Batch tautomer generation and more with MolTPC

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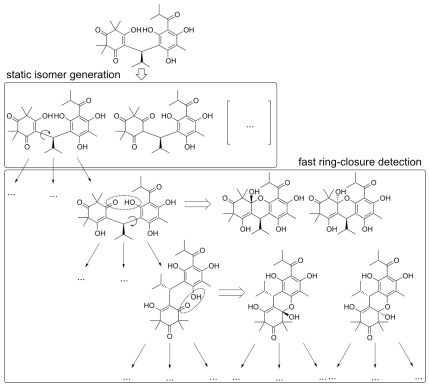
Besides all their conformational degrees of freedom, drug-like molecules and natural products often also undergo tautomeric interconversions. Compared to the huge efforts made in experimental investigation of tautomerism, open and free algorithmic solutions for prototropic tautomer generation are surprisingly rare. The few freely available software packages limit their output to a subset of the possible configurational space by sometimes unwanted prior assumptions and complete neglection of ring-chain tautomerism.

We described an adjustable fully automatic tautomer enumeration approach, which is freely available and also incorporates the detection of ring-chain variants. [1]

Furthermore, we provide functionality for the generation of reasonable protonation variants and a fast unified conformational as well as configurational search procedure.

All algorithms are implemented in the MolTPC framework and accessible on SourceForge via https://sourceforge.net/projects/moltpc/.



[1] Will, T., Hutter, M., Jauch, J., and Helms, V., *J. Comp. Chem.*, **2013**, *Vol. 34*, p. 2485-2492.