

Autumn 2018

Database News

Derwent Markush Resource on STNext[®]

The Derwent Markush Resource (file DWPIM) became publicly available October 1, 2018 on STNext, integrating the database for the first time into the classic STN[®] environment. DWPIM seamlessly integrates with the Derwent suite of files on STNext.

DWPIM has been implemented as a structure-based database encompassing more than 2.1 million Markush structures from 890,000 Derwent World Patents Index (DWPISM from Clarivate) documents. A total of 33 patent-issuing authorities are covered with US, EP and WO coverage back to 1978. DWPIM also includes INPI (French patent office) backfile data from 1961-1976. The major substance classes in DWPIM are organics and organometallics. Inorganic compounds, polymers, peptides and partially defined structures are also covered. DWPIM will be updated 82 times a year together with the Derwent files WPINDEX, WPIDS and WPIX. Cross-file searching with WPINDEX, WPIDS and WPIX is supported. Both Markush hit structures and DCR hit structures are fully integrated and available with all display formats in these files.

Structure Searching in DWPIM:

DWPIM offers the known STN structure search modes and scopes:

- Structure search: chemical structures can be drawn with the integrated structure editor or imported as .cxf or .str files to the structure editor. The search can be executed as substructure search (SSS) as well as closed substructure search (CSS).
- Search scope includes SAMPLE, FULL and BATCH search. SUBSET will be added at a later time.
- The STN/CAS conventions are preserved for all structure queries. Derwent nodes are fully supported for DWPIM on STNext.
- DWPIM results may also include structures for which the search process is not completed in the time allowed. (Note: this refers to the search time per structure and should not be confused with the overall system time-out of 30 minutes). These candidates are passed to the answer set and marked "iteration incomplete". These structures need to be examined manually to determine if they meet the search requirements. It may be possible to eliminate iteration incomplete answers by rerunning the search as a BATCH search.
- For DWPIM, structure searching has been developed for the structure editor only. Command line structure search (Graph-Node-Bond) should not be used for query building.

Crossover capabilities to WPINDEX, WPIDS, and WPIX:

- DWPIM structure searching and crossover to the Derwent files WPINDEX, WPIDS, and WPIX uses the classic STN crossover functionality and is similar to the CAS REGISTRY®/CAplusSM crossover.
- DWPIM results can be refined with a set of roles within WPINDEX, WPIDS, and WPIX. For example, this allows the preparation of compounds to be easily searched.

Derwent subscribers with access to fragmentation codes can refine Markush results in DWPI and make use of frag codes assigned for chemical reactions, pharmaceutical activities, formulation types and other applications.

In WPINDEX, WPIDS and WPIX combined Markush HIT Structure Display Formats with substructure highlighting support efficient relevance checking:

- AHITSTRUCTURE with assembled hit structures
- BHITSTRUCTURE a brief hit structure display with all query-relevant groups
- FHITSTRUCTURE with the full Markush hit structures displayed

STNext Features for DWPIM

- Scripting functionality for manual alerts in DCR/DWPIM/DWPI (WPINDEX, WPIDS or WPIX), enabling cross-file searching
- Reporting options include transcript in RTF, PDF, TXT and ZIP (TXT plus folder of images) formats

[Register](#) to learn more at an e-seminar October 25, 2018.

BLAST® Alignment Reports in STNext

STNext now supports the combination of sequence alignment data with bibliographic/substance information to create BLAST Alignment reports. [Learn more](#) about generating an alignment report. An updated version of the CAS REGISTRY® BLAST client was also released in September and it is available for [download](#).

Structure Attribute Display Enhancements in STNext

Now display all available detail about structures, such as element counts, variable node saturation, and ring system characteristics. The expanded structure display information is available in structure searchable databases in STNext, but not in other STN classic platforms. It also provides categories for the various structure attributes (e.g., Variable node attributes), allowing you to more quickly zero in on the information you're looking for. [Learn more](#) about the attribute display re-organization.

Structure Editor in STNext Includes More Derwent Nodes

The Structure Editor includes Derwent DWPIIM/DCR generic nodes as well as DWPIIM super atoms. Structure drawings can include variable nodes for metals, carbon chains, carbocycles, heterocycles as well as DWPIIM-specific groups (also referred to as super atoms). Super atoms available include Acyl groups (ACY), Protecting groups (PRT) and Unspecified groups that include or exclude hydrogen, and more.

1. Access the super atoms and generic nodes by clicking the red X button in the left hand toolbar.

The screenshot displays the Structure Editor window. The central canvas shows a chemical structure of 2-(2-acetylphenoxy)acetaldehyde. The left-hand toolbar contains various drawing tools, with the 'X' button highlighted in red and an arrow pointing to it with the text 'Click the X button'. The right-hand panel, titled 'Attribute Values', lists various properties for the selected node, including Bond Type, Bond Value, Node Type, Generic Definition, Match Level, Element Count Level, and Other Node Attributes. The bottom status bar shows the molecular formula C₉H₈O₃ (164.16) and a 'Save & Upload' button.

The variable lists in the right hand column are Derwent-specific. Note the miscellaneous nodes are for DWPIIM only and will not be compatible with other files such as MARPAT®. However, structures drawn with MARPAT generic nodes can be searched in DWPIIM, but not vice versa. For example, if you draw a structure with an HY (heterocycle) variable, STNext knows to search that same structure in DWPIIM with HEA, HET or HEF at that same node.

