Siphonify—Managing Chemical Structures with Style

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Features Available

- An easy-to-use tool to manage chemical structures similar to how music files and documents are managed
- Provide a convenient repository for searching and browsing of "registered" chemical structures
- Support for basic form of chemical registration (insofar as to recognize when two structures are the "same")
- Built-in support for structure standardization and normalization
- Batch and interactive compound registration
- Various search forms; e.g., keyword, substructure, similarity, exact, etc.
- Support for "smart" collections and filters
- Advanced set operations on collections and filters

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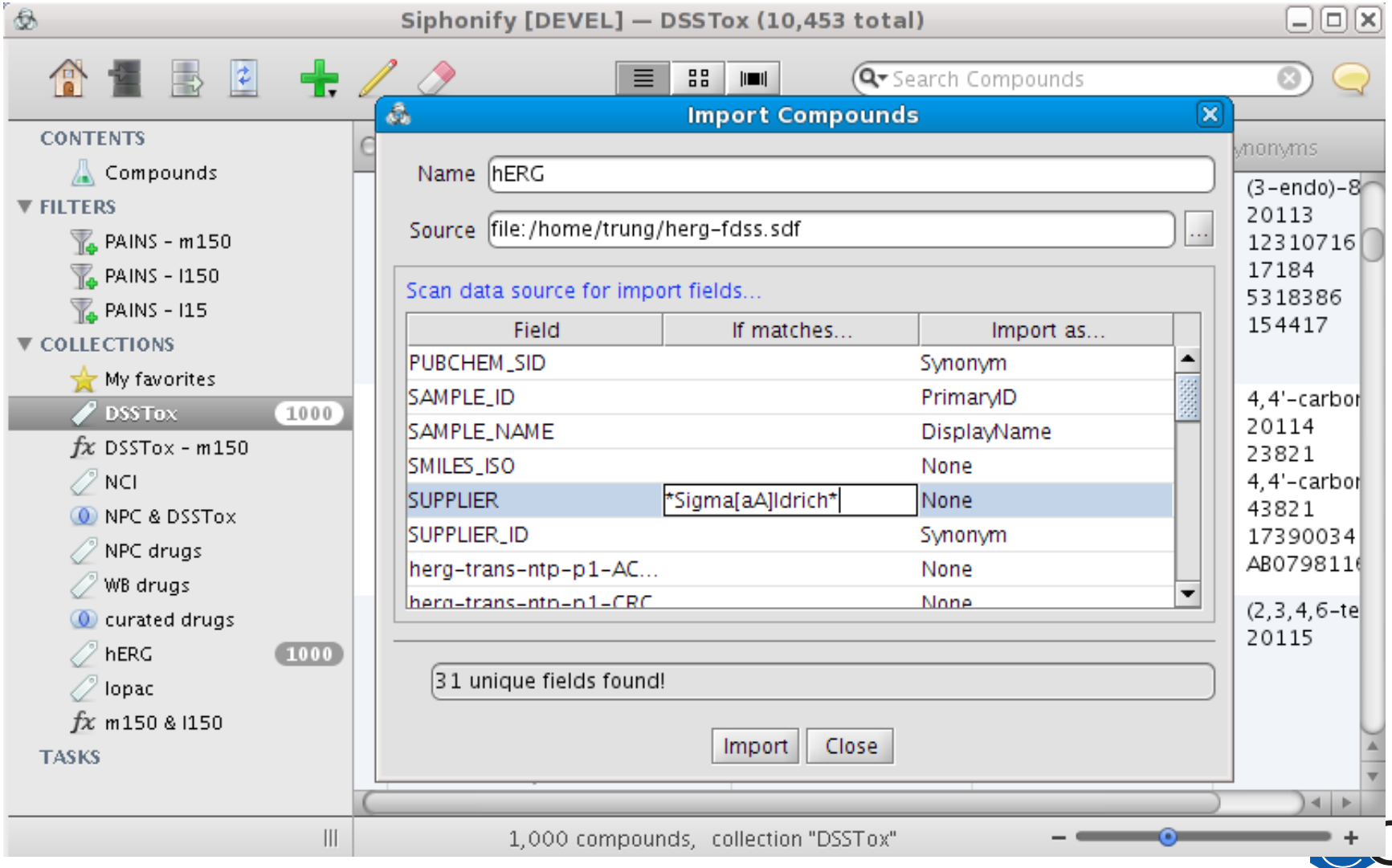
Features in the Work

