

RELEASE NOTES:

Functionality Enhancements to DWPIM

Summary:

Search and retrieval quality of the Derwent Markush Resource (DWPIM) database has been improved by fixing several major issues from the field of closed substructure search, repeating groups, matching of A, Q and XX node, ring lock function, searching hybrid ring systems.

Details:

- Ring and chain expansion allows matching to extended fragments:
 - Chain nodes have at least 1 free site and can therefore match to other chain nodes:
 - CHK → CHE
 - CHE → CHY
 - Ring nodes have at least 2 free sites and can therefore match to other ring nodes:
 - Cb → HEF
 - CYC → ARY, HEF
 - HET → HEF
 - HEA → HEF
 - ARY → HEF
 - The ring expansion can be prevented by assigning the attributes „mono“ and „ring lock“.
- Some issues from the DWPIM manual (Oct 2018) listed under “Warning” have been resolved:
 - Limitations 1) – 3) from chapter 3.5.2
 - Repeating Groups in combination with ring lock function correctly
 - Repeating Groups starting with 0 (e.g. [0-3]) function correctly
 - Repeating Groups without upper or lower limit (e.g. [2-] or [-2]) function correctly
 - Limitations 1) and 3) from chapter 4.1.
 - Derwent Superatom XX can now be used in queries.
 - Superatom Dye can be used for queries.
 - Search for Hybrid Rings Containing the Superatom XX (chapter 8.2)
 - The match level combination of Any and Atom in rings can now be used in query structures.
Note: XX is the only Superatom which is allowed (i.e. indexed) in rings.
 - The closed substructure search (CSS) functions properly. In the previous version CSS delivered non-H substituted hits in some instances.
- Issues pertaining ring locked structures have been resolved.
- Atom to Atom matches with A- and Q- node are now available.