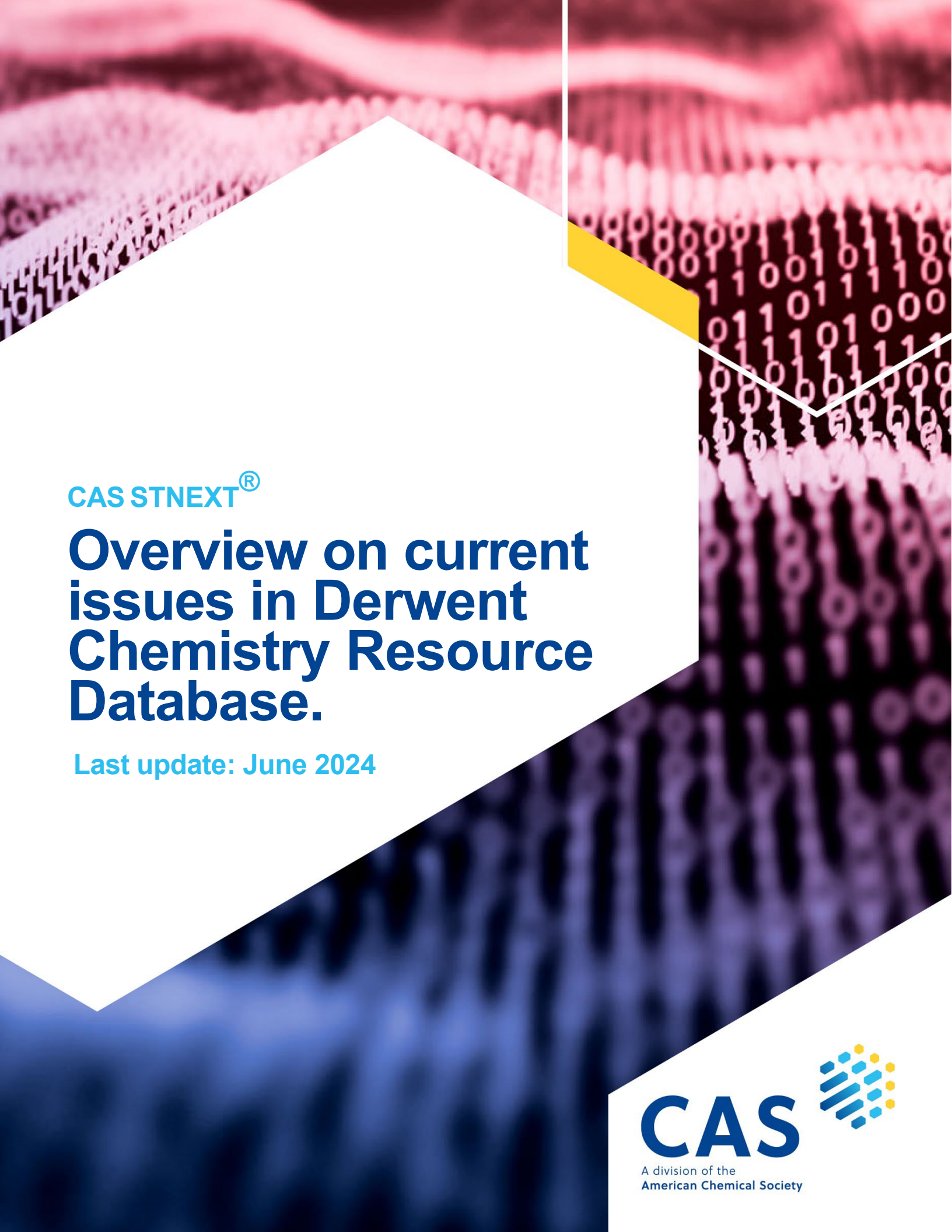

CAS STNEXT®

Overview on current issues in Derwent Chemistry Resource Database.

Last update: June 2024

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This document summarizes all known issues that can affect the results of structure searches in the Derwent Chemistry Resource (DCR) database.