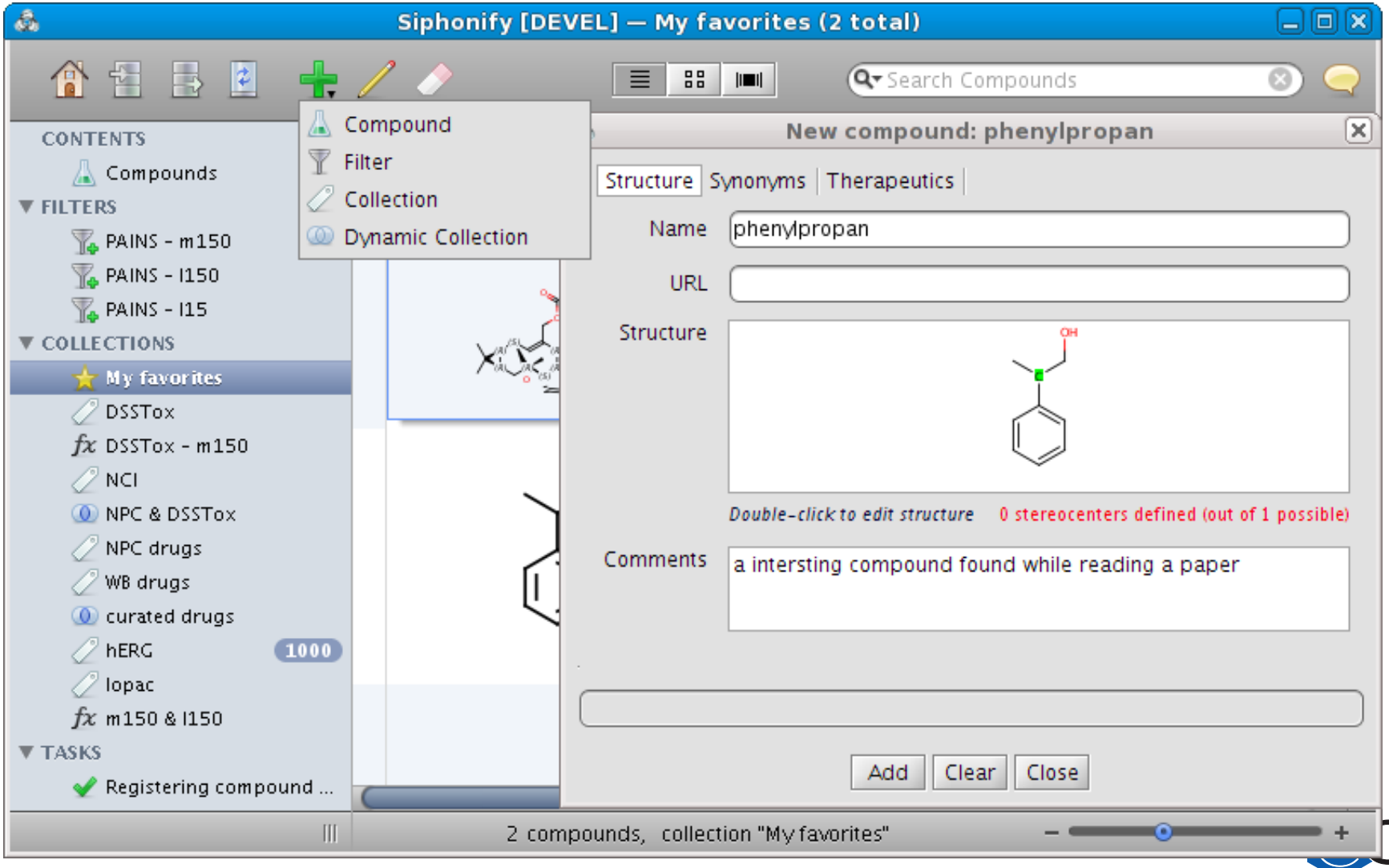
- Importing and searching of well-known public data sources (e.g., ChEMBL, PubChem, etc.)
- Integrate other tools available on `http://tripod.nih.gov`
  - Automated R-group analysis
  - Scaffold-based analyses and visualizations
- Automatic deployment of validated filters and well-known collections (e.g., curated drugs)
- Sharing of filters and collections
- Deployment of QSAR/QSPR models
- Improve on performance

