

### List of most relevant publications

M. Alcolea Palafox. "Structure and conformational analysis of the anti-HIV reverse transcriptase Inhibitor AZT using MP2 and DFT methods. Differences with the natural nucleoside thymidine. Simulation of the 1<sup>st</sup> phosphorylation step with ATP" *Physical Chemistry Chemical Physics*, **16**, 24763-24783 (2014) DOI: 10.1039/c4cp03695f

M. Alcolea Palafox, S. K. Rathor, Rachna Rastogi, Daisy Bhat, V. Bena Jothy, V.K. Rastogi. "Vibrational Spectroscopy: A tool for characterization of nucleic acid constituents: Cytosine and Uracil" *Asian J. of Physics*, **24** (1), 33-59 (2015)

M. Alcolea Palafox, V.K. Rastogi. "The biomolecule of 5-chlorocytosine: Geometry of the six main tautomers in the isolated state by DFT calculations, and interpretation of the FT-IR and FT-Raman spectra in the solid state". *Asian Chemistry Letters*, **19** (1), 1-25 (2015)

M Alcolea Palafox, Daisy Bhat, S. Khanna, S.P. Yawale, V. Bena Jothy, and V.K. Rastogi. "FTIR and FT-Raman spectra, ab initio and density functional computations of the vibrational spectra, molecular geometry, and some molecular properties of biomolecule: 5-Fluorocytosine". *National Conference on Role of Optics and Philosophy in Environment Protection, ROPEP-2015*, pp. 37 Tinsukia (India) 10-11 Marzo (2015)

Anupma, M. Alcolea Palafox, D. Bhat, M. Jane Alam, J.K. Vats, R.S. Gupta, and V.K. Rastogi. "FTIR and FT-Raman spectra, ab initio and density functional computations of the vibrational spectra, molecular geometry, and some molecular properties of 2-chloro-3-methylbenzotrile". *National Conference on Role of Optics and Philosophy in Environment Protection, ROPEP-2015*, pp. 38-39, Tinsukia (India) 10-11 Marzo (2015)