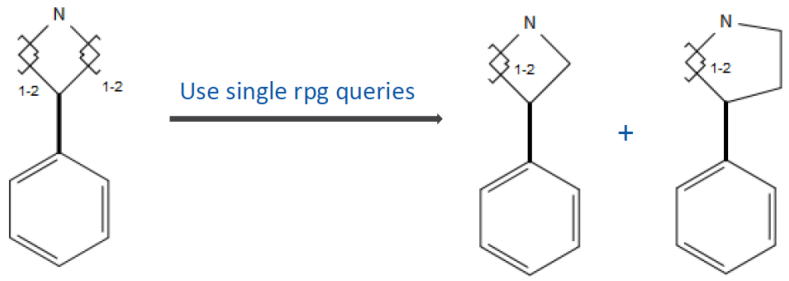
If you need support concerning your structure query or regarding DCR in general, please contact EMEAhelp@cas.org.

1.Within rings only one repeating group (rpg) per ring is allowed

In case of two or more repeating groups within the same ring incorrect results are obtained.

There is no workaround other than drawing out all possible combinations for every additional repeating group.

Example:



2. Variables for carbon chains, AK, CHK, CHE and CHY may not be used within drawn carbon chains

If the variable for any carbon chain, AK, or the Derwent generic nodes for carbon chains, CHK, CHE or CHY are used within drawn carbon chains, no results are found in structure searches.

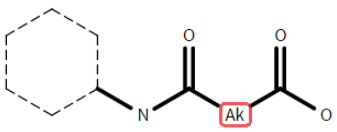
Please consider this also when you use the affected variables as an R-group or as a repeating group.

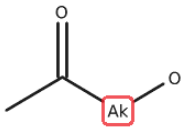
However, variables for carbon chains work without problems in terminal positions.

Affected variables:

AK	Any carbon chain
Derwent generic nodes	
CHK	Alkyl
CHE	Alkenyl
CHY	Alkynyl

Examples:



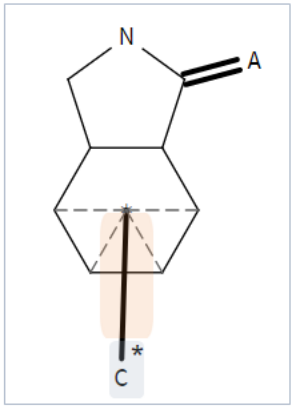


Workarounds need to be developed individually. One possibility is the replacement of the variables by drawn carbon groups with suitable attributes and, if necessary, repetitions of these groups.

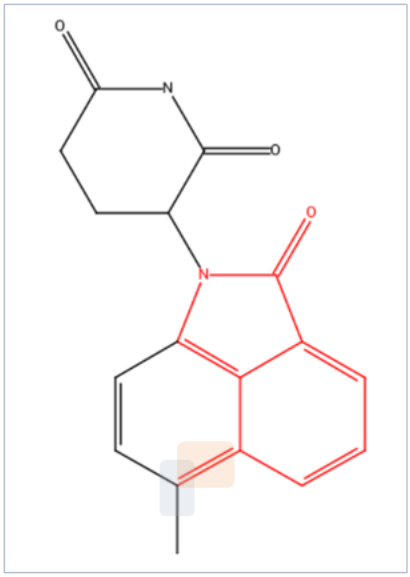
3.Bond attribute ignored for groups with node type ring bound via variable attachment points (VPA)

If a group with node type ring is attached to a ring via VPA, the VPA bond, which has bond type chain by default, is misinterpreted as bond type ring/chain. As a consequence, additional records with condensed ring systems are retrieved.

Example:



Node type: Ring
VAP bond type: Chain



Condensed rings

Workarounds need to be developed individually. The use of the Look Ring Fusion tool can be an option but needs to be considered carefully. Otherwise relevant structures may be missed.

4. Attribute non-hydrogen count is ignored for variables

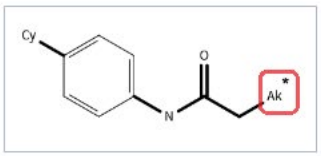
When the attribute non-hydrogen count is applied to variables this limitation is ignored when the structure is searched.

For example, if non-hydrogen count 1 is assigned to a variable to prevent substitution at the generic group, the search will return too many hits. Since the restriction is ignored, substituted substances are found in addition to the desired ones.

