to improve their action.



Alzheimer’s disease is a disorder of the central nervous system accompanied by memory deterioration, and progressive impairment of daily life activities. Aging of an organism is a biochemical process. Therefore, the injection of chemicals can influence this process.

There are collections of molecules, which have impact upon Alzheimer’s disease. However, the existence of more effective pharmaceutical agents is possible. How one can define these molecules?

One of the possible ways is the Monte Carlo method. The main idea can be represented by the following steps.

Step 1: Collecting of molecules, which can be utilized for treatment of Alzheimer's disease.
Step 2: Extraction of molecular features, which take place in molecules with very high impact upon treatment of Alzheimer disease.
Step 3: Extraction of molecular features, which take place in molecules with weak impact upon treatment of Alzheimer disease.
Step 4: Using computer one can build up random combinations of the above-mentioned fragments (this is essence of the Monte Carlo method).
Step 5: Experimentalist should define molecules, which can be synthesized and tested.

In fact, the above-mentioned steps contains many special operations. For instance, the fourth step is computational experiments, which can be carried out with the CORAL software, where the

SMILES are start point.

Publication

Searching therapeutic agents for treatment of Alzheimer disease using the Monte Carlo method.
Toropova MA, Toropov AA, Raška I Jr, Rašková M.
Comput Biol Med. 2015 Sep