Interactive evolutionary algorithms and data mining for drug design

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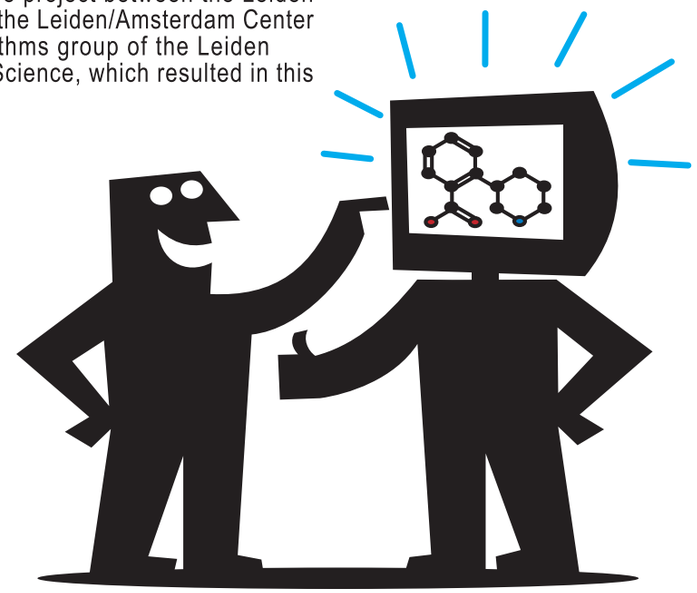
Interactive Evolutionary Algorithms and Data Mining for Drug Design

Of Molecules, Machines and Men

Interactive Evolutionary Algorithms and Data Mining for Drug Design' describes a number of investigations on how one can use the computer to generate new ideas for drugs.
First, it discusses experiments in data mining which were used to find substructure patterns in chemical databases; frequent and infrequent molecular fragments and fragment combinations which can be used to create novel compounds that can enhance the diversity of drug screening libraries. Second, it describes the development and use of a computer program based on an interactive evolutionary algorithm, the Molecule Evoluator. Similar to the philosophy of the Nobel-prize winning chemist Linus Pauling “The best way to have a good idea is to have a lot of ideas”, the Molecule Evoluator can generate many different molecular structures, either completely novel or based on a user-defined template. A chemist can then select or modify these ideas for his or her own purposes. We also describe how the Molecule Evoluator was used to design a series of biologically active compounds.

About the author: **Eric-Wubbo Lameijer** (1976) has studied medicinal chemistry at the Free University of Amsterdam with minors in cheminformatics and theoretical organic chemistry. After receiving his master's degree, he pursued his PhD at Leiden University in a collaborative project between the Leiden division of medicinal chemistry of the Leiden/Amsterdam Center for Drug Research and the algorithms group of the Leiden Institute for Advanced Computer Science, which resulted in this thesis.



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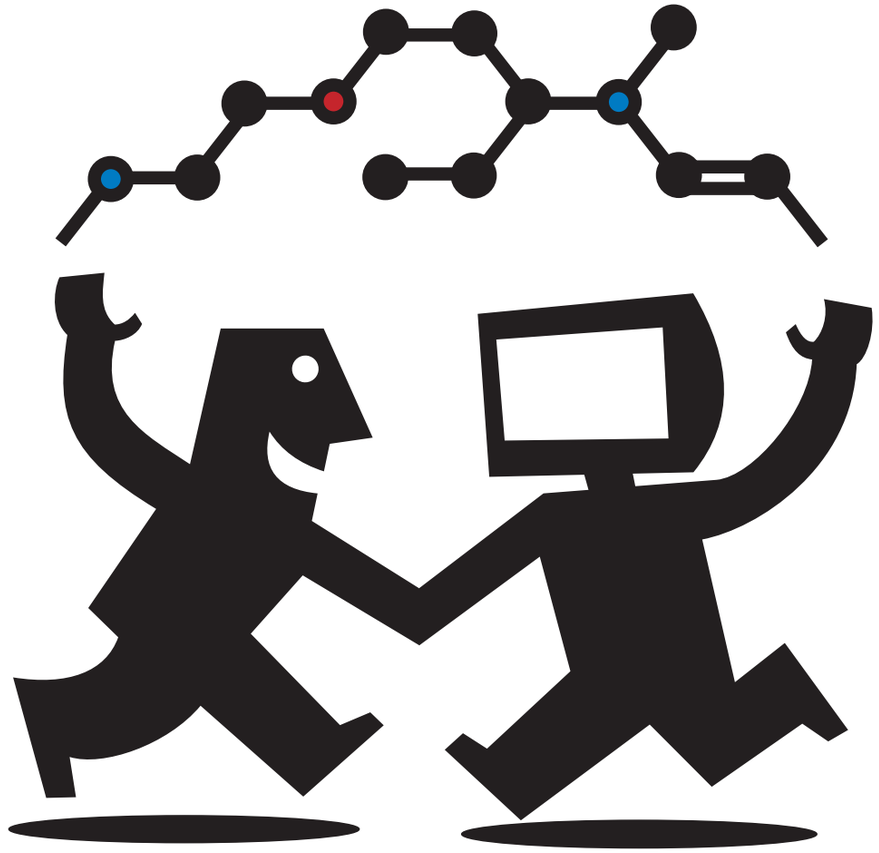

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