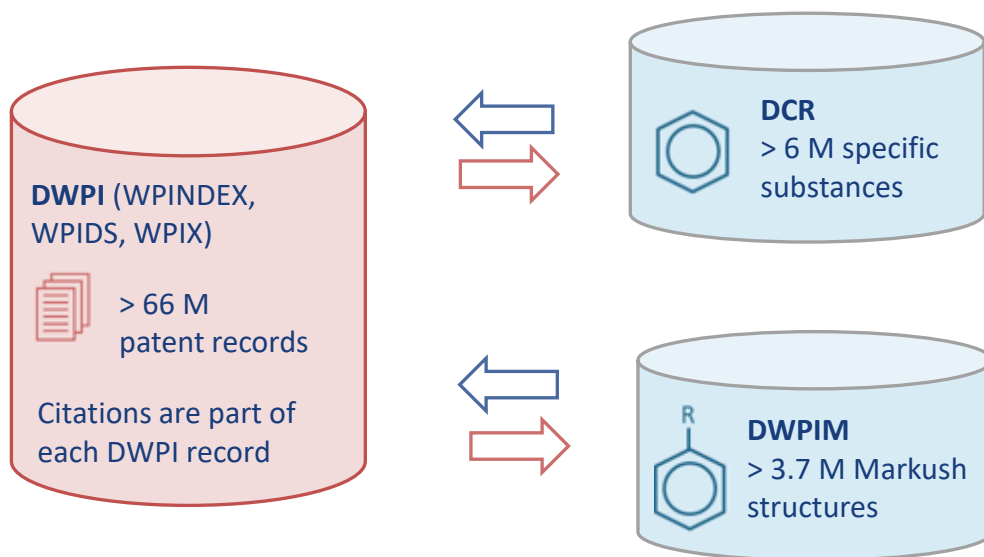


CAS STNext[®]

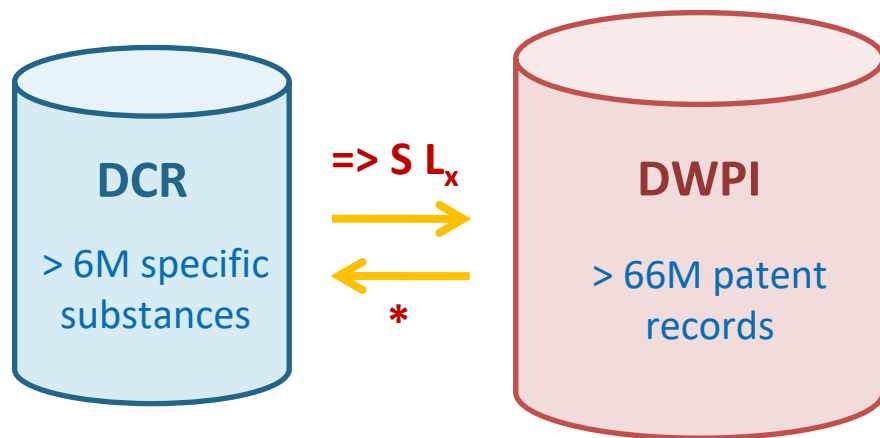
DERWENT CHEMISTRY RESOURCE (DCR)

© 2025 American Chemical Society. All rights reserved.

The DCR database is a companion file to Derwent World patents Index (DWPI)



The DCR database on STNext - highlights



- Simple workflow with DWPI
- HIT structure highlighting
- Derwent superatoms and isotopes (D, T)
- Higher system limits for structure searching
- Enhanced structure displays

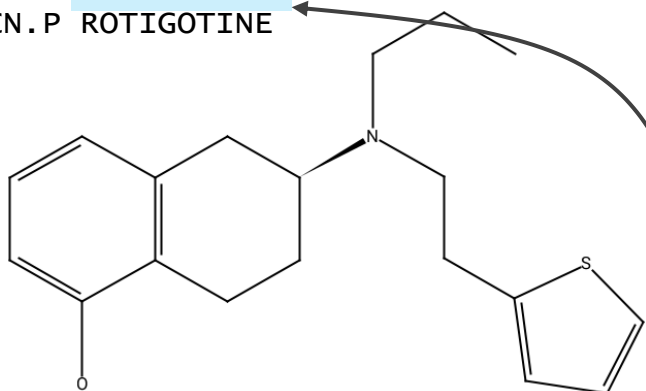
DCR and associated databases WPINDEX, WPIDS and WPIX

DCR substance records are linked to corresponding patent documents in DWPI through their DCR Accession Number.