Support for regular expression of individual import fields



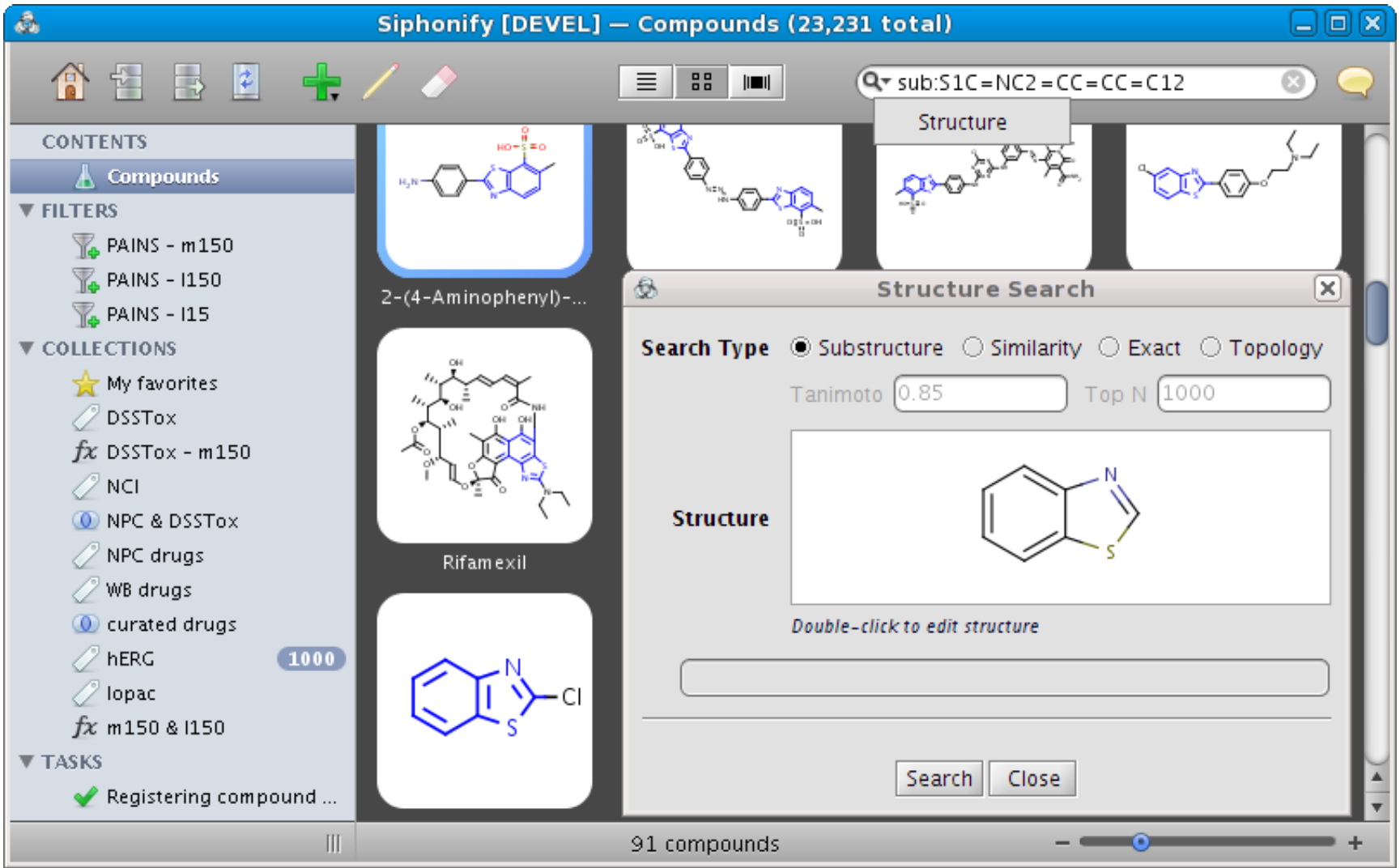
Basic Usage
Interactive import

Add a new compound to the "`My favorites`" collection



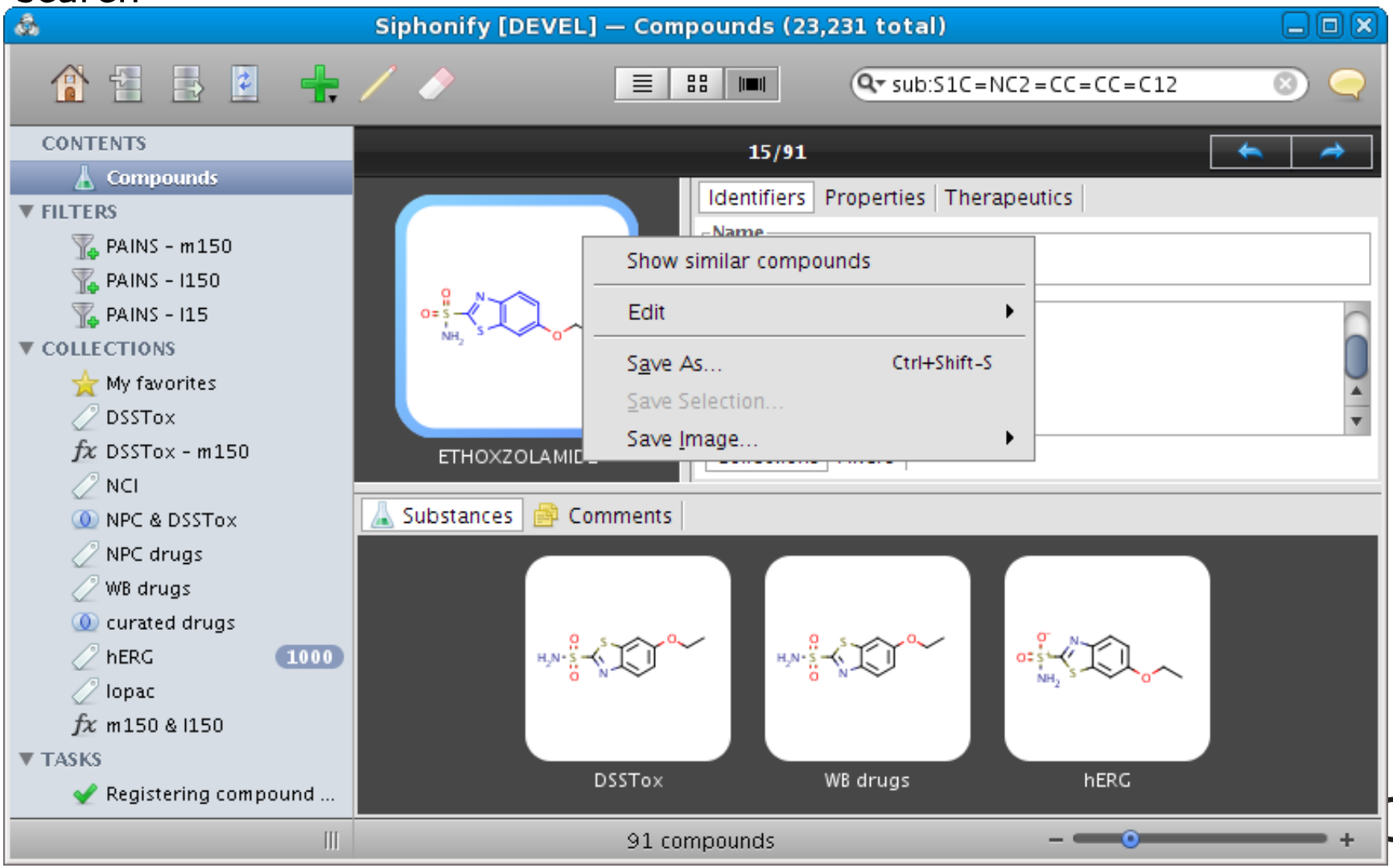
