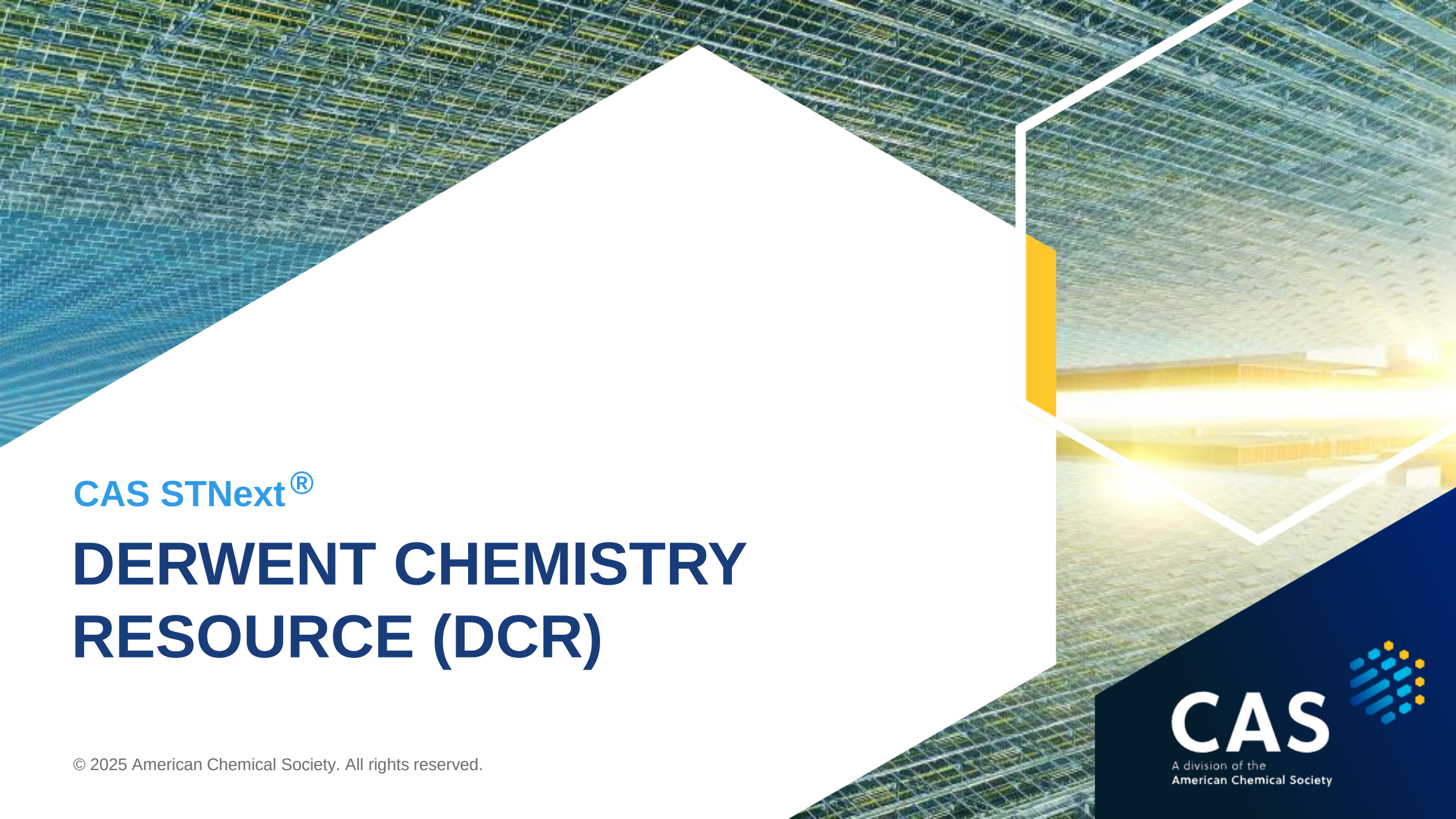

CAS STNext®

DERWENT CHEMISTRY RESOURCE (DCR)