DCR

AN DCR-101539
CN.P ROTIGOTINE

DCR

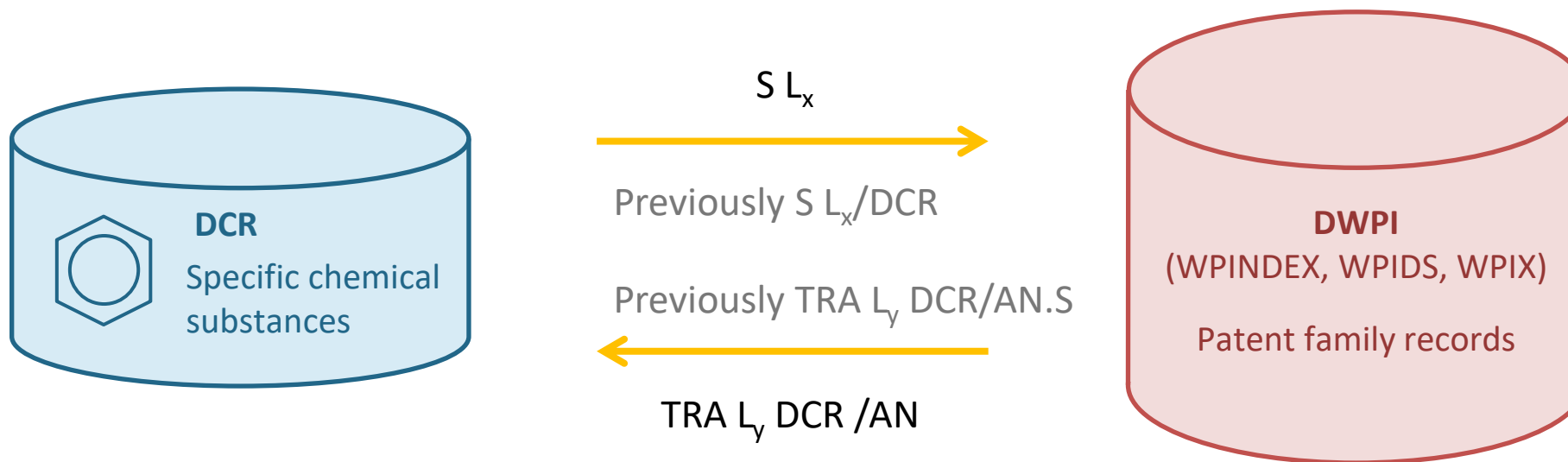


DWPI

AN 2014-v21559 [201480] WPIX
TI Method for delivering e.g. fentanyl with specified viscosity to human patient suffering from chronic hepatitis C by physician, involves actuating electrochemical actuator such that actuator deflects by exerting force in fluid reservoir
AB USE - Method for delivering drug fluid e.g. therapeutic agent such as opioid/non-opioid narcotics e.g. fentanyl, remifentanyl, sufentanil, morphine, hydromorphone, oxycodone and salt, non-steroidal antiinflammatories (NSAID) e.g. diclofenac, naproxen, ibuprofen and celecoxib, local anesthetic e.g. lidocaine, tetracaine and bupivacaine, dopamine antagonist e.g. apomorphine, **rotigotine** and ropinerole, ...
IT UPIT 20141212
...
DCR-72366-USE; DCR-127393-CL DCR-127393-USE; DCR-7556-CL
DCR-7556-USE; DCR-99408-CL DCR-99408-USE; DCR-108590-CL
DCR-108590-USE; DCR-89506-CL DCR-89506-USE; DCR-87611-CL
~~DCR-87611-USE~~ DCR-101539-CL DCR-101539-USE; DCR-25857-CL
DCR-25857-USE; DCR-109039-CL DCR-109039-USE; DCR-88306-CL ...

DCR Accession Numbers facilitate crossover

DCR - DWPI



Consistent workflow across STN

Crossover DCR database – DWPI files

=> **FIL DCR**

=> S L1 SSS FULL (L2)

=> **FIL WPIX**

=> S L2

=> D FULL HITSTR

- Chemical substance searching and crossover to associated database is consistent for STN database pairs:
- Registry – CAplus
- DWPIM - DWPI files (WPINDEX; WPIDS, WPIX)
- DCR – DWPI files.

