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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, an 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...

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