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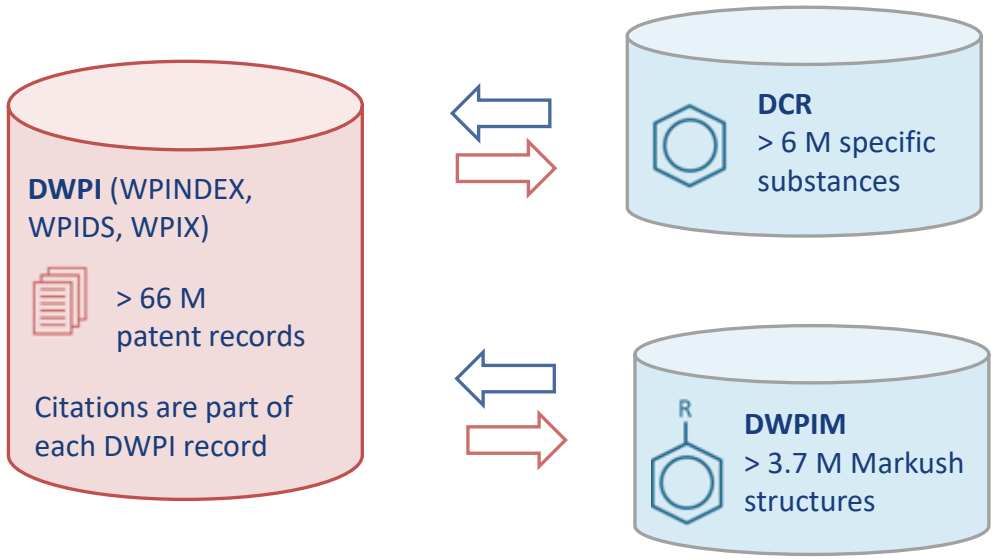
The DCR database is a companion file to Derwent World patents Index (DWPI)



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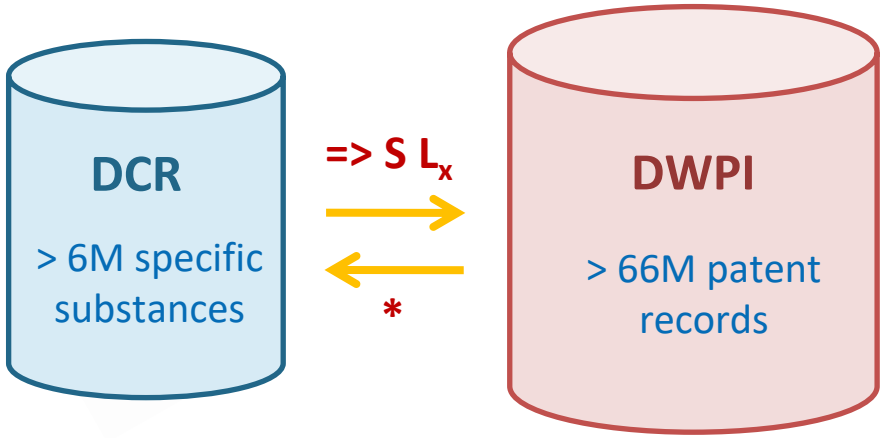
The DCR database on STNext - highlights



* => TRA DCR /AN

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

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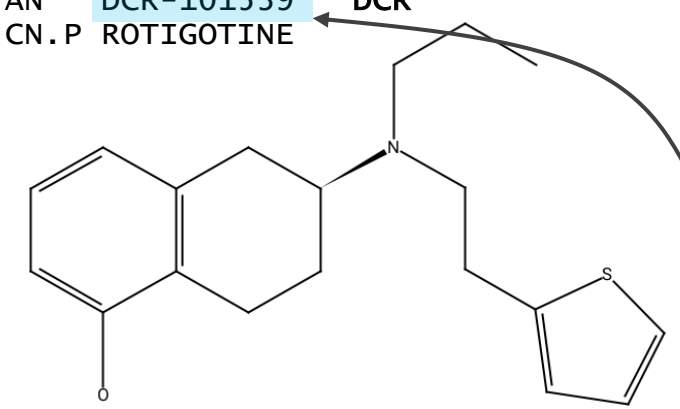
DCR and associated databases WPINDEX, WPIDS and WPIX

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

DCR

AN DCR-101539 **DCR**
CN.P ROTIGOTINE



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 antinflamatories (NSAID) e.g. diclofenac, naproxen, ibuprofin and celecoxib, local anesthetic e.g. lidocaine, tetracaine and bupivicaine, 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 ...

