

Symyx ISENTRIS 3.1 Key New Features

The Symyx ISENTRIS 3.1 informatics system replaces Symyx's industry-leading ISIS software, while also giving scientists the freedom to create, manage, and share fully searchable local databases and work offline.

General

- Reaction and molecule clustering in ISENTRIS client and ISENTRIS for Excel—the ability to select a field and group all information into unique bins, cherry-pick and further cluster on bins.
- Automatic molecule and reaction searches for desktop applications. Runs through a cascade of searches until the application finds a hit.
- Set or writable .NET controls for insert/update and delete functionality
- Admin control of ISENTRIS client and Personal Data Source functionality
- Preservation of end-user sort in the history
- Fully searchable help for the API and application functionality
- Ability to associate vocabularies with query fields using SQL
- Search performance improvements across WAN
- Improved performance for multi-instance support
- Microsoft® Vista SP1 and Office 2007 support for all desktop applications
- Additional Linux 5 support
- Additional support for Microsoft Visual Studio 2008 .NET development

Symyx ISENTRIS client

- Reaction planner: SSS and Similarity product searches such that if the exact product is not found, the search automatically expands to include similar products you may like to synthesize.
- Improved QueryByForm configuration: Now a single-button click to use a form in both query and the browse environment.
- Improvements to the reaction browsing query and browsing forms
- Improved browsing of the Symyx Available Chemicals Directory (ACD) including shopping cart with export to SDF file facilities and supplier address reporting.
- Personal data source support
 - Ability to work offline with personal data sources
 - Full molecule and reaction search and browse capabilities
 - Create a Personal Data Source from a file (SDF file, RDF file, XDF file)
 - Create a Personal Data Source from a definition
 - Edit an existing Personal Data Source definition
 - Create a personal database from an existing recordset
 - Insert, update and delete data in an ISENTRIS Personal Data Source
 - Wrap and unpack personal data for sharing personal data sources
 - Import files (SDF file, XDF file and RDF file) into an existing data source with collision checking

ISENTRIS for Excel

- SSS and Exact match searches of Microsoft Excel spreadsheets
- Molecule and reaction-based enumeration of results into ISENTRIS for Excel
- Rgroup decomposition to support exact and substructure decomposition (decomposes structures with open valencies)
- Unique SMILES and unique SMILES convertor to support Rgroup decomposition workflows
- On and off switch for ISENTRIS for Excel add-in
- Import an SDF file or XDF file directly into Excel
- Personal data source support
 - Ability to work offline with personal data sources

- Full molecule and reaction search and browse capabilities
- Create a personal database from a spreadsheet
- Import files (SDFFile, XDFFile and RDFFile) into an existing data source with collision checking
- Create a personal database from an existing recordset
- Wrap and unpack personal data for sharing personal data sources

Symyx Draw

- Full support for polymers, mixtures, and formulations - Sgroups
- Enhanced sketch cleaning
- Name-to-structure
- Structure-to-name
- Canonical SMILES
- 3D query support
- Start up time for embedded renditor
- Microsoft Vista and Office 2007 support

Minor enhancements:

- Symbol Chooser
- Layout orthogonally
- Alternate display for star atom: zig-zag style as recommended by IUPAC
- 3D rotation tool
- Data Sgroup tool

DSBuilder

- Improvements to DSBuilder user interface and insertion of additional missing functionality
- Ability to collapse and group tables
- Ability to navigate connections for highly link tables or IDSeS
- Ability to publish a data source context directly to the admin console



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