

# **Tautomerism: Methods And Theories**

**Theoretical Study of Molecular Structure, -**

Theoretical Study of Molecular Structure, Tautomerism, and Geometrical Isomerism of Moxonidine: Two-Layered ONIOM Calculations

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<http://www.sciencedirect.com/science/article/pii/S0166128003005463>

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Methods for tautomer enumeration, -searching and -duplicate filtering J zsef Szegezdi, Zsolt Mohcsi, Tamás Csizmazia, Szilárd Dörntös, Papp György Pirok,

[http://www.chemaxon.com/app/uploads/2010/07/Methods\\_for\\_tautomer Enumeration\\_searching\\_and-duplicate\\_filtering-Szabolcs\\_Csepregi-ChemAxon.pdf](http://www.chemaxon.com/app/uploads/2010/07/Methods_for_tautomer Enumeration_searching_and-duplicate_filtering-Szabolcs_Csepregi-ChemAxon.pdf)

### **7 Tautomer-Selective Spectroscopy of Nucleobases, -**

Tautomerism: Methods and Theories, First Edition. Edited by Liudmil Antonov. 1967 Tautomer-Selective Spectroscopy of Nucleobases, Isolated in the Gas Phase

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Theories used include B3LYP density functional (CBS) methods. Tautomerism and pK<sub>a</sub> behaviour of 1-hydroxypyrazoloquinolines and pyrazoloisoquinolines (2001) <http://citeseerx.ist.psu.edu/viewdoc/summary?doi=10.1.1.22.4058>

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