Basic Usage

Initiating (sub-) structure search



Basic Usage
Implicit neighbor search

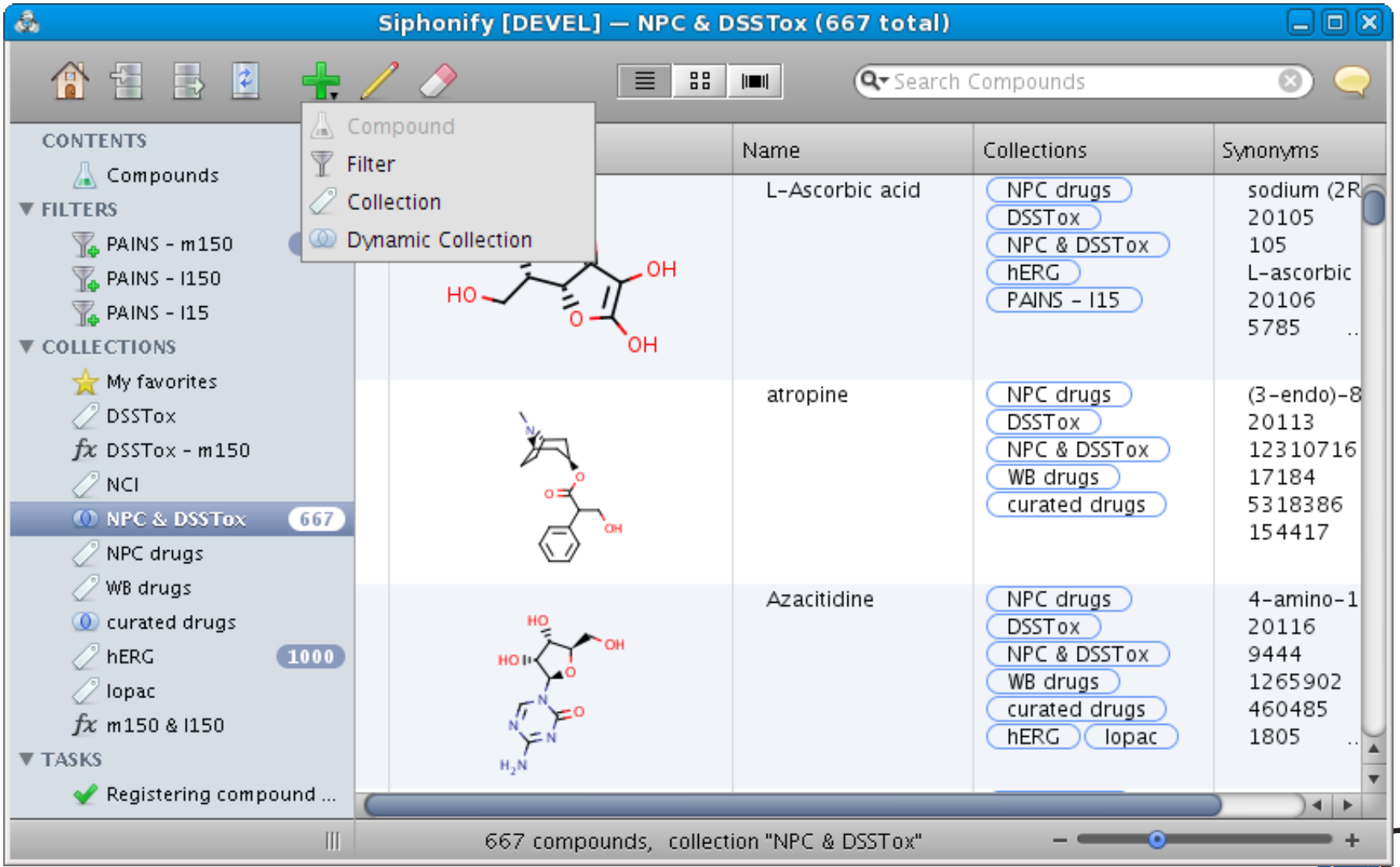
Right-click on any structure to perform implicit neighbor/similarity search



