

# Seminario de Química Orgánica

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Aula de Seminario - Departamento de Química Orgánica

“Tautomerism and Hydrogen Bonding in 1,3-Diketones -  
Insights from Solid-State NMR Spectroscopy”

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“Our research has focused on  $^1\text{H}$ ,  $^{13}\text{C}$  and  $^{17}\text{O}$  NMR studies of several 1,3-diketones that exist as the enol tautomer in the solid state (e.g., dibenzoylmethane). The enol tautomer of these compounds are stabilized by intramolecular O--H--O hydrogen bonds, many of which are classified as low-barrier hydrogen bonds (i.e., O -- O separations less than  $\approx 2.5 \text{ \AA}$ ). We have carried out systematic one- and two-dimensional NMR experiments of dibenzoylmethane and curcumin, both of which are examples of molecules that have LBHBs. Some interesting two-bond deuterium isotope effects on the  $^{13}\text{C}$  chemical shifts in the enol tautomer of 1,3-diketones will be presented. As well, recent results illustrating the value of solid-state NMR in characterizing two polymorphs of curcumin will be discussed (e.g., see: M.A. Matlinska, R.E. Wasylishen, G.M. Bernard, V.V. Terskikh, A. Brinkmann and V.K. Michaelis, *Crystal Growth & Design*, **2018**, DOI: 10.1021/acs.cgd.8b00859). Our experimental data are supplemented by plane-wave density functional theory (DFT) computations”.