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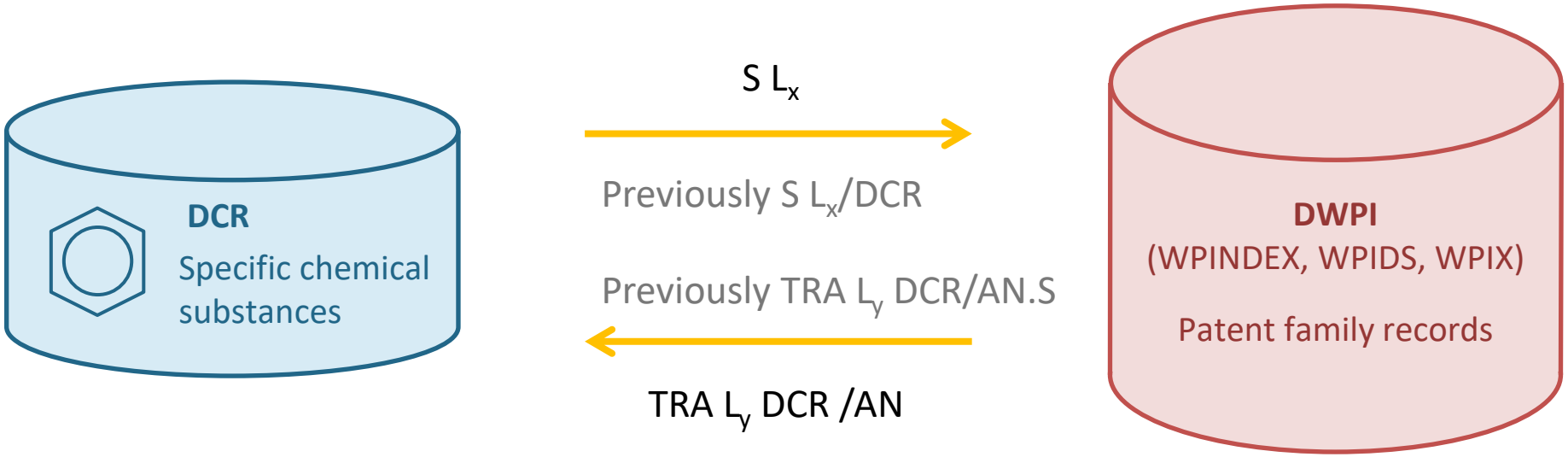
DCR Accession Numbers facilitate crossover DCR - DWPI



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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.

