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CRYSTAL STRUCTURE DETERMINATION OF A N-ACYLHYDRAZONE DERIVATIVE: LASSBIO-1733

Costa, F.N.[1],*; Silva, T.F.[2]; Sato, J.A.P.[1]; Barroso, R.C.[3]; Braz, D.[4]; Lima, L.M.[2]; Barreiro, E.J.[2] and Ferreira, F.F.[1]

[1]*Center of Natural and Human Sciences, Federal University of ABC, Santo André, SP, Brazil*

[2]*LASSBio, Institute of Biomedical Sciences, Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil.*

[3]*Physics Institute, State University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil.*

[4]*Program of Nuclear Engineering, Federal University of Rio de Janeiro, Rio de Janeiro, RJ, Brazil.*

**** fanny.costa@ufabc.edu.br***

The methodology of structure determination from X-ray diffraction data has been employed as a tool able to define the configurational and conformational aspects of the new bioactive compounds, which are directly related to the biological activity. In this work, X-ray powder diffraction (XRPD) was used to carry out the crystal structure determination of LASSBio-1733, which was initially obtained as part of a project of synthesis of novel anti-inflammatory and analgesic leads with a *N*-acylhydrazone scaffold. The measurements were performed at room temperature on a Stoe STADI-P powder diffractometer in transmission geometry by using a CuKα_1 (λ = 1.54056 Å) wavelength. LASSBio-1733 crystallizes in an orthorhombic crystal system, space group $P2_12_12_1$, with unit-cell dimensions a = 25.2049(13) Å, b = 10.2952(6) Å, c = 5.2333(3) Å, $\alpha = \beta = \gamma = 90$ °, V = 1357.99(13) Å^3. The structure was energy-minimised with dispersion-corrected density functional theory (DFT-D).[1] Additionally, other experimental techniques were employed in characterization of this compound.

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[1] Streek, J. v. d. & Neumann, M. A. (2010). *Acta Crystallogr. B* **66**, 544-558.