Easy current awareness searches via scripts

The screenshot displays the STNNext web interface. At the top left is the STNNext logo. Below it, a navigation bar includes a 'Return to Session' link and a 'Structures (41)' section. A toolbar contains icons for file operations and a search bar labeled 'Search Files by Name'. A list of files is shown, with 'Structure_Cy_Repeating_Group' selected, displaying its chemical structure and a timestamp. A magnifying glass highlights the 'My Files' dropdown menu, which lists 'Alerts', 'Transcripts', 'Structures', 'Scripts', and 'Biosequences'. A text box on the right states 'In-application file storage and management'. Below the file list, a script editor shows a sequence of commands for deleting, updating, and uploading a structure file. A 'Run' button is at the bottom of the script editor. To the right, a 'Validation' panel shows a 'Success' message: 'No errors detected'. A text box on the left states 'Reference to structure file'.

STNNext

Return to Session

Structures (41)

Move to Folder Search Files by Name Import Biosequence

Structure_Cy_Repeating_Group 2021 Apr 13 1:41 PM

Edit

My Files

- Alerts
- Transcripts
- Structures
- Scripts
- Biosequences

Upload

In-application file storage and management

Reference to structure file

Save As Upload Download Refresh Copy Validate

```
1 => DEL HIS
2 :Y
3 => fil DCR
4 GET _update LABEL="Enter latest DCR update date"
5 => s _update/upwx
6 upload LNUM _str1 <Structure_Cy_Repeating_Group>
7 => s _str1 sss subset=L1 full
8 ECHO "Compounds with bibliographic changes in WPI"
9 => fil windex
10 => S L3
11
```

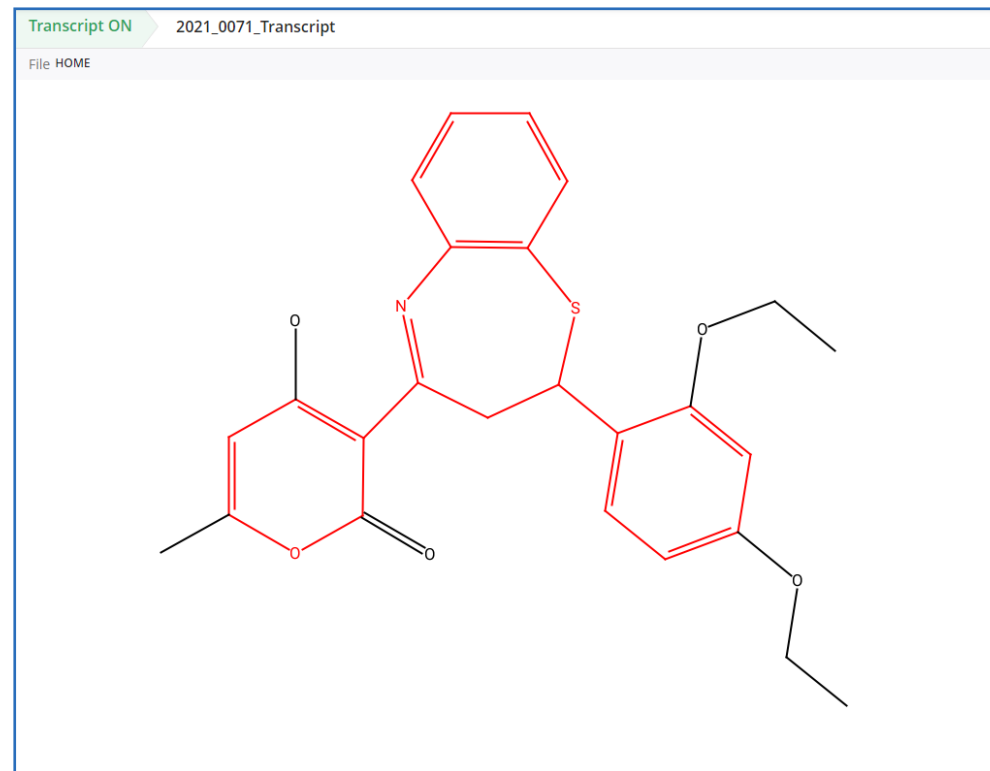
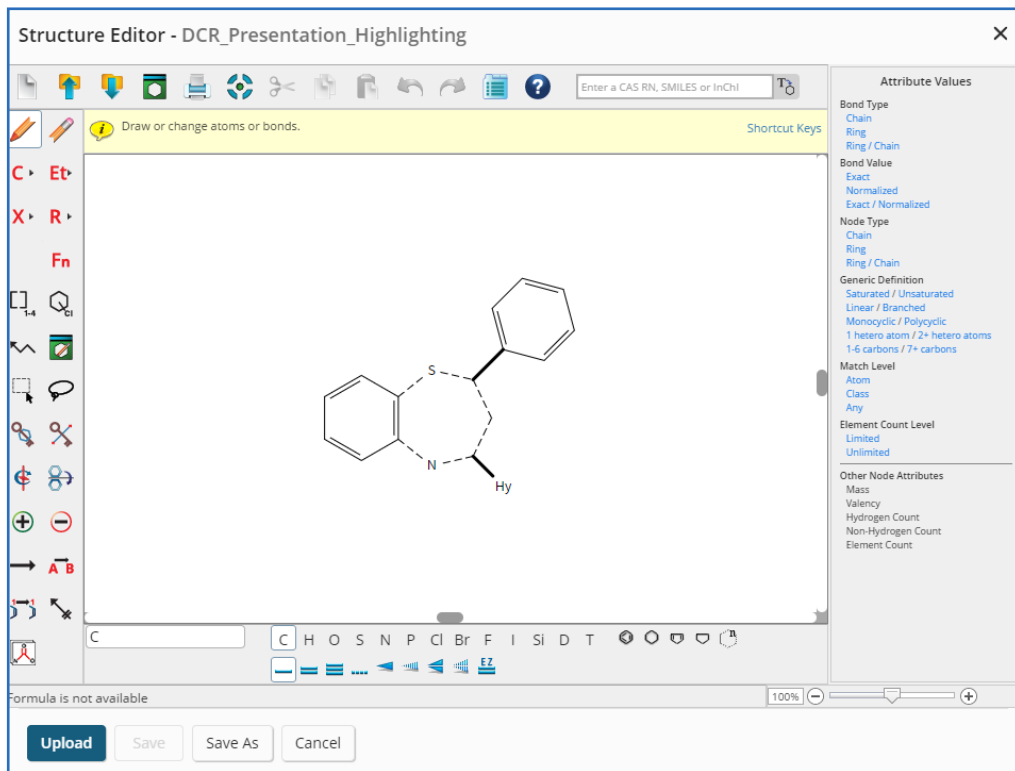
Run Save Cancel