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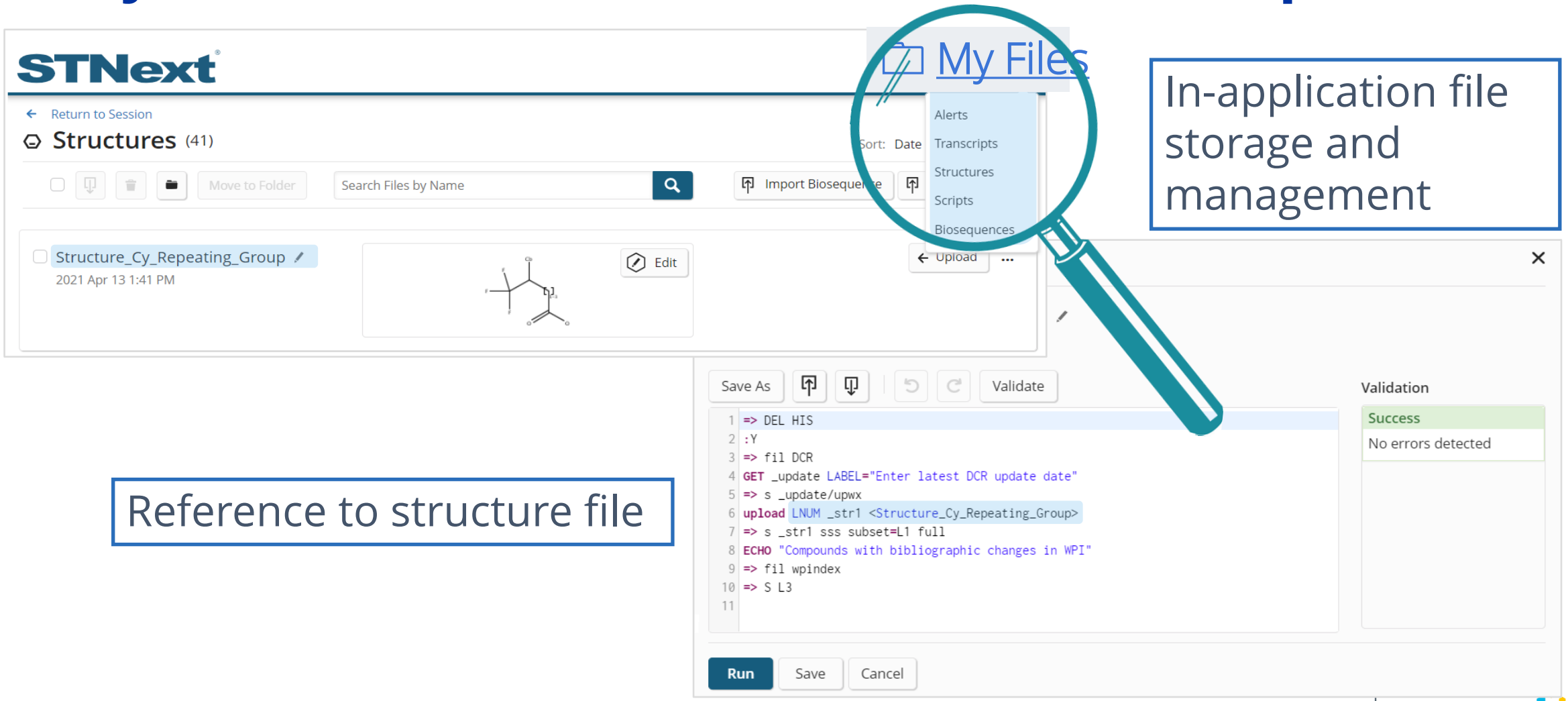
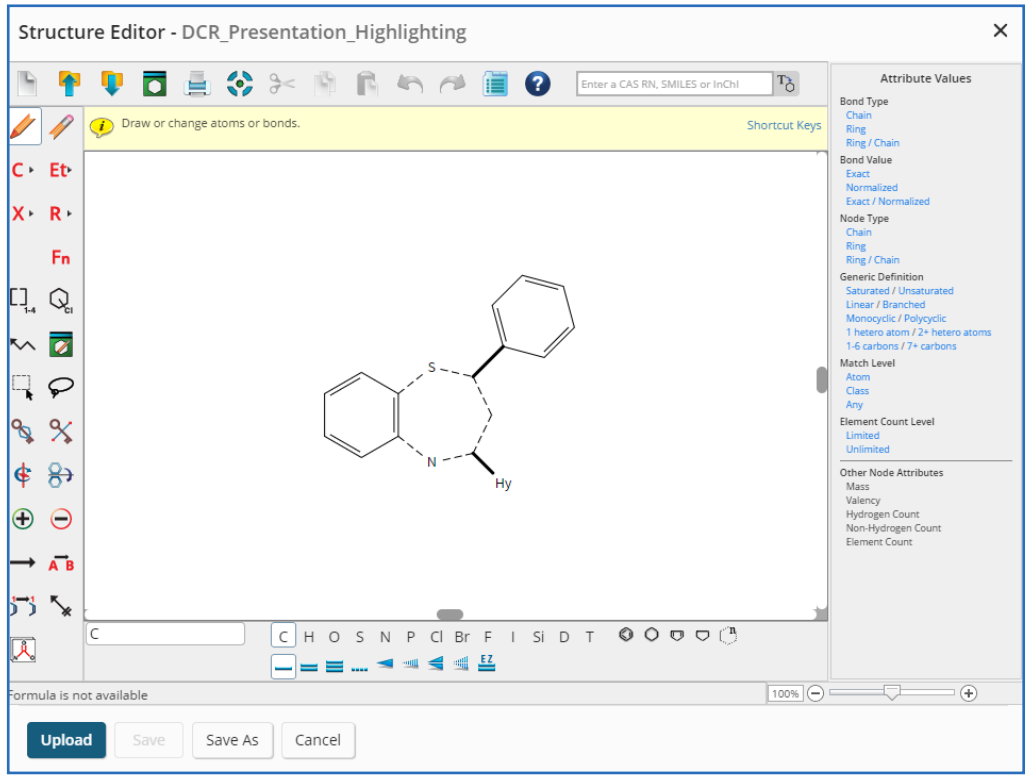
Easy current awareness searches via scripts

