dotmatics
knowledge solutions

Datasheet

REACTION WORKFLOWS

Reaction Workflows is a graphical environment that lets scientists build and execute data processing workflows to perform common cheminformatics tasks, such as library enumeration, structure normalization and compound profiling.

DEFINING A WORKFLOW

Users build workflows in a drag-and-drop environment by selecting and connecting nodes that provide inputs and outputs or perform actions. Nodes are configured with data and then the workflow is run to generate results. Figure 1 shows a simple example with two sets of input reagents (blue), a generic reaction (yellow), and the resulting library structures

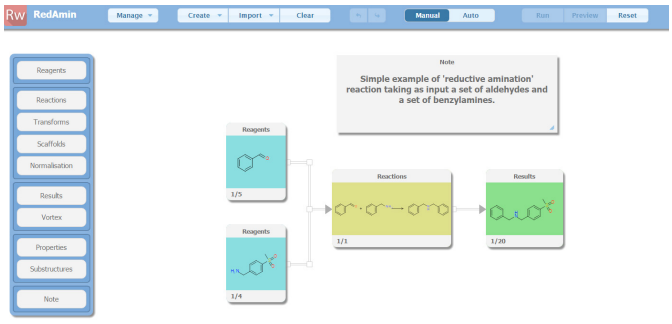

Figure 1 : Simple Enumeration Workflow

Nodes are prepopulated with sets of data such as commercial reagents or literature reactions, and the users can expand these collections themselves. Once results are generated they can be viewed as shown in Figure 2, sent to additional processing nodes or exported

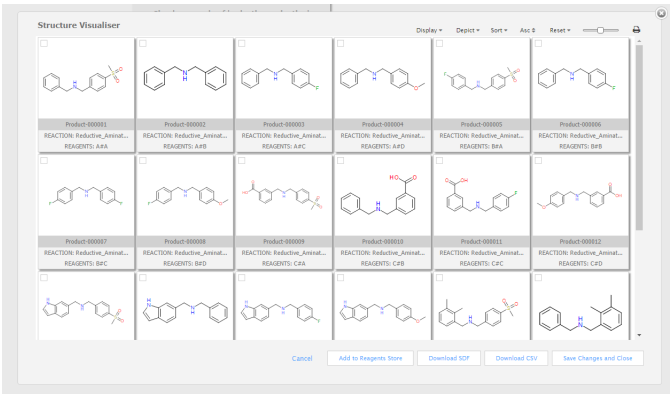

Figure 2: An enumerated library viewed from the results node

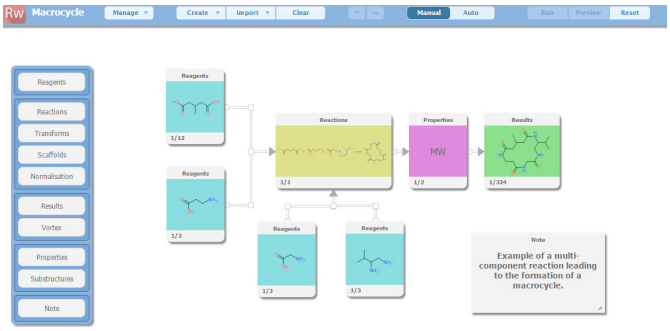

Figure 3: Reaction based enumeration

NODES AND STORES

A rich set of data processing nodes are available to build workflows

- Cheminformatics action nodes – reaction-based enumeration (see figure 3), chemical transformation, scaffold-based enumeration (see figure 4), structure normalization
- Calculate/filter nodes – by molecular properties and substructures
- Visualization nodes – structure grid visualizer, view/select in Vortex
- Input/output – SD, smiles, CSV files or interactive molecular drawing
- Note – document the workflow for sharing

Nodes are prepopulated with extensive content (Stores) to allow users to be productive straightaway

- 50+ standard literature reactions (see Figure 5), 100+ standard transformations, more than 1500 library scaffolds and 60+ normalization rules
- Common eMolecules reagents lists from Dotmatics ChemSelector
- Common property profiles such as rule of 3/5 and substructure profiles such as PAINS filters
- Stores can be augmented with user/group/company data and collections

