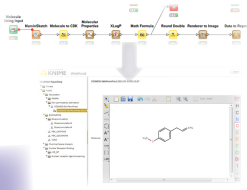
COSMOS KNIME Workflows: *In Silico* Models for Toxicity

COSMOS KNIME WebPortal

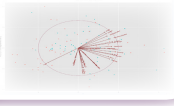
- KNIME workflows integrate access to chemical databases, data processing and analysis, modelling approaches, profiling of structures and calculation of properties in a flexible way.
  Workflows are adaptable in the desktop version.
- The WebPortal version allows for a **wizard-like execution** in a web browser without software installation.



First COSMOS Models Publicly Available in WebPortal!

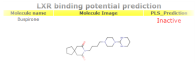
Chemical Space Analysis

- Upcoming – a preliminary step before modelling to find analogues:
  includes multivariate analysis of descriptors and properties, as well as important functional groups



Receptor Binding and Structural Alerts

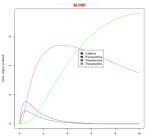
- Prediction of potential binding to nuclear receptors related to steatosis



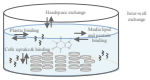
- Upcoming: screening using structural alerts for protein/DNA binding and hepatotoxicity

Biokinetics

- **Physiologically-Based Kinetic (PBK)** models to simulate concentration-time profiles and internal dose metrics for dermal or oral scenarios



- Extrapolation of *in vitro* intracellular concentrations with the **Virtual Cell Based Assay**

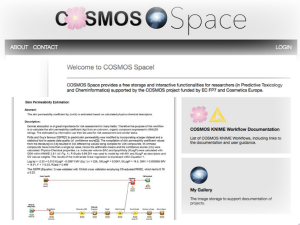


- Human bioaccumulation factor (hBCF)
- Gastrointestinal absorption
- Skin permeability

Updates on releases and upcoming web tutorials: www.cosmostox.eu

Documentation of Models in COSMOS Space

- **COSMOS Space** facilitates sharing of predictive toxicology resources (models, data, workflows, documentation), links to the COSMOS Database and COSMOS KNIME workflows.
- **Description and user guidance** are available in COSMOS Space for all KNIME WebPortal workflows.



Free access at
http://knimewebportal.cosmostox.eu
Registration via http://cosmosspace.cosmostox.eu