Validation

Success

No errors detected

Hit Structure Highlighting



Support for analyzing results of generic structure searches efficiently.

Derwent superatoms for structure searching

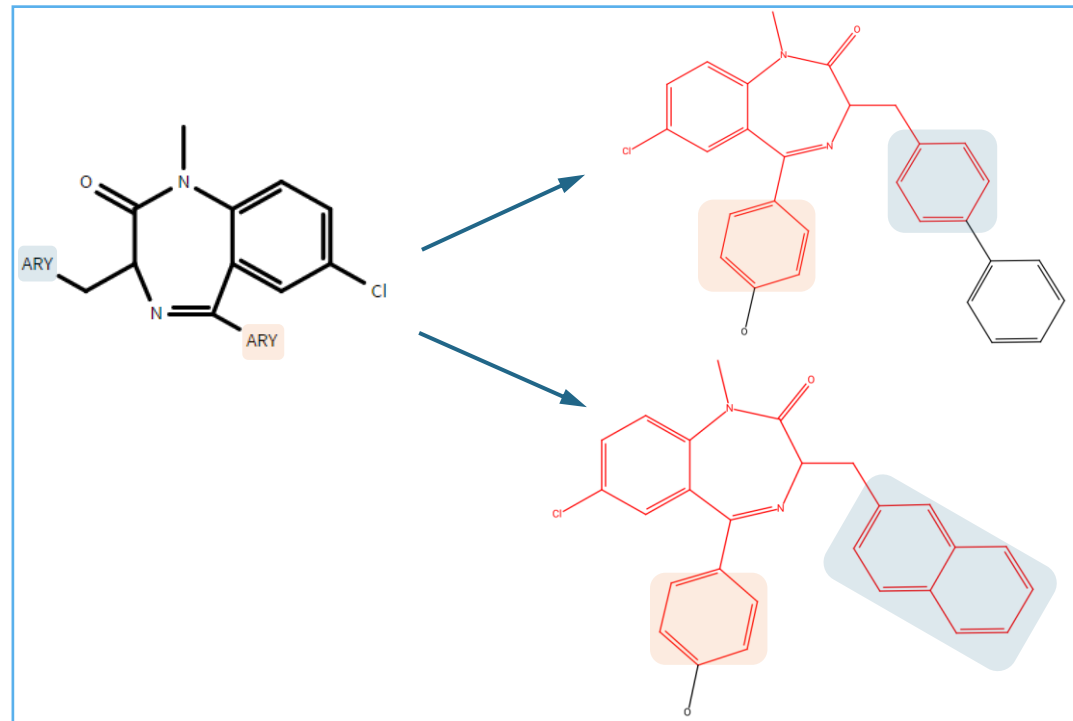
Variables

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

Derwent (DWPIM/DCR) generic nodes

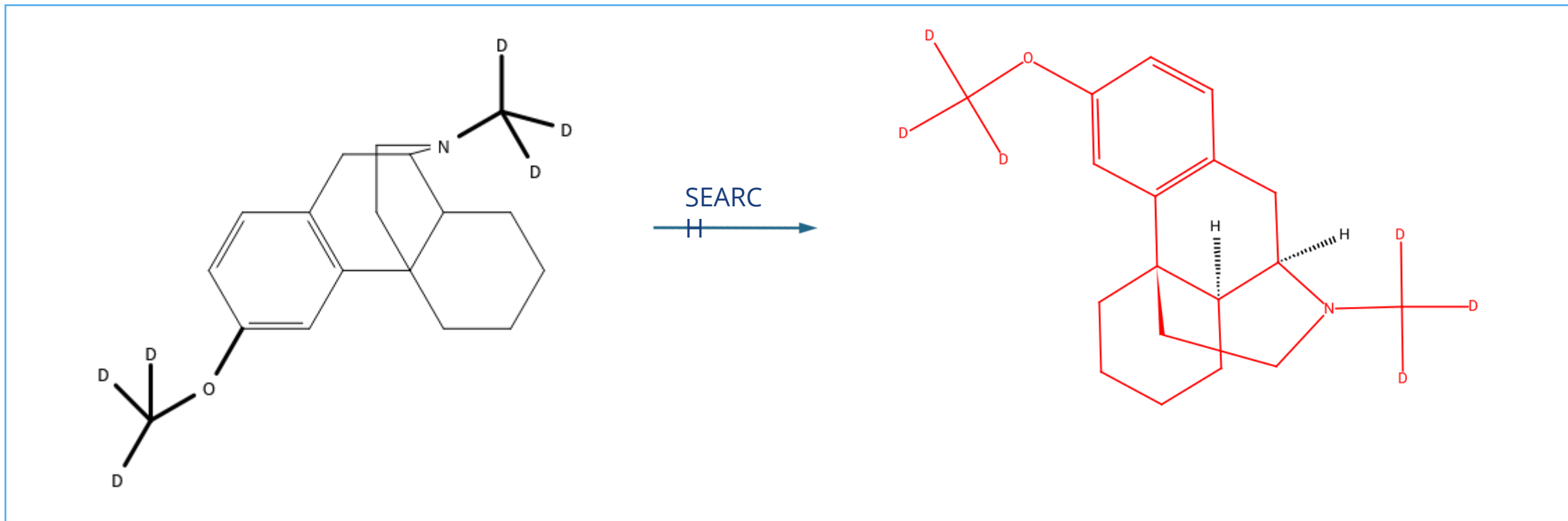
- Metals
- Carbon Chains
- ▼ Carbocycles
 - ARY Carbocycle (at least one benzene)
 - CYC Cycloaliphatics (all others)
- Heterocycles
- Miscellaneous (DWPIM only)

Close



Enhanced retrieval capabilities for generic structure searches.

Isotopes D and T for structure searching



Increase search precision by specifying hydrogen isotopes in your query.

