Subject: Re: Suggestion: tautomer-check
Posted by thomas on Mon, 11 May 2020 18:59:48 GMT
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This is, of course, and important issue. Having the right tautomer to start with is crucial for any reliable prediction.
The intention behind the work on the published tautomer database is to allow others and ourselves to work on algorithms
to predict the most prominent tautomer. If we had such an algorithm with a reasonable performance at hand, we could use
it as input before training any prediction model. It also would allow to normalize pKa databases to improve or develop
algorithms to more reliably predict pKa-values, which is also in big demand. We have it in the pipeline, but it will
take time...