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Overview on current issues in REAXYSFILESUB

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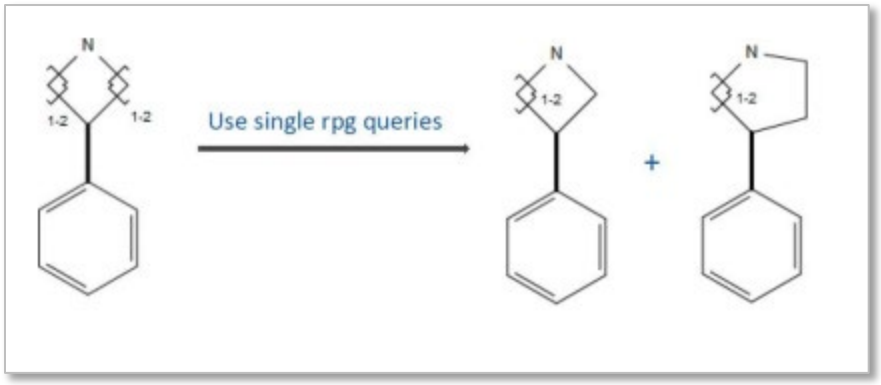
This document summarizes all known issues that can affect the results of structure searches in the REAXYSFILESUB database as of June 2025. If you need support concerning your structure query or regarding ReaxysfileSub in general, please contact EMEAhelp@cas.org.

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

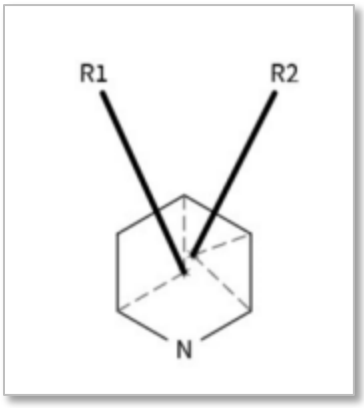
In case of two or more repeating groups within the same ring incorrect results are obtained. There is no workaround other than drawing out all possible combinations for every additional repeating group.

Example:



Only one variable point of attachment (vpa) per ring is allowed

Currently not recommended is, e.g., the following structure query:



Not all possible combinations are retrieved

Stereo search is not working correctly

To ensure completeness of searches it is recommended to use “flat” structures.

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

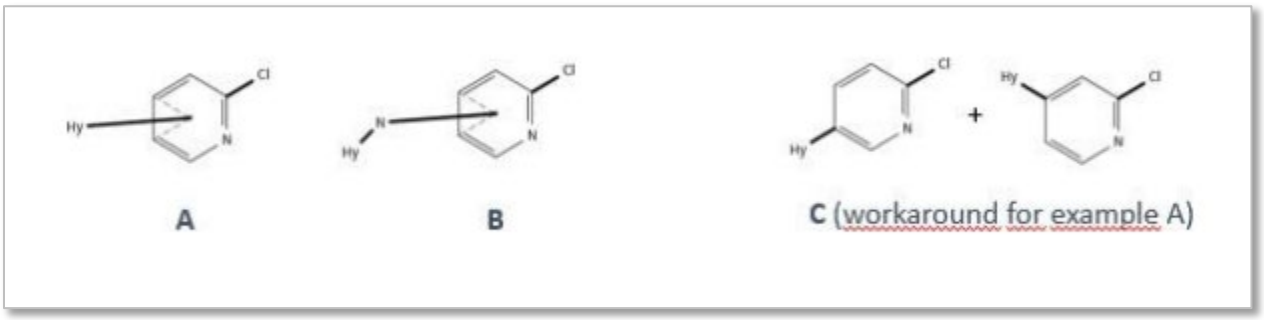
The problem only applies to directly VPA connected generic ring or chain nodes (example A). If there is at least one atom in the VPA between the generic ring or chain node and the main molecule, the problem does not exist (example B).

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).

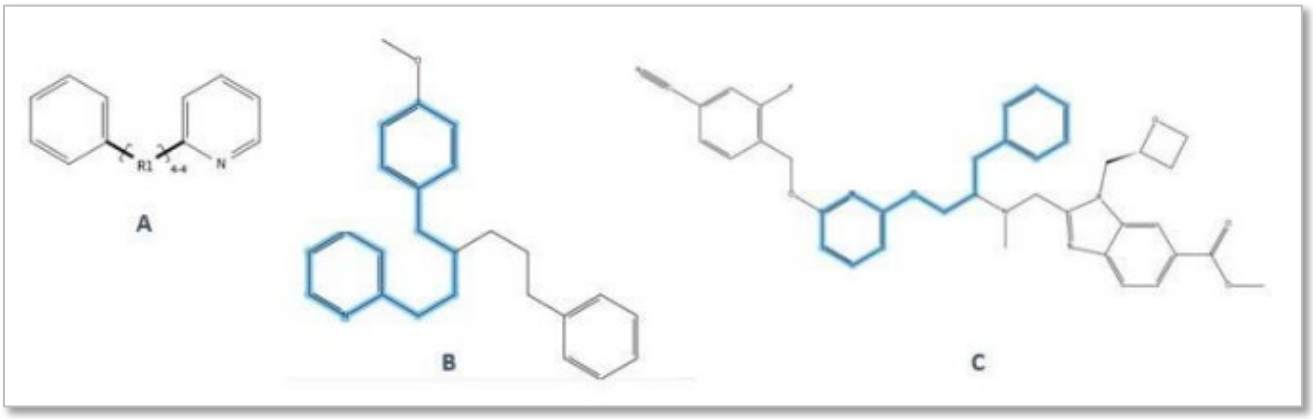
Examples:



R-groups within repeating groups may led 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 (above) with R1=C,O only yields 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.

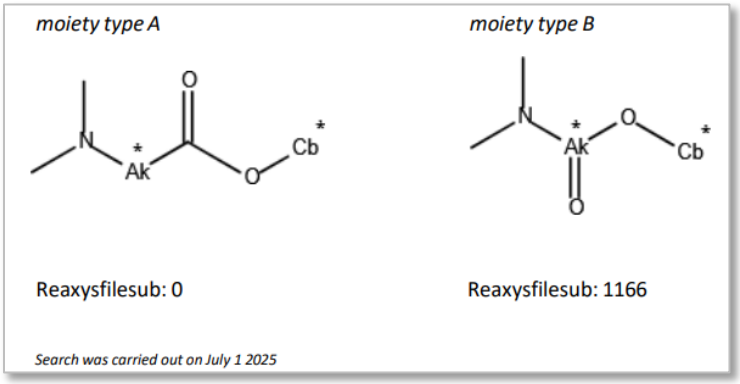
Avoid “Ak-C” moiety in structure searches

Query structures which contain an Ak carbon chain node adjacent to a specific carbon (both moieties optionally substituted) may lead to incorrect results.

Instead, only the Ak node alone should be used.

Example: SSS fullsearch

- Incorrect results for moiety type A
- Correct results for moiety type B



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