Structure search and crossover limits

Structure Search Scope	Answers
Online SAMPLE	50
Online FULL	1,500,000
Batch FULL	1,500,000
Crossover DWPI Files	200,000

Helpful new search options

BI	Basic index contains fragments of CNS, CN.P, SY, MF and CT.	S BENZOIC (S) ACID (W) HYDRAZIDE
FA	Available information for a compound.	S L1 and DDRN/FA
NC, NC.TOT	Field codes for multi-component substances consistent with other STN structure files.	NC Number of components (previously NFRAG) NC.TOT Total number of components (previously NC) MF C12 H20 O4 . 2 Na SMF C12 H20 O4 *1; Na *2; TOTAL *3; TYPE *2
ELS, ELS.CNT	Element Symbol may be combined with Element Symbol Count by (S) proximity.	S C/ELS (S) 16/ELS.CNT or S 16 C/ELS => C16 H9 F6 N3
CMF, CMF.CNT	Component Molecular Formula may be combined with its ratio in multi-component substances by (S) proximity.	S H2O/CMF (S) 5/CMF.CNT
MF, CMF	Molecular Formula and Component Molecular Formula indexing with and without blanks.	E C12H20/MF,CMF or E C12 H20/MF,CMF

Consistent field codes for multi-component substances in STN

NC, NC.TOT	NC Number of components (previously NFRAG)									
	NC.TOT Total number of components (previously NC)									
	MF	C12	H20	04	.	2	Na			
	SMF	C12	H20	04	*1;	Na	*2;	TOTAL	*3;	TYPE *2

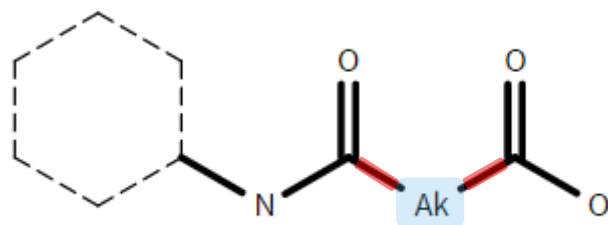
Structure search results may differ

Structures with certain features are processed differently by the new structure search engine:

- Cycles and complex structures with more than one repeating group
- Variables with attributes, e.g., non-hydrogen count
- Variable Ak and Derwent Nodes CHK, CHE, CHY as part of carbon chain or used as repeating group
- Group with node type ring bound via variable attachment points

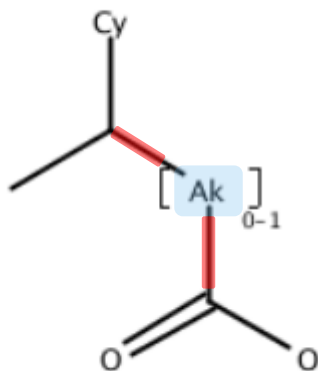
Individual workarounds are possible!

Variable Ak as part of carbon chain



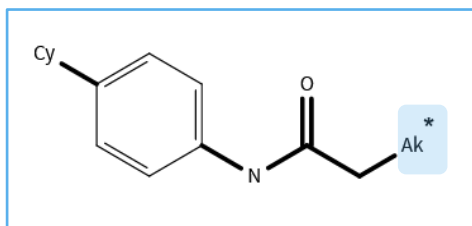
0 Answers

Please consider when you work with R-groups!