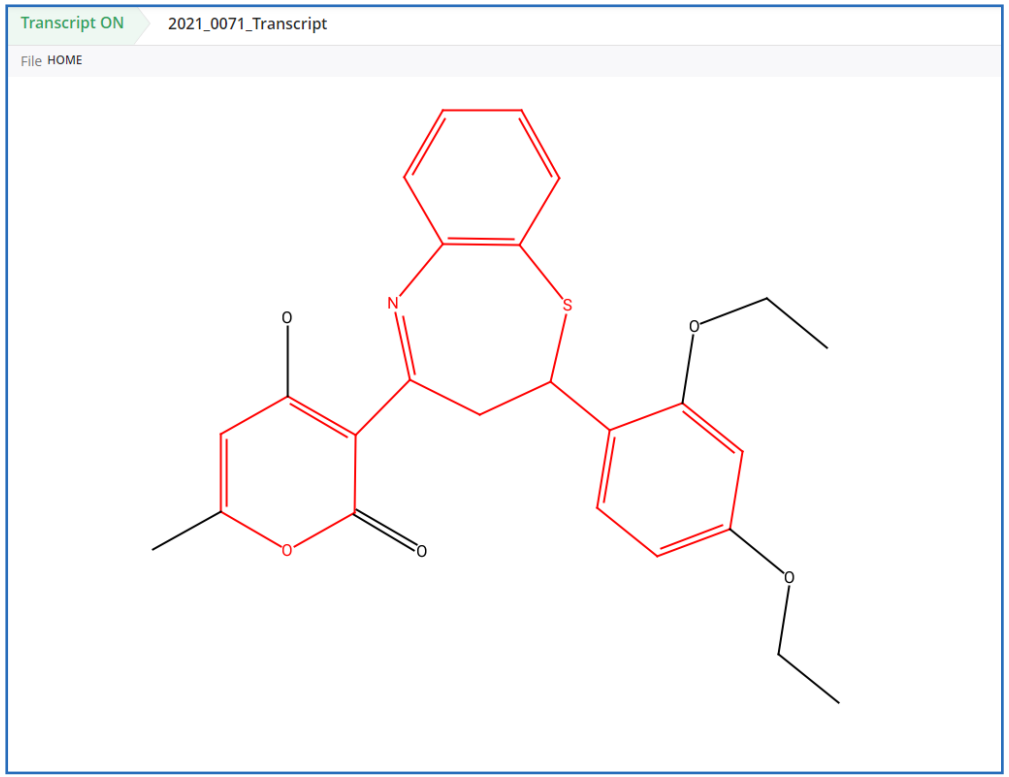


In-application file storage and management

Reference to structure file

Hit Structure Highlighting





Support for analyzing results of generic structure searches efficiently.

