



Recently reported issues concerning the Derwent Markush Resource (DWPIIM) on STNNext[®]

Status as of December 10, 2019

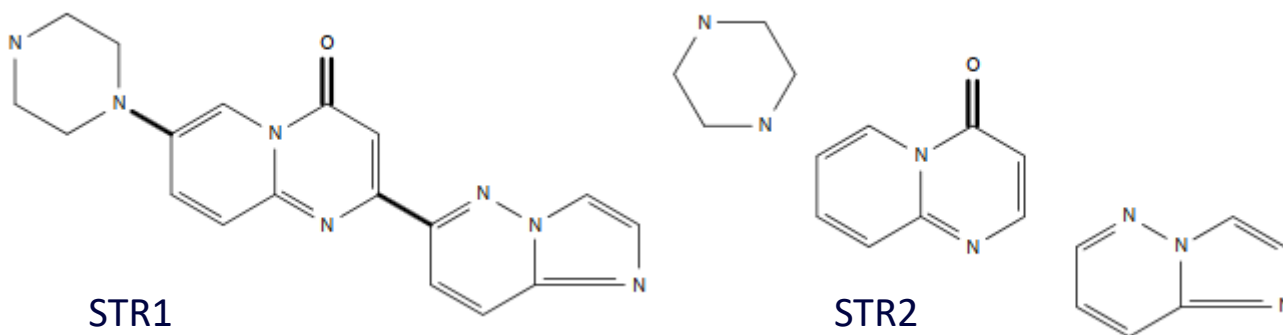
We are currently working on these issues and will inform you as soon as they are solved.

If you need support concerning your structure query or regarding DWPI in general, please contact our helpdesk@fiz-karlsruhe.de.

1. Query Structures containing several Fragments do not work correctly

Hit records may be missed due to a matching problem.

Example: STR2 does not include all hits retrieved with STR1



➔ Make sure to use only a single query structure in the editor

2. STNext: Adjust bond value for Carboxylic acid derivates to exact/normalized (e/n)

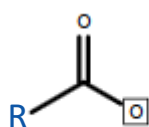
Carboxylic acid derivates as well as corresponding phosphoric, sulfonic and selenic acid derivates are defined with normalized bonds in the STNext structure editor (as shortcuts or drawn, see table below). In order to achieve correct matching in DWPIIM those bonds need to be set to exact/normalized. This can be done either by drawing a respective group with locked heteroatom (bonds are automatically set to e/n in the editor) or by changing the normalized bonds of the Hydrogen containing group manually.

The bond value of the shortcuts cannot be changed and therefore those shortcuts should not be used at all!

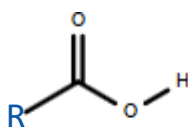
The following groups are affected:

-COOH	-OPO3H2	-SO3H	-SeO3H
-CO2H	-OSO3H	-SO2H	-SeO2H
-COSH	-PO3H2		
-CSSH	-PO2H		
-CS2H			

How to draw those groups correctly:



e/n (default)

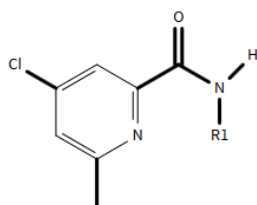


Switch from n (default) to e/n

3. Differences between STNext and new STN for DWPIIM

In STNext a drawn Hydrogen is substituted by the corresponding H-count. If a query structure contains both, an H within an R-group as well as a drawn H, matching takes place with an H in the R-group. Consequently a “free site” is generated which could be substituted with a substituent not present in the query structure. Therefore the answer set on STNext might include false positives.

Example:



R1: H, SO₂, Hy

Results (for SSS)
STNext: 3302
nSTN: 2443

False positive Hit on STNext (CHK substituent)

