CHEMOPROP – CHEMICAL PROPERTIES ESTIMATION SOFTWARE SYSTEM

CHEMOPROP OVERVIEW

- QSARs for physical chemistry, environmental fate and ecological and human toxicology
- Quantitative and categorical models, decision trees, automated read-across
- Structure import, editing, export

OSIRIS Webtool (http://osiris.simpple.com/OSIRIS-ITS/welcome.do)
- Support for automated model selection
- Quantitative and categorical models, decision trees, automated read-across

DATABASE MODULE

- Structure import, editing, export
- Database search (structures, data)
- Link to external databases (ODBC, SQL)
- Structure module
- Structure-related information
- Structure retrieval from database
- Structure code
- Compound list either with or without links to external informatics
- Tools for visualization
- Generation of Terminal (topological, valence, A, B, C) and molecular structures (chemists, biologists)
- Search or substructures
- Structure search in WWW

FURTHER INFORMATION

- Windows XP SP3 or Vista or 7
- .NET Framework 2 or higher
- Web Resources:
- Alternatively, from www.ufz.de select Divisions, Ecological Chemistry, Methods, click on the ChemProp link

RECENT DEVELOPMENTS

- USZ Models and Models with USZ Participation
  - New and improved USZ models for air/blood, air/blood, air/fat, and fat/blood partitioning
  - New read-across model for BCF
  - Automated searching scheme for BCF

- Literature Models
  - Blood/blood partition coefficient
  - Structural alerts for narcosis
  - Other improvements
  - Rule example for structural alerts

ACKNOWLEDGMENT

The ChemProp development has been supported significantly by the EU integrated project OSPER (Optimized Strategies for Risk Assessment of Industrial Chemicals Through Integration of Non-Test and Test Information, GOCE-CT-2007-017177, 2007-2011) (www.ospere-project.org). Additional financial support is gratefully acknowledged from the former EU Projects 2.0-km (Full-data and Uncertainty Approaches for Assessing Health Risks in Future Environmental Scenarios) contract No. 507957, and CAESAR (Computer Assisted Evaluation of Industrial Chemical Substances) according to Regulation (EEC) No. 1272/2001, the German Federal Environmental Agency (UBA), Electricité de France (EDF), and the Water Resource Commission of South Africa, Environmental Risk Assessment and Management (GOREW), Brussels, and the Long Range Research Institute (LRTI) of the European Chemical Industry Council (CEFIC), Brussels. Currently further developments are supported by the IGF project (EMRNL.SA.01.17.BG.01) of the UFA Düsseldorf through the AIF within the framework of the BGF.