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Computational NMR, IR/RAMAN calculations in sodium pravastatin: Investigation of the Self-Assembled Nanostructure of Pravastatin-LDH (Layered Double Hydroxides) Systems[1] PHILIPPE PETERSEN, VANESSA CUNHA, MARCOS GONÇALVES, HELENA PETRILLI, VERA CONSTANTINO, Universidade de Sao Paulo, INSTITUTO DE FíSICA, DEPARTAMENTO DE FíSICA DE MATERIAIS E MECÂNICA TEAM, INSTITUTO DE QUíMICA, DEPARTAMENTO DE QUíMICA FUNDAMENTAL TEAM — Layered double hydroxides (LDH) can be used as nanocontainers for immobilization of Pravastatin, in order to obtain suitable drug carriers. The material's structure and spectroscopic properties were analyzed by NMR, IR/RAMAN and supported by theoretical calculations. Density Functional Theory (DFT) calculations were performed using the Gaussian03 package [1]. The geometry optimizations were performed considering the single crystal X-ray diffraction data of tert-octylamonium salt of Pravastatin [2]. Tetramethylsilane (TMS), obtained with the same basis set, was used as reference for calculating the chemical shift of 13C. A scaling factor was used to compare theoretical and experimental harmonic vibrational frequencies. Through the NMR and IR/RAMAN spectra, we were able to make precise assignments of the NMR and IR/RAMAN of Sodium Pravastatin.

[1] Frisch, M.J. et al. Gaussian 03, Revision A.1, Gaussian Inc., Pittsburgh, PA,(2003).
[2] Sato, S.; Furukawa, Y. J. Antibiot. 41, 1265-1267 (1988).

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