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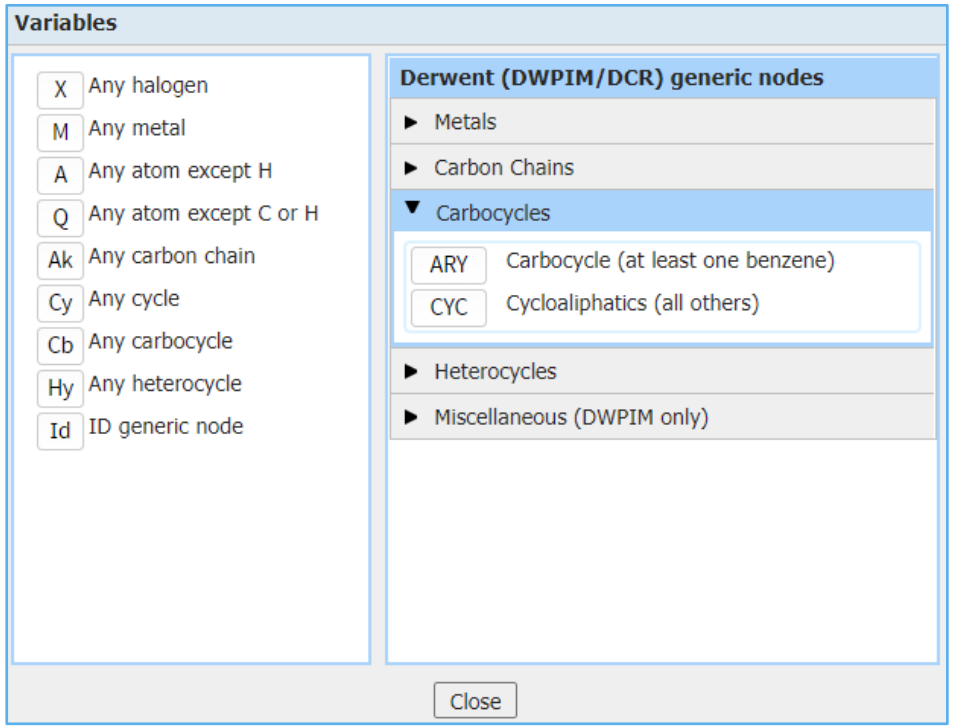
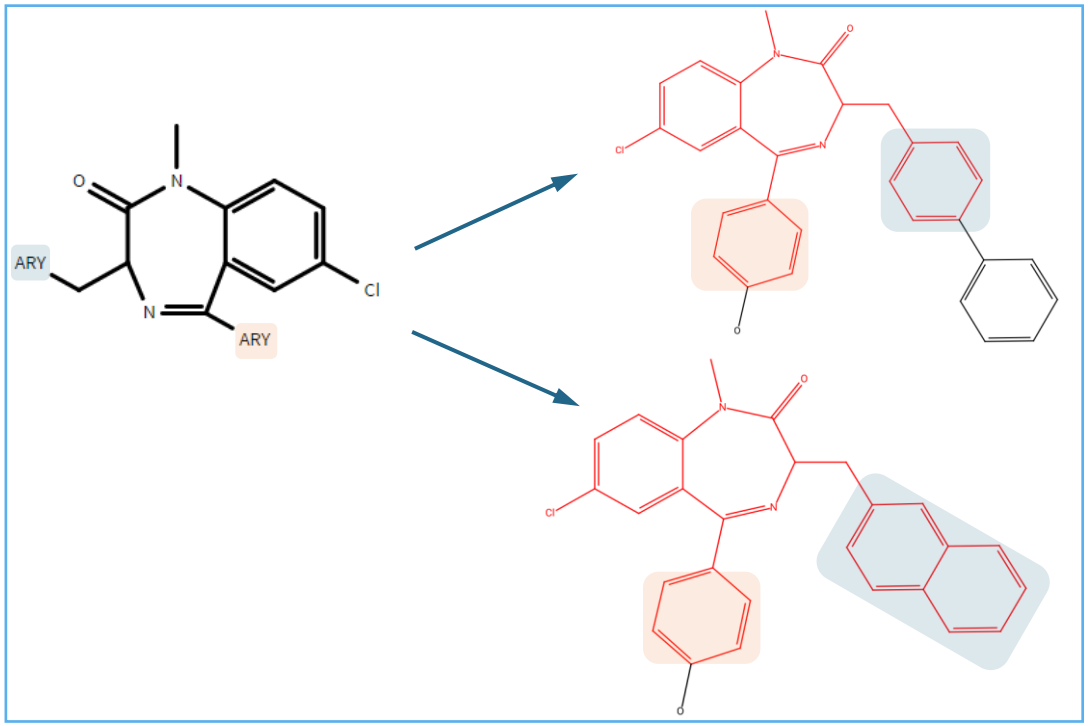
Derwent superatoms for structure searching





Enhanced retrieval capabilities for generic structure searches.