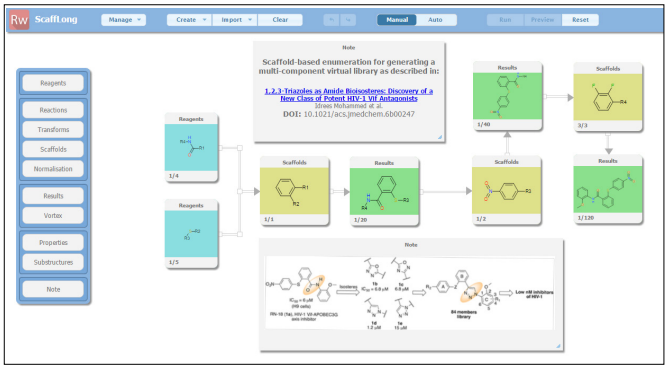

Figure 4: Scaffold based enumeration

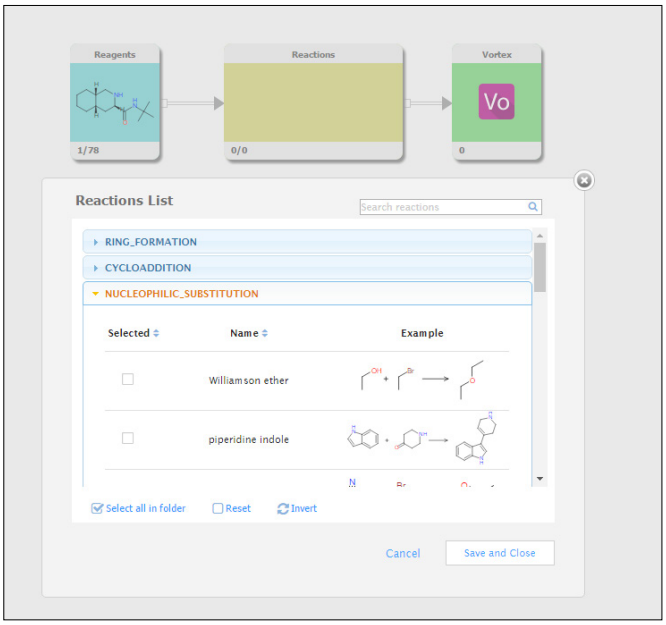

Figure 5: Browsing the reaction store to populate the reaction node

SCIENTIFIC WORKFLOWS

With a large, flexible set of available nodes, users can build workflows to solve a wide variety of cheminformatics tasks. Common use cases include

- Synthetic Library enumeration – enumerating a synthetic compound library for an ELN experiment
- Virtual Library enumeration and profiling – enumerating all possible compounds that could be made with known reactions and available reagents, which will then be filtered for those with good properties and/or predicted active with virtual screening methods, to select a subset as candidates to make and test
- Structure normalization for registration – encoding company structure standardization and normalization rules for corporate registration
- Compound idea generation – proposing new chemical series via lead hopping, or alternative molecules to avoid liabilities in existing leads
- Chemistry file clean up – cleaning up chemistry files from collaborators or the literature prior to further processing

BENEFITS

- **Efficient development** – graphical programming is faster and more efficient than scripting for cheminformaticians, and produces a self-documented result that is much better for reuse and sharing
- **Captures best practice** – the workflows allow experts to capture their best practice and then distribute to non-experts to configure with their own data and execute
- **No programming skills required** – easy to use for scientists to produce their own ad-hoc workflows without any knowledge of programming or scripting
- **Immediate productivity** – the easy to learn graphical environment combined with extensive content already built into the nodes, means that users will be up and running very quickly
- **Integrated** – seamlessly integrated into the Dotmatics suite – Browser hitlists become data sources in the reagent node, push and pull to Vortex for analysis and visual selection
- **Accessible** – the client is web-based for easy deployment, server can be hosted in the cloud or on-premise

dotmatics.com

Info: info@dotmatics.com
Sales: sales@dotmatics.com
Support: support@dotmatics.com
Careers: careers@dotmatics.com

Head Office UK

Phone: +44(0)1279 654 123
Fax: +44(0)1279 653 088
The Old Monastery
Windhill
Bishops Stortford
Herts
CM23 2ND
UK

North America West Coast

Phone: +1 855 808 8332
6050 Santo Road
Suite 270
San Diego
CA 92124
USA

North America East Coast

Phone: +1 855 808 8332
800 West Cummings Park
Suite 2950
Woburn
MA 01801
USA

Japan

Phone: +81 3 6895 7390
Shinbashi Tokyu Bldg 3F
4-21-3
Shinbashi
Minato-ku
Tokyo 105-0004
Japan

South Korea

Phone: +82 31 278 7038
Fax: +82 31 278 7039
iOffice Building, 1034-16
Ingye-dong, Paldal-gu
Suwon, Gyeonggi-do
442-834
South Korea

dotmatics knowledge solutions