

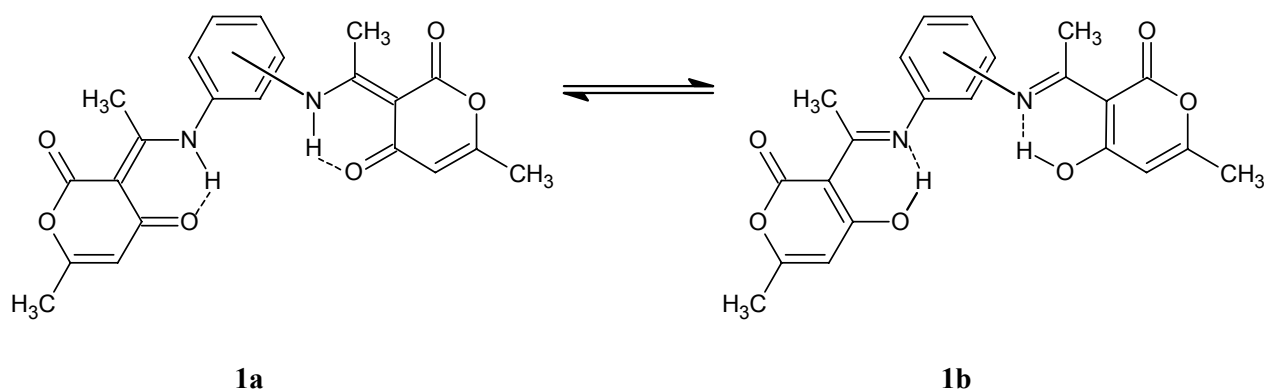
## Hydrogen Bonding and Deuterium Isotope Effects in $^{13}\text{C}$ NMR Spectra of Phenylene Enaminones Derived from Dehydracetic Acid

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Enaminones have been recently a subject of comprehensive studies due to their wide applications in organic synthesis [1] and coordination chemistry, as well as their potential pharmacological importance. Studies have shown that enaminone derivatives possess anti-inflammatory, anticonvulsant, antimalarial and cardiovascular activities.

Hydrogen bonds are an important structure and reactivity factor, and also a bioactivity modulator. The aim of this work is to investigate the intra- and intermolecular hydrogen bonding structure in solution of enaminones derived from dehydracetic acid by employing NMR and DFT methods. X-ray structural analysis has confirmed the existence of the keto-amine form (**1a**) in the solid state, stabilized by formation of intramolecular H-bonds [2]. However, the fundamental question is whether the nature of the intramolecular H-bond  $\text{N}-\text{H}\cdots\text{O}$  and the proton transfer (Fig. 1) will be affected by solvents of different proton donor and acceptor abilities and the substitution pattern (*ortho*, *meta*, *para*) of enaminone isomers. In order to get further insight into these interactions secondary deuterium isotope effects on  $^{13}\text{C}$  chemical shifts have been measured and analyzed.



**Fig. 1:** Tautomerism in phenylene enaminones derived from dehydracetic acid (1a = keto-amine form, 1b = hydroxy-imine form).

[1] A.Z.A. Elassar, A.A. El-Khair, Tetrahedron 59 (2003) 8463-8480.

[2] M. Cindrić, T. Kajfež Novak, K. Užarević, J. Mol. Struct. 750 (2005) 135-141.