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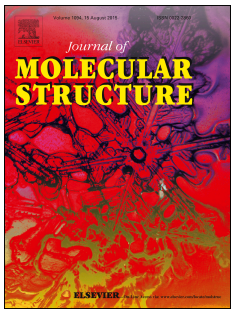

A combined experimental and *in silico* characterization to highlight additional structural features and properties of a potentially new drug

Isadora T.S. Bastos, Fanny N. Costa, Tiago F. Silva, Eliezer J. Barreiro, Lídia M. Lima, Delson Braz, Giuseppe M. Lombardo, Francesco Punzo, Fabio F. Ferreira, Regina C. Barroso

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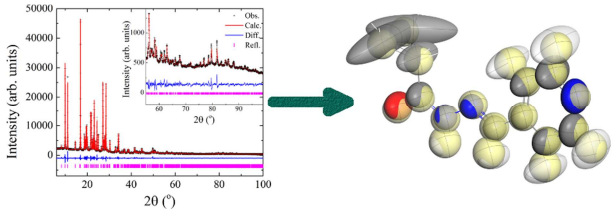

Inference of anisotropic atomic displacement parameters by integrating X-ray powder diffraction data and a molecular dynamics calculation.