

ChemicalToolBoX

Cheminformatics inside the Galaxy

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"Cheminformatics is the use of computer and informational techniques, applied to a range of problems in the field of **chemistry**. These **in silico** techniques are used in **pharmaceutical companies** in the process of **drug discovery**."

Aim:

Starting a Cheminformatic Galaxy Community

- Data Source
 - paint your structure
 - download the NCBI PubChem
 - enhanced upload tool
- molecule datatypes as first class citizen
 - 30 different converters
 - Built-in parallelism

- orphan tool dependencies
 - Open Babel
 - RDKit
 - Chemfp
 - matplotlib
 - numpy
 - scipy

- Tools (>30)
 - Filtering
 - Descriptor Calculation
 - Drug/Natural Product likeness prediction
 - Similarity Search
 - Substructure Search
 - Chemical clustering
 - Conformer Generation
 - Image to Structure
 - ...

dark script matter?



github:

<http://bit.ly/chemicaltoolbox>

Tool Shed:

<http://testtoolshed.g2.bx.psu.edu/view/bgruening/chemicaltoolbox>

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