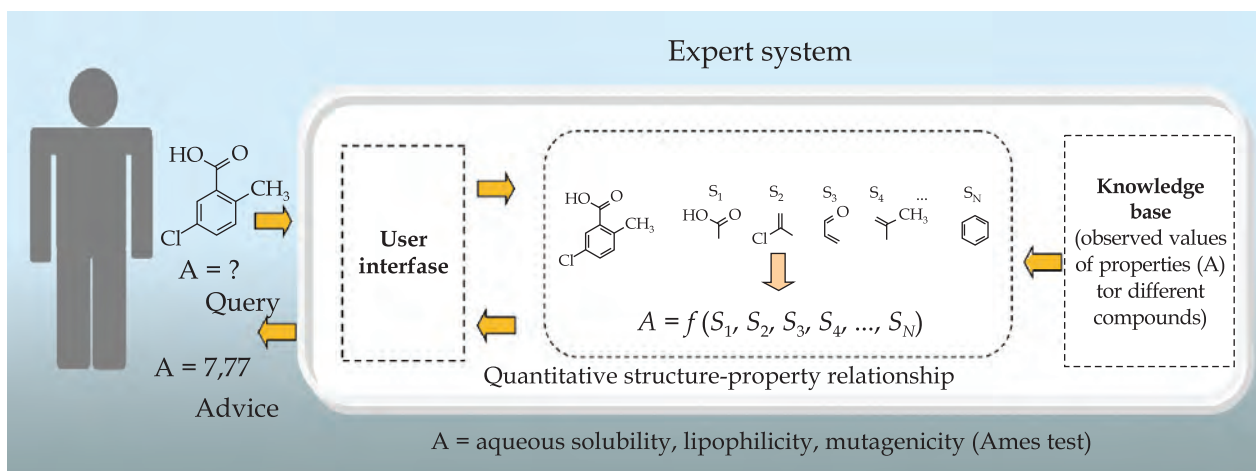


COMPUTER EXPERT SYSTEM FOR PREDICTING AQUEOUS SOLUBILITY, LIPOPHILICITY, AND MUTAGENICITY OF BIOLOGICALLY ACTIVE COMPOUNDS



Areas of Application

Based on the chemical structure of organic compounds the expert system predicts their aqueous solubility, lipophilicity, and mutagenicity (the Ames test). The predicted values of these properties can be used as filter in medicinal chemistry to create new drugs and bioactive compounds. The system enables to replace expensive screening of these properties by computer experiment

Specification

The expert system is implemented as computer program designed for using in the operating system Windows XP / Vista / 7/8/10. Recommended configuration: Pentium III or higher, 1 Gb RAM, 250 Mb hard disk space. Input information: file with the chemical structure of organic compound. Output information: predicted values of properties

Advantages

The expert system has no analogs in Ukraine and meets international standards predicting aqueous solubility, lipophilicity, and mutagenicity of biologically active compounds

Stage of Development. Suggestions for Commercialization

IRL8, TRL5
Installation of program and staff training, upon request

IPR Protection

IPR2

Contact Information

Tetiana V. Mikhaylova, A.V. Bogatsky Physico-Chemical Institute of the NAS of Ukraine;
+38 067 706 10 94, e-mail: office.physchem@nas.gov.ua