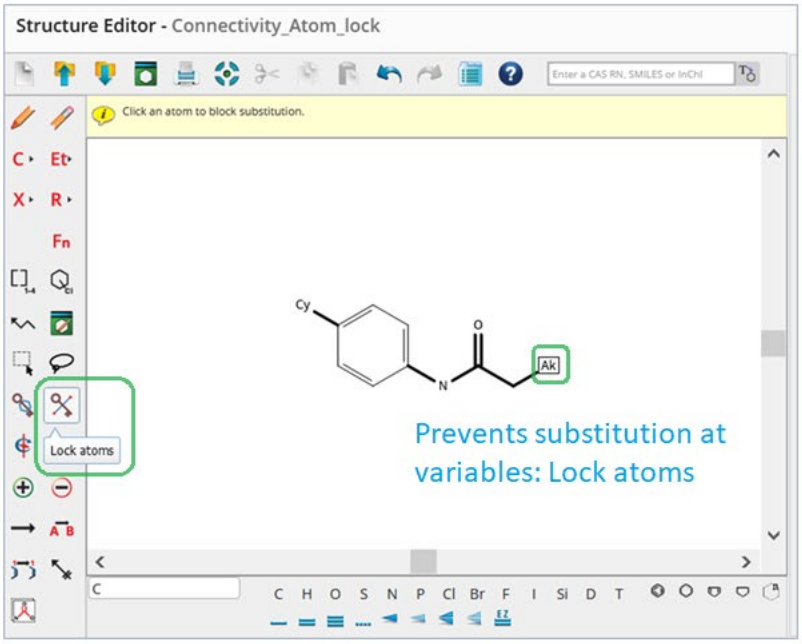
This affects all variables and Derwent generic nodes.

To completely prevent substitution on variables, the Lock Atoms option can be used as an alternative.

Example:



Ignored in structure searches:
Non-hydrogen count



5. Usage of generic ring and chain nodes via variable attachment points (VPA) can lead to incorrect results

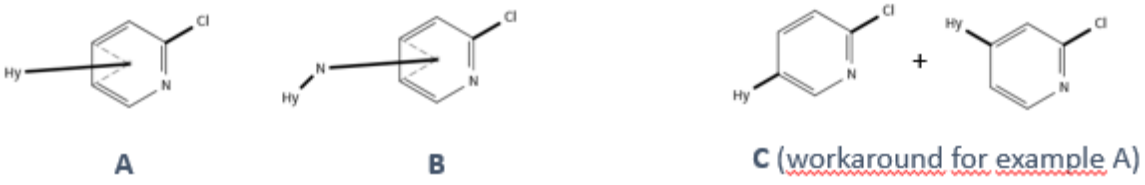
The problem only applies to directly VPA connected generic ring or chain nodes (example A). If there is at least one atom in the VPA between the generic ring or chain node and the main molecule, the problem does not exist (example B).

The following nodes are affected:

- Cy, Cb, Hy, CYC, ARY, HEA, HET, HEF
- Ak, CHK, CHE, CHK

The only practicable workaround for this issue is to use the respective individual structures encoded in the VPA query (example C).

Examples:



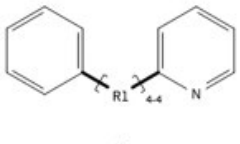
6.R-groups within repeating groups may lead to incomplete results

The variants within R groups within repeating groups do not provide mixed results but only results of one of the occurring variants.

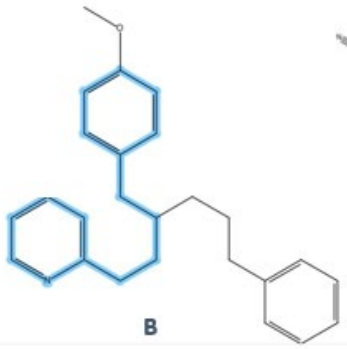
Examples:

Query structure A with R1=C,O does only yield results with either C‘s (example B) or O‘s but not mixed results (example C).

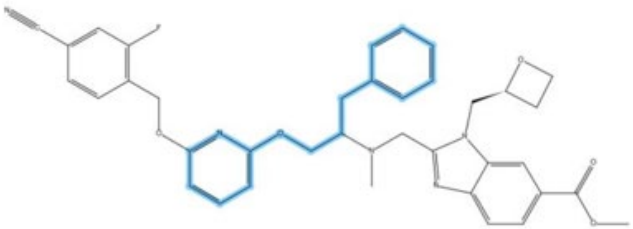
The only practicable workaround is to search for structures with mixed variants separately as individual structures.



A



B



C

Solution images are included for illustrative purposes only. Your experience may vary based on recent enhancements or product license.

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