Collections and Filters

Creating collections

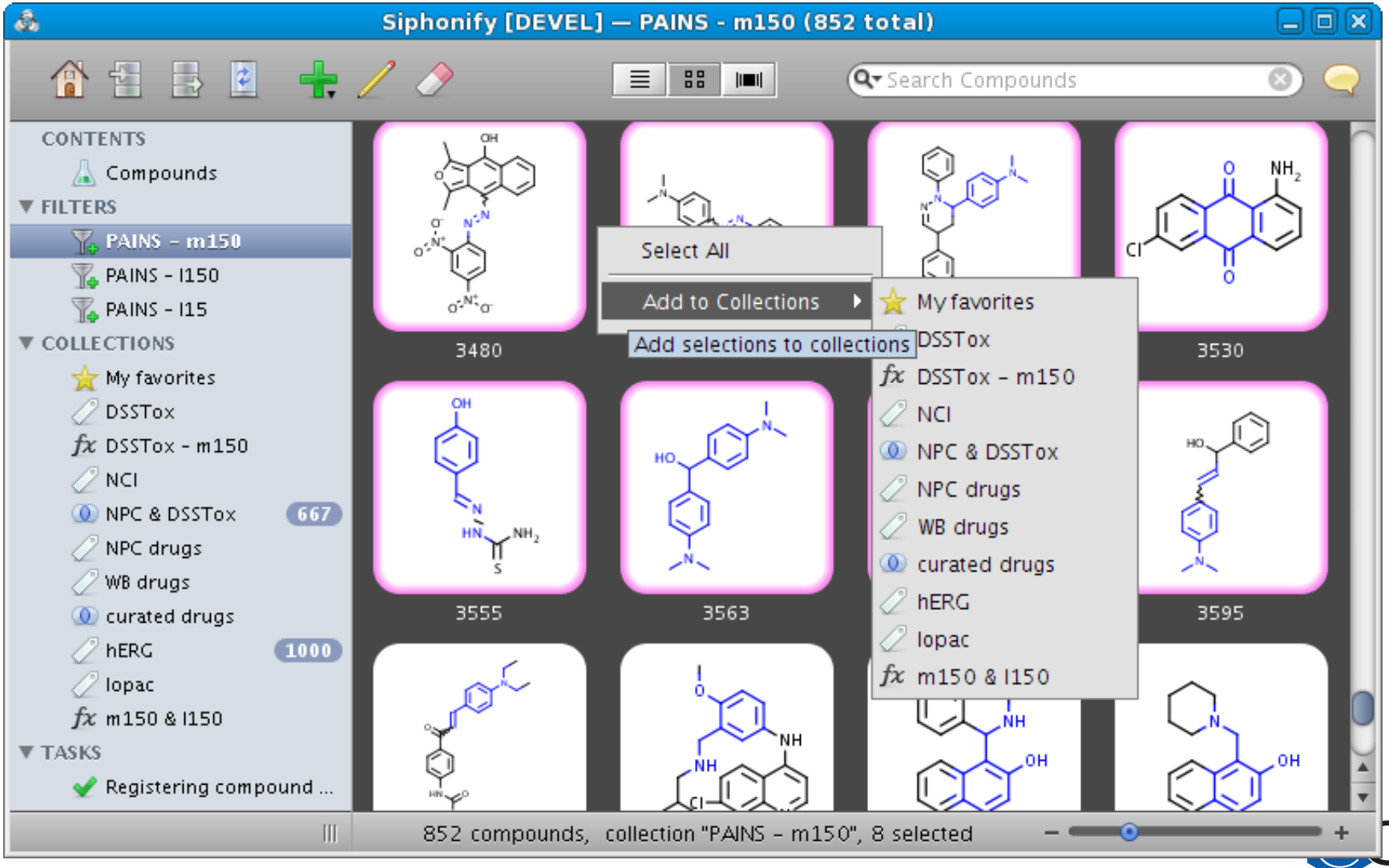
Collections and filters are “tags” on chemical structures



