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Density Functional Study of the structural properties in Tamoxifen[1] ROMEO DE COSS-MARTINEZ, JORGE A. TAPIA, Facultad de Ingenieria, Universidad Autonoma de Yucatan, RAMIRO F. QUIJANO-QUIÑONES, Laboratorio de Quimica Farmaceutica, Facultad de Quimica, Universidad Autonoma de Yucatan, GABRIEL I. CANTO, Centro de Investigacion en Corrosion, Universidad Autonoma de Campeche — Using the density functional theory, we have studied the structural properties of Tamoxifen. The calculations were performed with two methodological approaches, which were implemented in SIESTA and Spartan codes. For SIESTA, we considerate a linear combination of atomic orbitals method, using pseudopotentials and the van der Waals approximation for the exchange-correlation potential. Here we analyzed and compared the atomic structure between our results and other theoretical study. We found differences in the bond lengths between the results, that could be attributed to code approaches in each one.

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Romeo de Coss-Martinez
Facultad de Ingenieria, Universidad Autonoma de Yucatan

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