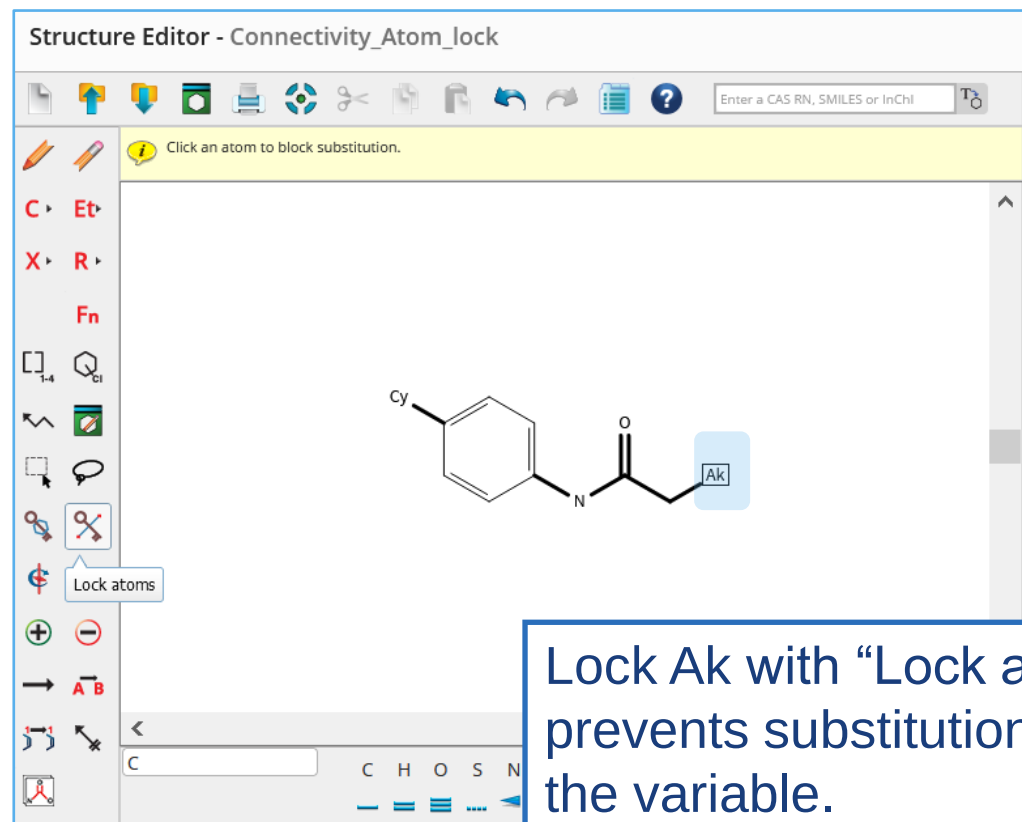


Retrieves only answers with $[Ak]_0$

Variables with attribute non-hydrogen count: Workaround with “Lock atoms”

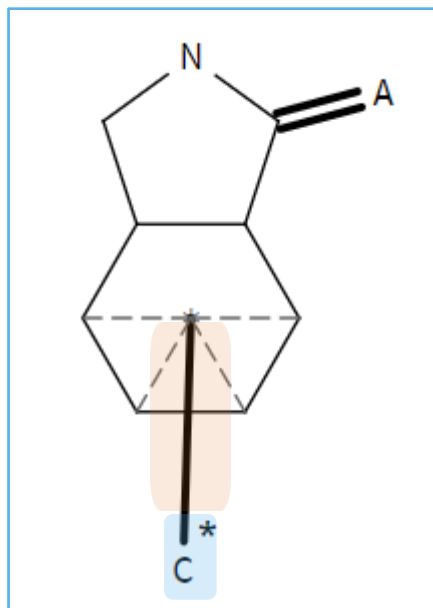


Structure with attribute non-hydrogen count at Ak retrieves too many hits.



Lock Ak with “Lock atoms” prevents substitution at the variable.

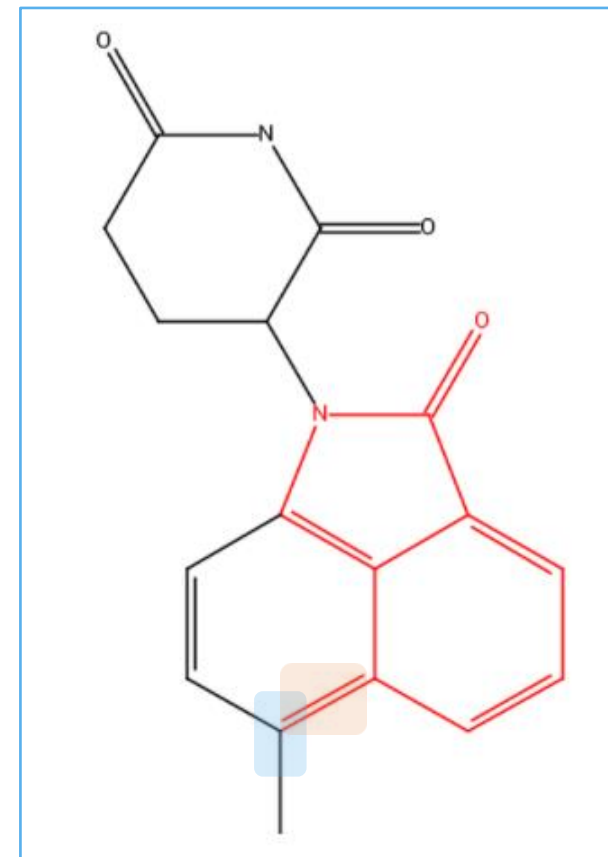
Group with node type ring bound via variable attachment points (VAP)



Node type ring
VAP bond type chain



Retrieves also
condensed structures



For more information...

CONTACT

CAS
help@cas.org
cas.org

FIZ Karlsruhe
EMEAhelp@cas.org