Collections and Filters

Editing collections

Right-click on a selected set of structures to add to a collection

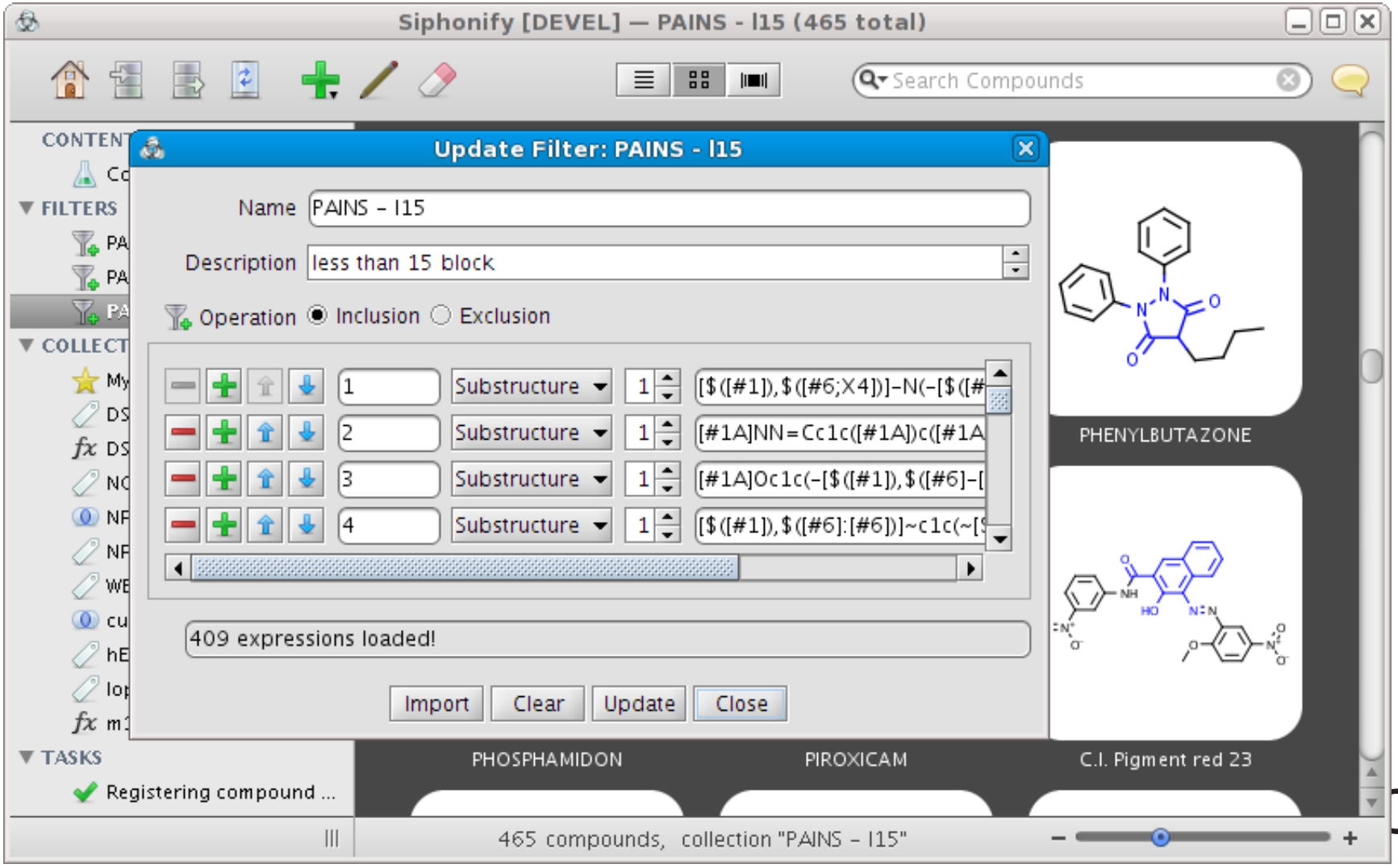


Collections and Filters

Creating filters

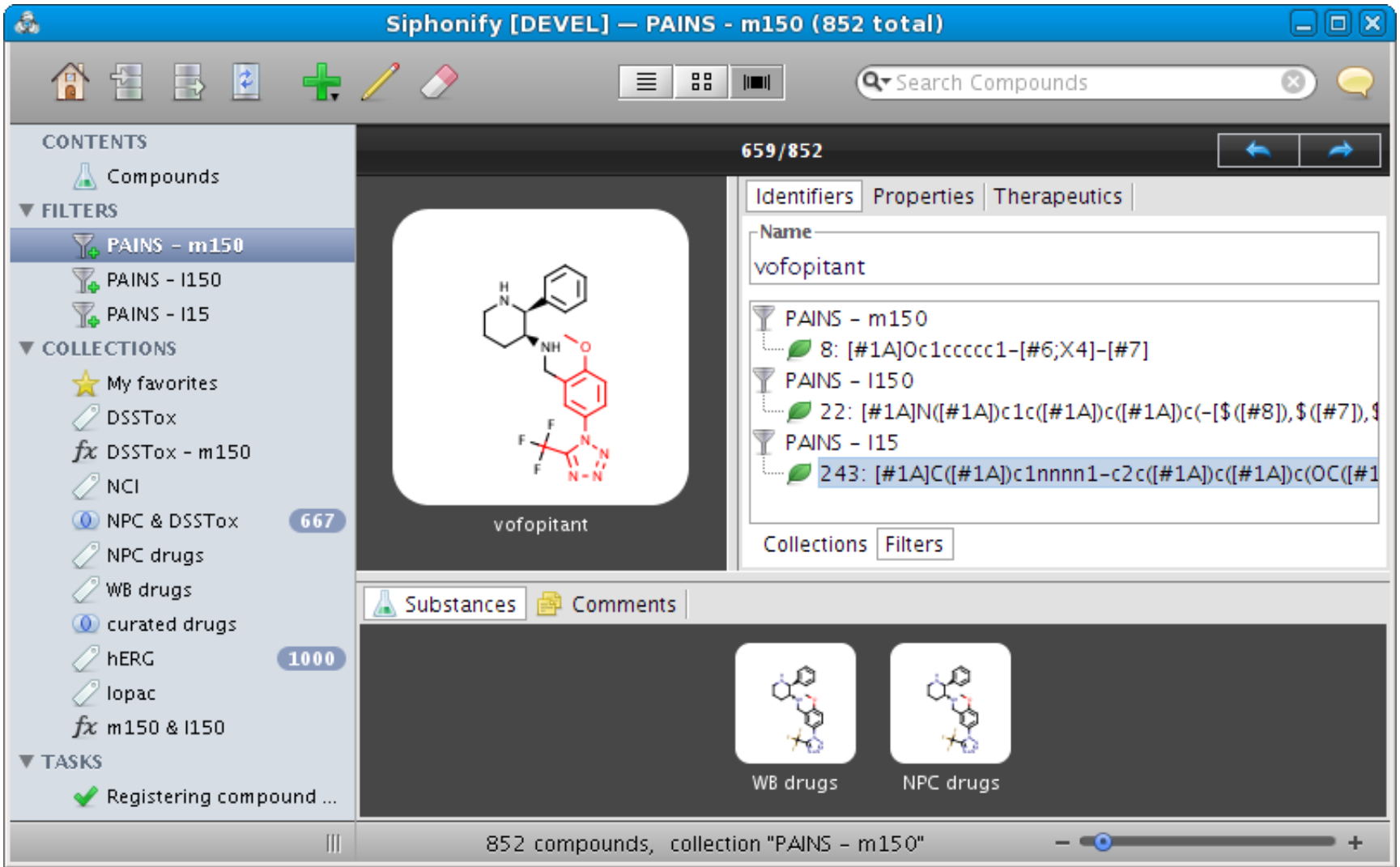
Below are the PAINS filters available at

