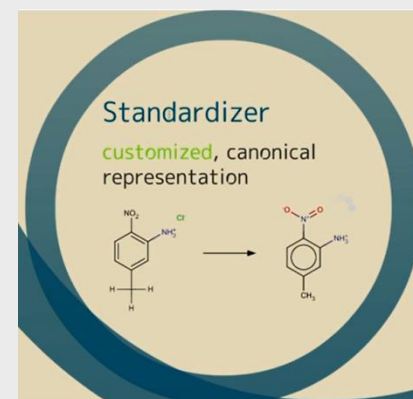


Standardizer and Structure Checker at Boehringer Ingelheim

UGM 2014 ChemAxon / Edith Richter

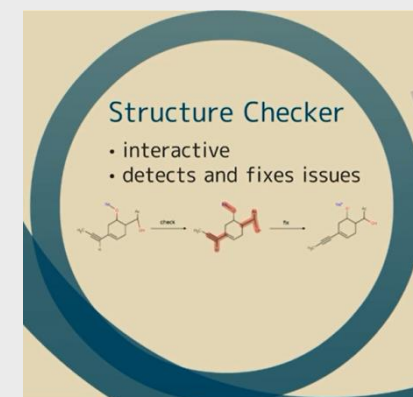
Standardizing is equivalent to

„Translation“



Structure Checking is equivalent to

„Spell Checking“



Structure Checking with Fixing is equivalent to

„Autocorrection“



Review and Discuss Existing Rules



Decide about Standardizing and Structure Checking

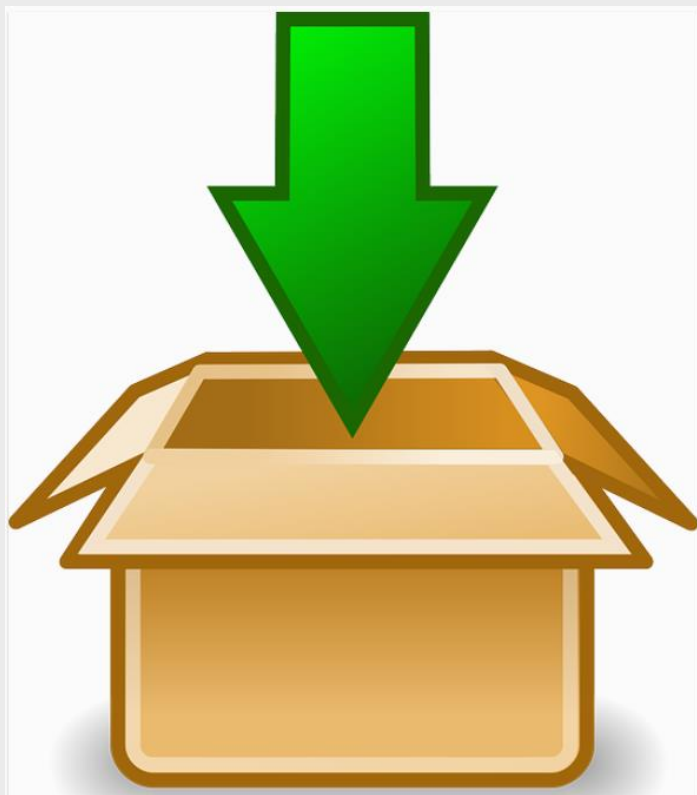


Implement Customized Checkers with ChemAxon



Provide Templates

Templates for Database Cartridge



and Marvin Tools



- enable identical structure checker across different tools
- enable to be compliant with internal guidelines

Packages

- Provides functions for single- and multistep checks and fixings
- Provides functions for automated checks

Database Tables

- Store the default checker and standardizing configuration
- Store customized results messages for checks
- Store dedicated structures for tests

Basic Checkers

- As Abbreviated Group / Pseudo Atom etc.

Substructure Checkers

- Working with SMARTS defined substructures
- Can be set individually
- Very flexible approach

Customized Checkers

- Provided as consultancy projects
- Good experiences by now
- Easy to implement both for DB Cartridge and for Marvin Tools