

# Enhancing the Galaxy Tool Shed

<http://usegalaxy.org/toolshed>

<http://wiki.galaxyproject.org/Tool%20Shed>

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The Galaxy Team

# The Galaxy Tool Shed is an App Store

- The Tool Shed is a fully functioning, online App Store when used in conjunction with the enhanced Galaxy features that complement it
- The Tool Shed enables installation of Galaxy utilities into any web accessible Galaxy environment
- The Tool Shed uses mercurial repositories to contain Galaxy utilities
- The Tool Shed enables acquisition of updates for Galaxy utilities installed into a Galaxy environment

# What are Galaxy Utilities?

- **Tools** for data analyses
- **Data** (acquired using specialized Data Manager tools)
- **Custom Datatypes**
- **Tool Dependency** definitions
- **Repository Dependency** definitions
- Exported **Galaxy Workflows**

Additional utilities will be supported in the future

# Tool Dependency Definitions

- A tool dependency definition is an XML file included in a Tool Shed repository named `tool_dependencies.xml`
- The file includes the recipe for installing and compiling all required tool dependencies into the Galaxy environment
- The dependencies framework supports defining dependencies that require other dependencies
- A specific dependency version will be installed only once, with any number of Galaxy utilities able to use it

# Repository Dependency Definitions

- A repository dependency definition is an XML file included in a Tool Shed repository named **repository\_dependencies.xml**
- The file defines relationships to any number of repositories
- Relationships at the repository level are defined as “simple”
- Relationships at the repository contents level (Galaxy utilities) are defined as “complex”

# Order matters!

- Some tool dependencies may require other tool dependencies to be installed first
- Repository dependency definitions provide support for ordering the installation of the dependency hierarchy

# Time matters too!

- Tool dependency definitions support relationships created for dependency compile time and for tool execution time

# Options for installation

- Galaxy utilities can be installed using either a browser or the Galaxy API for the Tool Shed



# An example

- Björn Grüning's chemicaltoolbox  
<http://testtoolshed.g2.bx.psu.edu/view/bgruening/chemicaltoolbox> incorporates all of these features

## Dependencies of this repository

▼ [Repository dependencies](#) – This is a metapackage, that will install several other tools.