Variables

X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
Ak	Any carbon chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle
Id	ID generic node

Derwent (DWPIM/DCR) generic nodes

- ▶ Metals
- ▶ Carbon Chains
- ▶ Carbocycles
- ▶ Heterocycles
- ▼ Miscellaneous (DWPIM only)
 - ACY Acyl group
 - DYE Chromophore or fluorescent group
 - POL Macromolecule
 - PEG Polymer end group
 - PRT Protecting group
 - XX Unspecified atom or group (excluding H)
 - UNK Unspecified atom or group (including H)

Close

2. Make your selection from the lists and then draw the connecting bond where you want to place the group.

Structure Editor

Draw or change atoms or bonds. Shortcut Keys

Enter a CAS RN, SMILES or InChI

Attribute Values

- Bond Type
- Chain
- Ring
- Ring / Chain
- Bond Value

Variables

X	Any halogen
M	Any metal
A	Any atom except H
Q	Any atom except C or H
Ak	Any carbon chain
Cy	Any cycle
Cb	Any carbocycle
Hy	Any heterocycle
Id	ID generic node

Derwent (DWPIM/DCR) generic nodes

- ▶ Metals
- ▶ Carbon Chains
- ▶ Carbocycles
- ▶ Heterocycles
- ▼ Miscellaneous (DWPIM only)
 - ACY Acyl group
 - DYE Chromophore or fluorescent group
 - POL Macromolecule
 - PEG Polymer end group
 - PRT Protecting group
 - XX Unspecified atom or group (excluding H)
 - UNK Unspecified atom or group (including H)

Close

Formula is not available

View Previous Structures... Cancel Save Save As Save & Upload

The screenshot shows the Structure Editor interface. In the center, a chemical structure is displayed: a benzene ring with an acetoxy group (-O-C(=O)-CH3) at the top position and a carbonyl group (-C(=O)-) at the ortho position. The carbonyl carbon is labeled with 'PRT'. A 'Variables' dialog box is open over the structure, with an orange arrow pointing from the 'PRT' label in the structure to the 'PRT' option in the 'Miscellaneous (DWPIM only)' section of the dialog. The dialog lists various generic nodes, including 'PRT' (Protecting group). At the bottom of the editor, there is a toolbar with various drawing tools and a text input field containing 'PRT'. The status bar at the bottom indicates 'Formula is not available' and provides buttons for 'View Previous Structures...', 'Cancel', 'Save', 'Save As', and 'Save & Upload'.

3. Proceed with your structure drawing.

Emtree® Thesaurus Updated in Embase®

The third Emtree thesaurus release for 2018 is now available within Embase. Now totaling 81,735 preferred terms and over 355,000 synonyms, Emtree added 766 new terms. Of the new terms added, 67 are drug terms, allowing you to keep up-to-date with the latest developments in the terminology of pharmacology and biomedicine.

In addition, there are also 699 new non-drug terms, including:

- Cell lines
- Bodies of water
- And more!

34 terms from Emtree May 2018 have been replaced. Customers running Alerts in Embase should check the new Emtree terminology and update their Alerts strategies as necessary to ensure continued comprehensive retrieval. [Review new and changed terms](#).

Top Reasons STN Search Professionals Switch to STNext:

- New features and improvements are added monthly! Take advantage of STN enhancements the moment they are available without the need to install any software updates or plug-ins.
 - Latest updates: BLAST alignment reports when sequence searching in CAS Registry and Markush searching of Derwent (DWPI) content
- Securely access STN content from any computer with convenient always-on access to your scripts, transcripts, stored search queries and SDI results.
- Leverage your hard-won skill using the STN command line interface. The same search language that you know and love in STN Express is also available in STNext.

Login into STNext with your standard STN credentials at next.stn.org and access the premier STN product.

Help Improve CAS Products

CAS is always looking for ways to improve our products and services, and we invite you to help!
[Complete a quick survey](#) to sign up.

Need help with STN? Contact the CAS Customer Center (help@cas.org)

CAS® Customer Center Tip

Scripting with data files in STNext

Q: I typically follow a consistent search strategy using key terms and specific substances. There can be some variation over time, but is there a way to automate or streamline my searches?

A: Yes. Scripts may be a useful tool. You have the option to save any query as a script and then run that script whenever you want. Furthermore, if you have lists of substances or search terms that you use frequently, STNext scripts can read data files and add search terms to your query. When you create and manage .data files in STNext, you establish consistent search terms that can be shared within your organization. [Learn about the OPEN, READ and WRITE scripting commands and see some example scripts.](#)

Save the Dates

Concept Life Sciences 5th "Synthesis in Drug Discovery & Development" Symposium

October 24, 2018
Alderley Park, UK

[Learn More](#)

American Chemical Society National Meeting & Exposition

March 31 – April 4, 2019
Orlando, FL

[Learn More](#)

eSeminar

The Derwent Markush Resource database
(aka DWPIIM) now on STNext

October 25, 2018

9:00am - 10:00am ET

or

2:00pm - 3:00pm ET

[Register](#)

**Contact your CAS representative to
discuss your organization's training
needs**