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Molecular Networks Announces the Release of Version 1.8 of MN.TAUTOMER

MN.TAUTOMER is Molecular Networks' fast and automatic, rule-based enumerator of tautomeric states of a chemical compound. The rules encoded automatically detect substructures in a given input structure that can undergo a tautomeric transformation. Currently, **MN.TAUTOMER** supports 17 of the most important types of tautomerism.

A brief summary of all major new features and improvements of **MN.TAUTOMER** version 1.8 are given in the following. Further details can be found in the program manual of **MN.TAUTOMER** that is downloadable from Molecular Networks' web server at www.molecular-networks.com/software/tautomer/mn_tautomer_manual.pdf.

Test copies can be downloaded from the Download Area at Molecular Networks' web server at www.molecular-networks.com/php/profile.php.

New Features and Improvements of MN.TAUTOMER Version 1.8

- (1) The new option `-nprefmax N` (N of type integer) internally generates all possible tautomers of an input structure and ranks them by applying the empirical scoring function (see program manual, section 1.3). Finally, only the N top ranked (most probable) tautomers are written out, i.e., each input structure is represented by a maximum number of N tautomers.
- (2) The new option `-percentprefmax F` (F of type float and in percentage, %) internally generates all possible tautomers of an input structure and ranks them by applying the empirical scoring function (see program manual, section 1.3). Finally, only the top ranked (most probable) tautomers are written out until the given threshold of $F\%$, whereas the unique tautomer is set to 100%. I.e., only those tautomers are written out that have a score of $\geq F\%$ compared to the unique tautomer.
Note. In contrast to the option `-nprefmax` (see above), the number of output tautomers may strongly vary for different input structures.
- (3) The new option `-typeN` (N of type integer) allows to apply only the specific tautomeric transformation rule N to the input structure and suppresses application of other transformation rules. Therefore, this option can be regarded as the opposite of the option `-notypeN` (see program manual, section 4.3). The application of more than one transformation rules can be forced by defining this option at the command line more than once.
- (4) A list of supported tautomeric transformation rules and their respective numbers N can be printed on the screen with the option `-types`.
- (5) The new option `-skiperrors` skips molecules (records) in a multi-record file which show some deficiencies or errors in the formatting or structure coding and continues processing the very next record without aborting the program run.