- ▼ [Repository chemical\\_data\\_sources](#) revision 955783ed181f owned by [bgruening](#)
  - Repository molecule\_datatypes revision a1474892287e owned by [bgruening](#)
- ▼ [Repository package\\_numpy\\_1\\_7](#) revision ad6ebe2c75ef owned by [bgruening](#) (prior install required)
  - Repository package\_lapack\_3\_4 revision a6b8f46acca7 owned by [bgruening](#) (prior install required)
  - Repository package\_atlas\_3\_10 revision 25dc49b0d6d5 owned by [bgruening](#) (prior install required)
- ▼ [Repository package\\_openbabel\\_2\\_3](#) revision 3a993ff17df5 owned by [bgruening](#) (prior install required)
  - Repository package\_eigen\_3\_1 revision b72b882b30b4 owned by [bgruening](#) (prior install required)
- ▼ [Repository package\\_sclpy\\_0\\_12](#) revision e4f395310680 owned by [bgruening](#) (prior install required)
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- ▼ [Repository opsin](#) revision 12640f433fd7 owned by [bgruening](#)
  - Repository molecule\_datatypes revision a1474892287e owned by [bgruening](#)
- ▼ [Repository rdkit](#) revision 0ab075fb42f9 owned by [bgruening](#)
  - Repository molecule\_datatypes revision a1474892287e owned by [bgruening](#)
  - Repository package\_rdkit\_2012\_12 revision 5b30ea84ba25 owned by [bgruening](#) (prior install required)
- ▼ [Repository confab](#) revision 6eb2a0358b9c owned by [bgruening](#)
  - Repository molecule\_datatypes revision a1474892287e owned by [bgruening](#)
  - Repository package\_eigen\_2\_0 revision 7293f118efef owned by [bgruening](#) (prior install required)
- ▼ [Repository natural\\_product\\_likeness](#) revision 5796e03c3cf9 owned by [bgruening](#)
  - Repository molecule\_datatypes revision a1474892287e owned by [bgruening](#)
- ▼ [Repository osra](#) revision d97d51e9bb95 owned by [bgruening](#)
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  - Repository package\_graphicsmagick\_1\_3 revision 34f511310435 owned by [bgruening](#) (prior install required)
- ▼ [Repository simsearch](#) revision 47d2bf691908 owned by [bgruening](#)
  - Repository package\_openbabel\_2\_3 revision 3a993ff17df5 owned by [bgruening](#)
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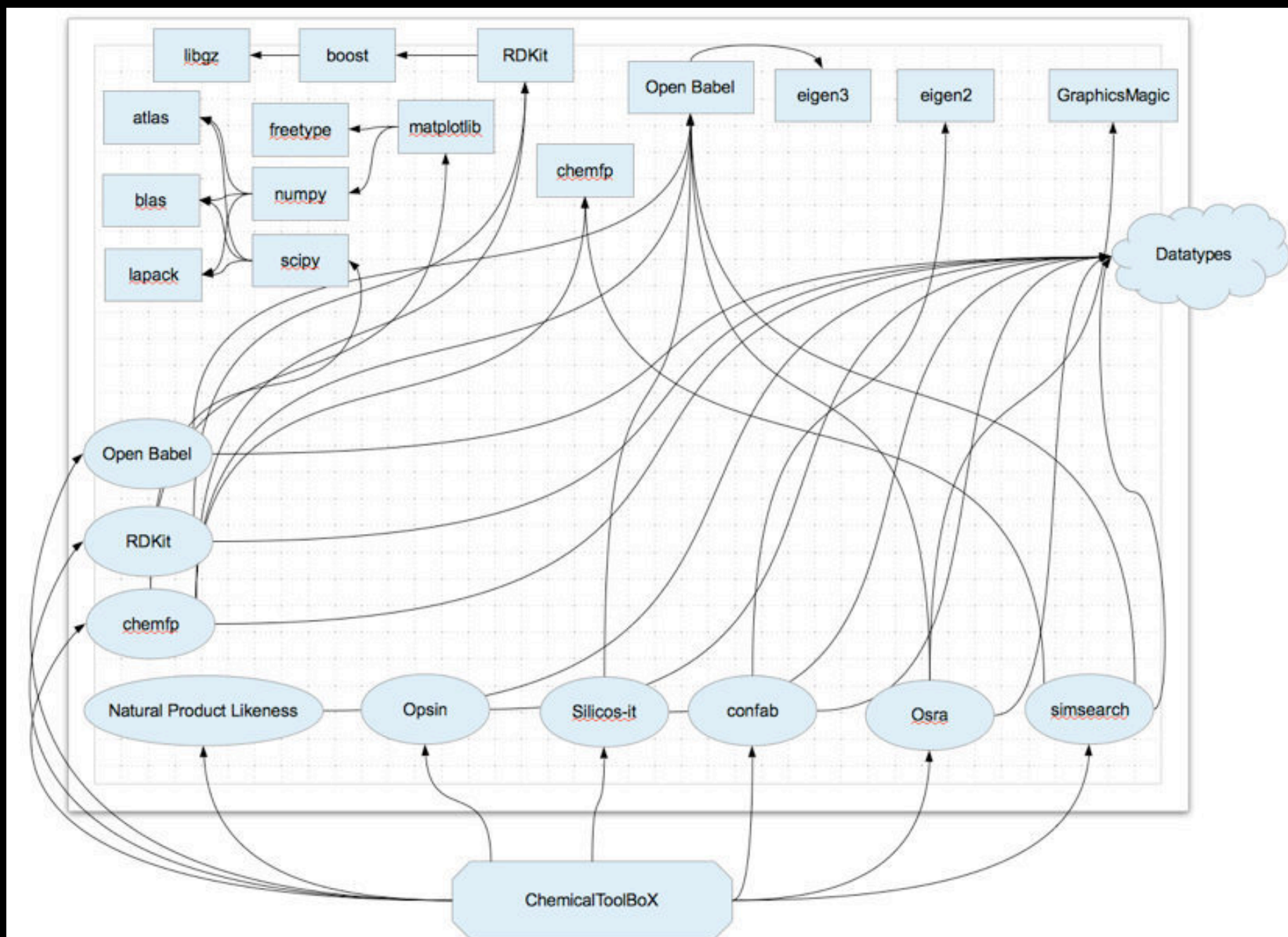
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# ChemicalToolBox Dependency Graph



# A demonstration using the Galaxy API

```
install_tool_shed_repositories.py
  --api 22be3b2e392a64
  -l http://localhost:8763
  --url http://localhost:9009/
  --name chemicaltoolbox
      -o bgruning
      -r 1018e3cee313
      --tool-deps
      --repository-deps
  --panel-section-name 'Chemical Tool BoX'
```

# Acknowledgments

Special thanks to:

- Björn Grüning, author of the chemicaltoolbox repository – <http://testtoolshed.g2.bx.psu.edu/view/bgruening/chemicaltoolbox>
- Dave Bouvier





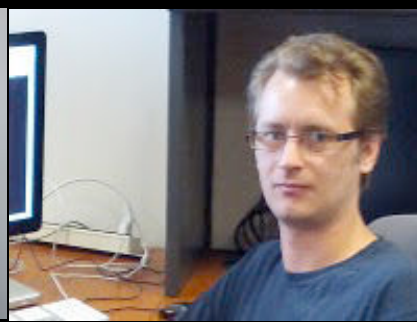
Enis Afgan



Dannon Baker



Dan Blankenberg



Dave Bouvier



Dave Clements



Nate Coraor



Carl Eberhard



Dorine  
Francheteau



Jeremy Goecks



Sam Guerler



Jen Jackson



Greg von Kuster



Ross Lazarus



Anton Nekrutenko



James Taylor

# The Galaxy Team

<http://wiki.galaxyproject.org/GalaxyTeam>

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