cheminformatics data management system

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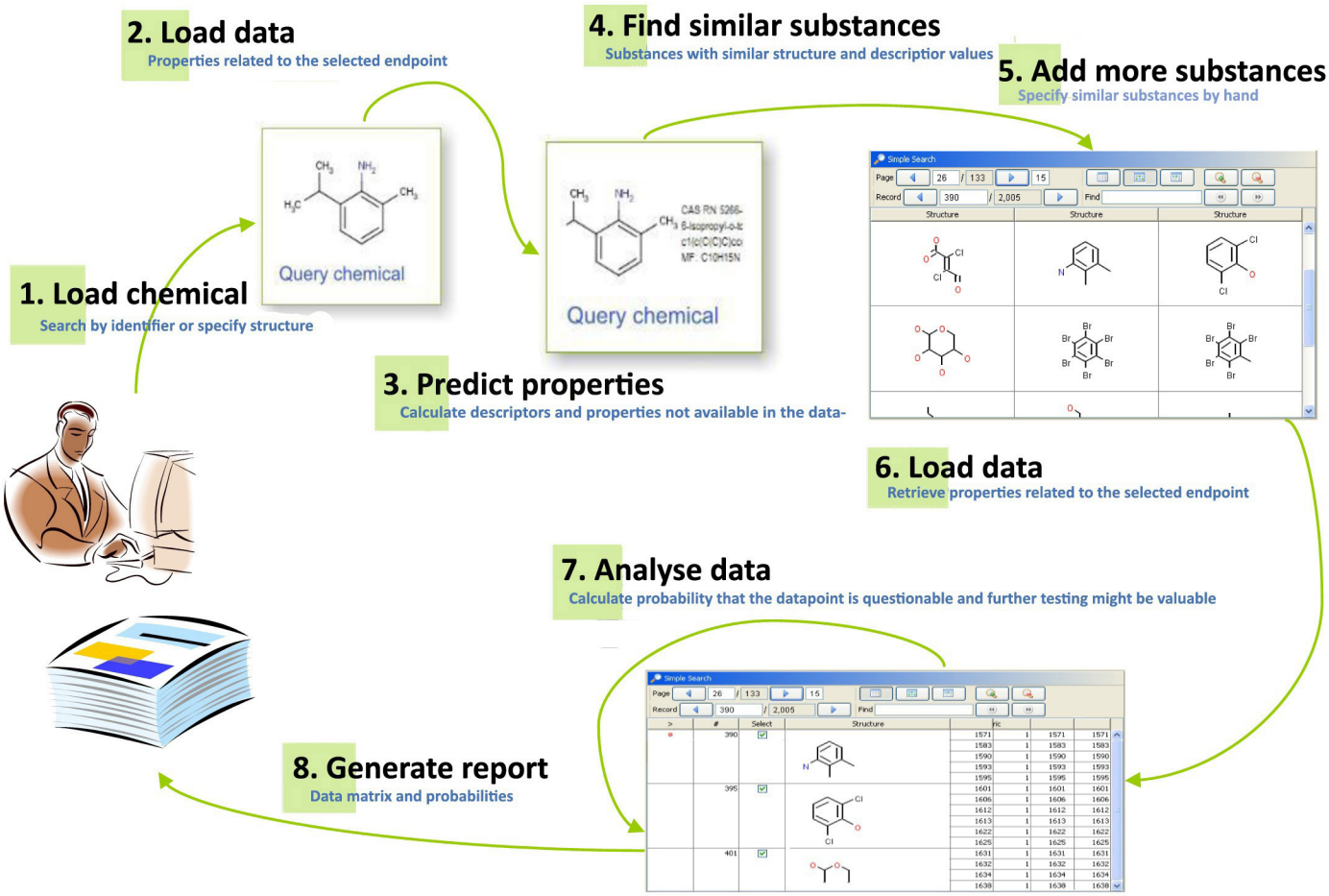
OVERVIEW

- AMBIT software is a set of libraries and tools
- various chemoinformatics functionalities for data management
- multiple Quality Assured datasets for REACH-relevant toxicological endpoints
- variety of flexible searches and mining of the data stored in the database

Unique features of AMBIT:

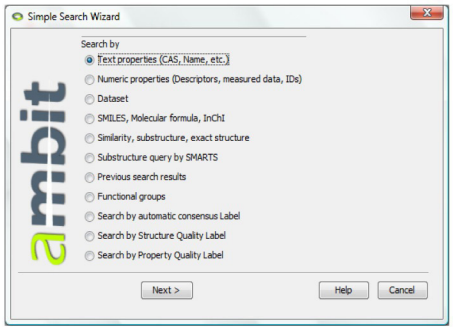
- ability to store and query multifaceted information about chemicals (structure, data, text)
- workflow engine to facilitating often repeated user's actions (e.g Analogue identification, PBT assessment are completed and can be applied in REACH).
- internal pKa calculation

Datapoint evaluation workflow



Querying capabilities

The above queries can be combined by OR and AND operators to form a more complex query.



AMBIT XT QualityAssured datasets

- **EINECS list**
- **ECETOC Aquatic Toxicity (EAT) Database**
- Supplement to ECETOC. 2003. Aquatic Hazard Assessment II. Technical Report No.91. European Centre for Ecotoxicology and Toxicology of Chemicals, Brussels, Belgium.
- **Bioconcentration factor (BCF) Gold Standard Database**
- Compilation of historical local lymph node assay data for the evaluation of skin sensitization alternatives.
- Gerberick GF, Ryan CA, Kern PS, Schlatter H, Dearman RJ, Kimber I, Patlewicz G, Basketter DA (2005). Dermatitis 16(4): 157-202.
- **Skin irritation and corrosion reference chemicals database (1995)**
- ECETOC Technical Report No.66

Acknowledgments

http://ambit.sourceforge.net