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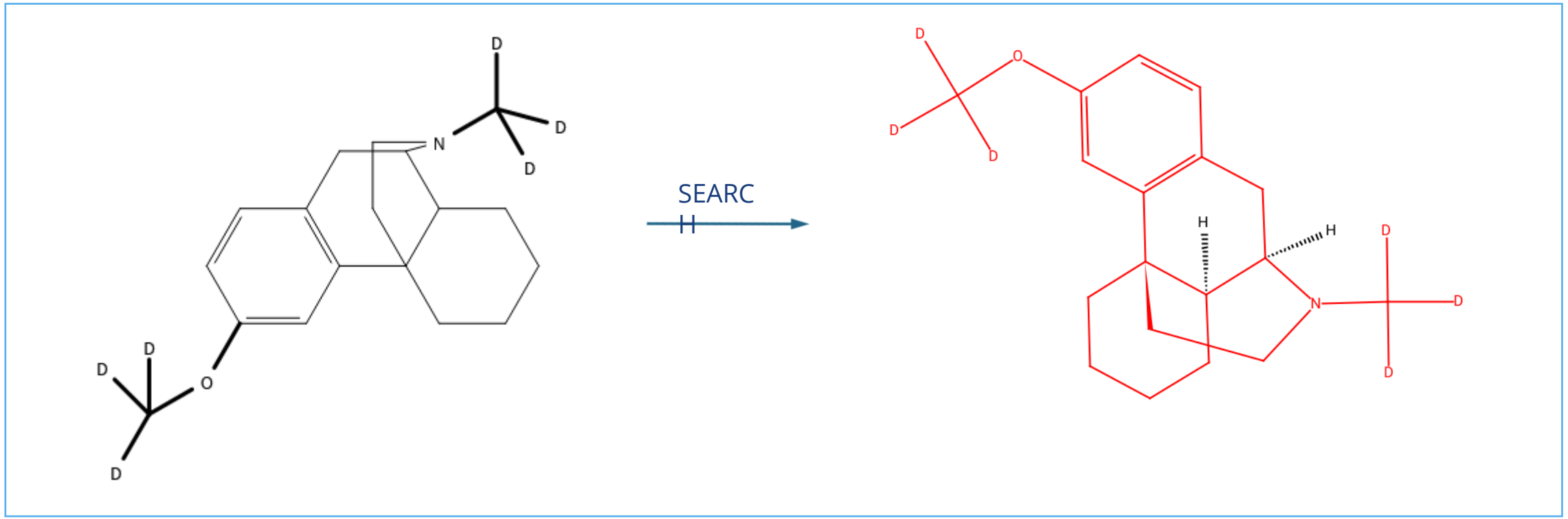
Isotopes D and T for structure searching



Increase search precision by specifying hydrogen isotopes in your query.

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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

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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

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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 O4 . 2 Na SMF C12 H20 O4 *1; Na *2; TOTAL *3; TYPE *2

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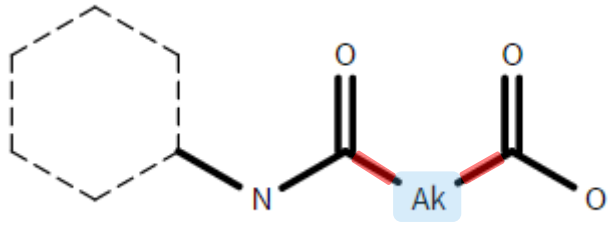
Structure search results may differ

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

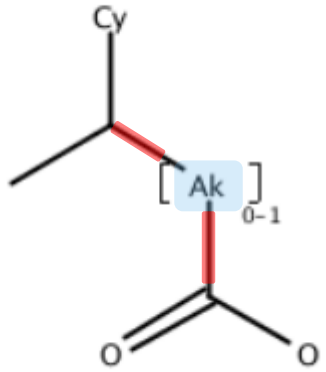
Individual workarounds are possible!

Variable Ak as part of carbon chain



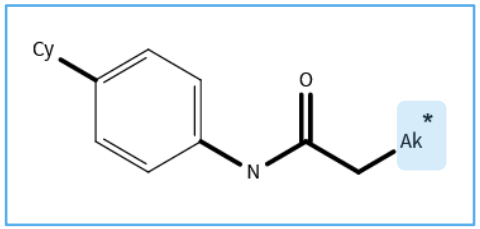
0 Answers

Please consider when you work with R-groups!