`http://blog.rguha.net/?p=850`



Collections and Filters

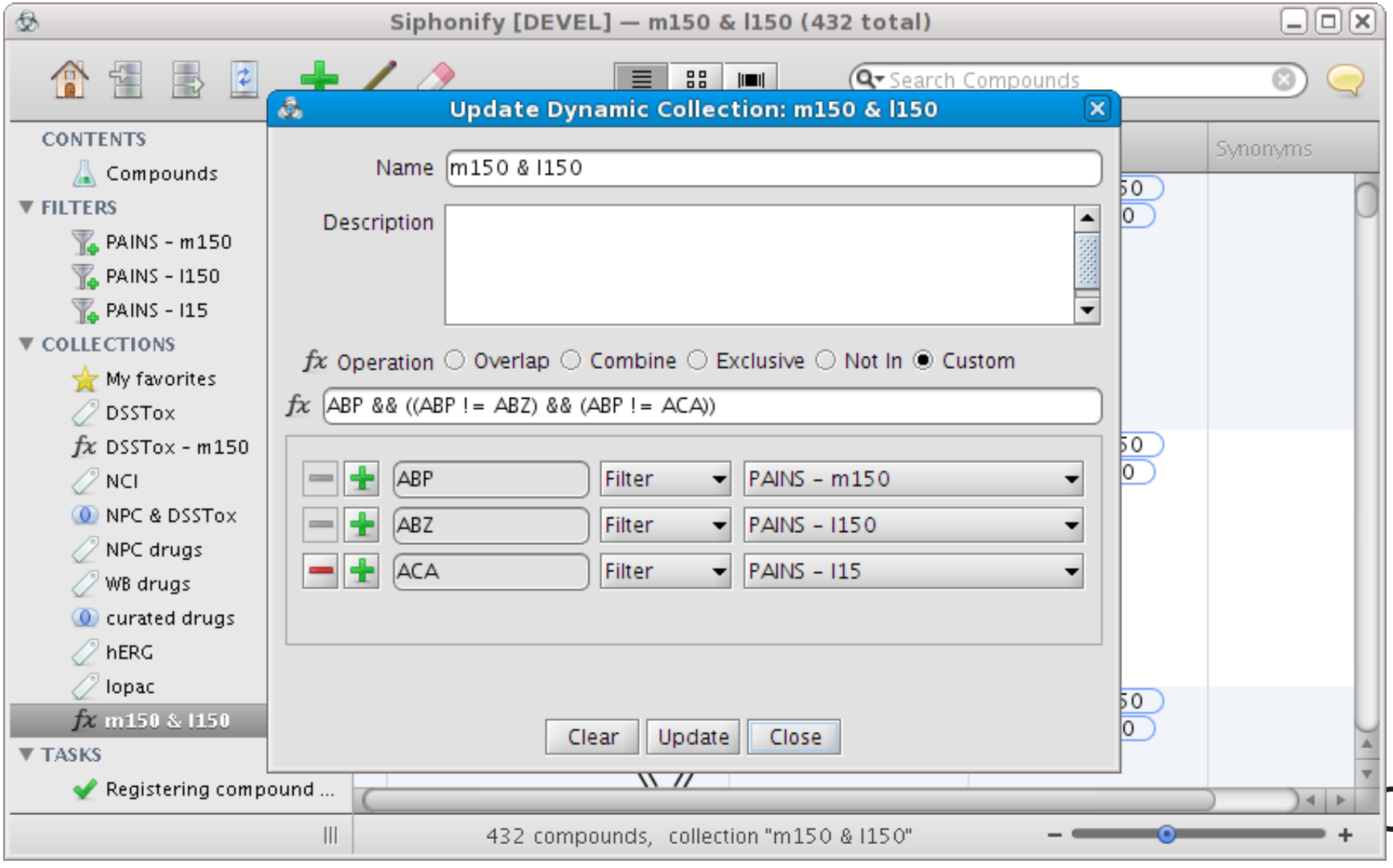
Examining individual filter rules



Collections and Filters

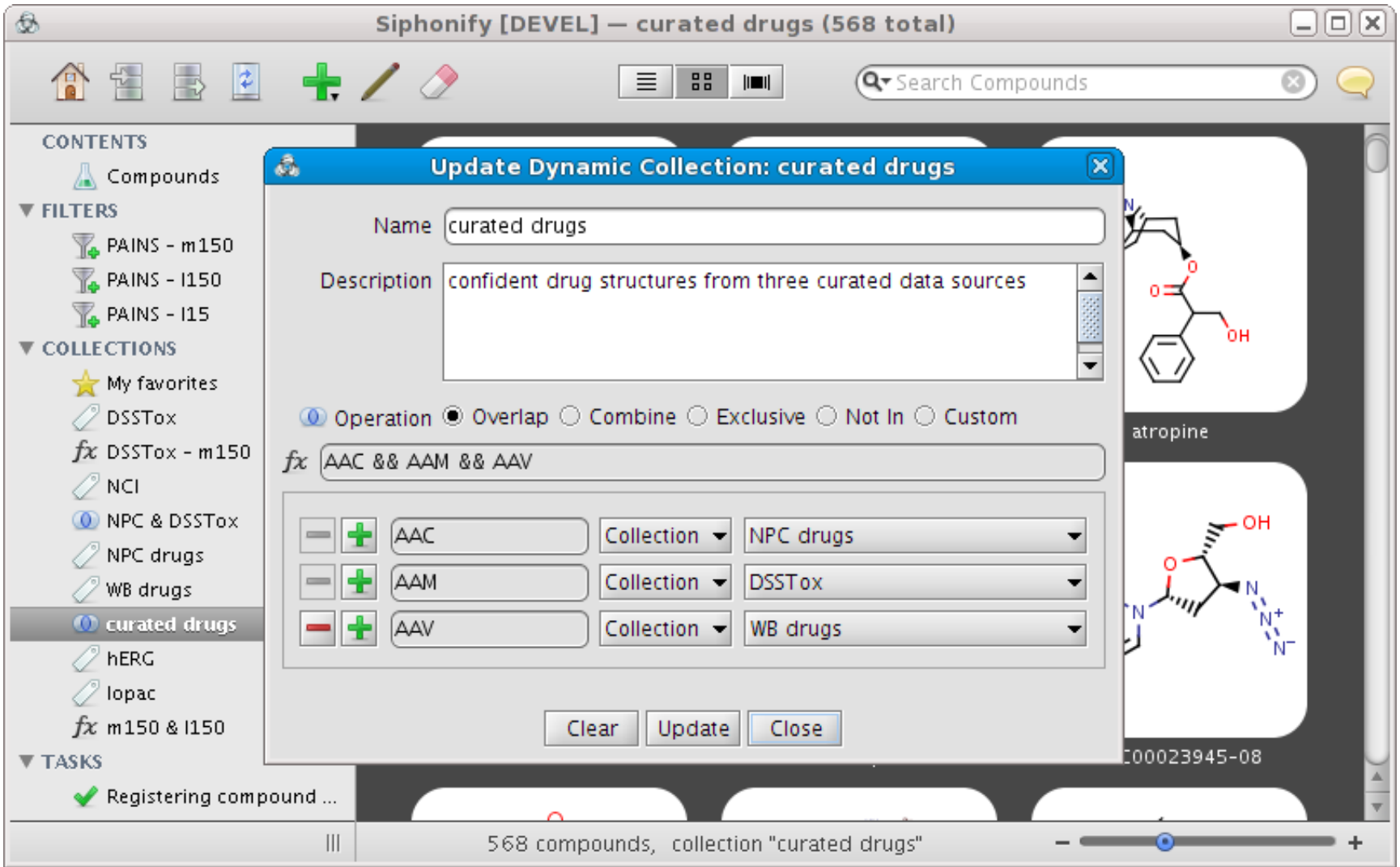
Operations on collections and filters

Basic set operations (e.g., AND, OR, XOR) are supported as well as advanced logic expressions



Collections and Filters

More operations on collections and filters



Availability

- Siphonify is available for download from here
  `http://tripod.nih.gov/siphonify`
- Please give us feedback either via email or the feedback button within the software 

Acknowledgements

Our informatics colleagues have been instrumental in the development of Siphonify:

- Rajarshi Guha's web-based filter tool—*siphon*—provides the initial inspiration.
- Noel Southall's original work on the `CanonicalForm` code serves as guidance for the structure standardization code within Siphonify. Any shortcomings are certainly our fault.