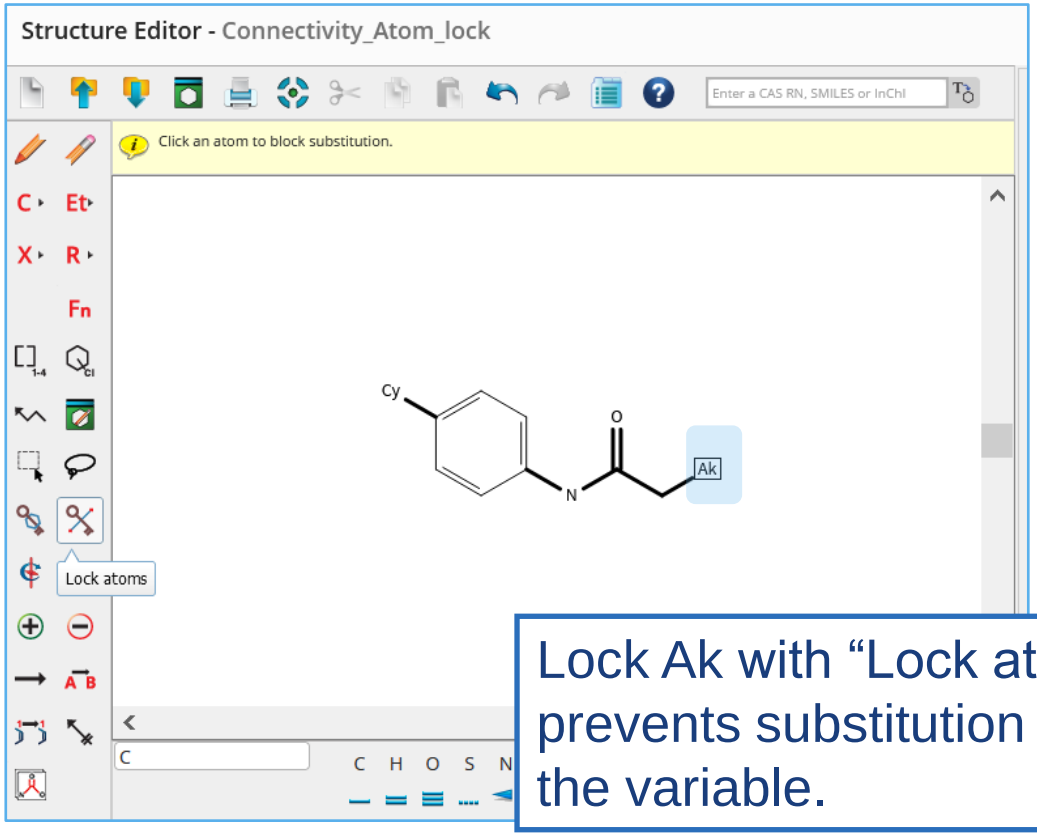


Retrieves only answers with $[Ak]_0$

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.

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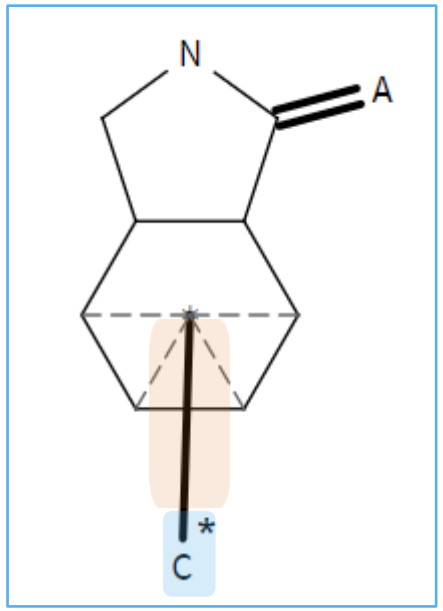
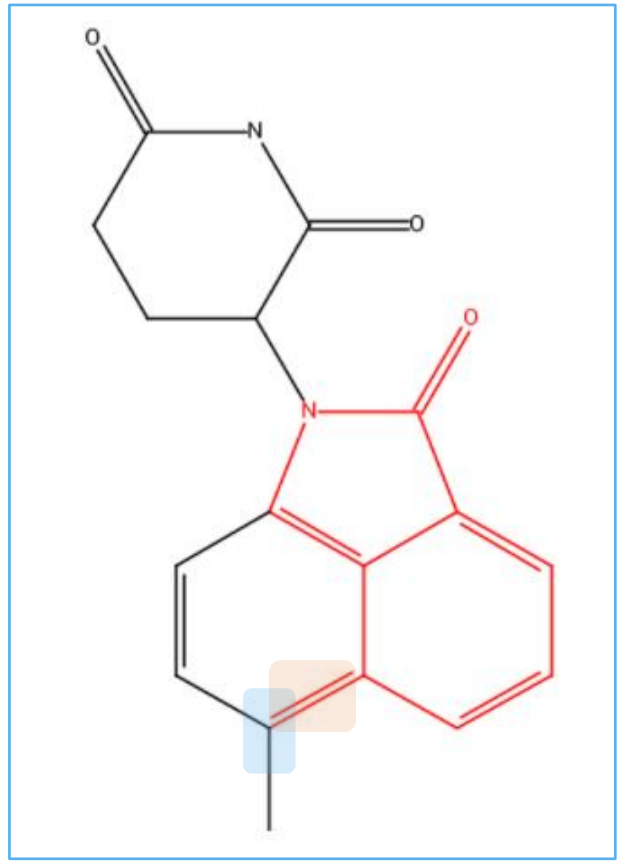
Group with node type ring bound via variable attachment points (VAP)



Node type ring
VAP bond type chain

Retrieves also
condensed structures



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