

Synthesis, characterization, spectroscopic properties and DFT study of a new pyridazinone family

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Nitrogen compounds are widely investigated due to their pharmacological properties such as antihypertensive, antinociceptive, antibacterial, antifungal, analgesic, anticancer and inhibition activities and lately even as pesticide. In this context, we present the synthesis of new compounds: (E)-6-(3,4-dimethoxyphenyl)-3-(3-(3,4-dimethoxyphenyl)acryloyl)-1-(4-R-phenyl)-5,6-dihydropyridazin-4(1H)-one (with R = [sbnd]H(1), -Cl(2), -Br(3), [sbnd]I(4) and [sbnd]COOH(5)) that was carried out by reaction of (1E, 6E)-1,7-bis(3,4-dimethoxyphenyl)hepta-1,6-diene-3,5-dione with a substituted phenylamine with general formula p-R-C₆H₄[sbnd]NH₂ (R = [sbnd]H (1), [sbnd]Cl (2), -Br(3), [sbnd]I(4) and [sbnd]COOH(5)). This is the first synthesis report of a pyridazinone using as precursors a curcuminoid derivative and a diazonium salt formed in situ. All compounds were characterized by EA, FT-IR, UV-Vis, Emission, ¹H- and ¹³C-NMR spectroscopy and the crystalline and molecular structure of 4 was solved by X-rays diffraction method. DFT and TD-DFT quantum chemical calculations were also employed to characterize the compounds and provide a rational explanation to the spectroscopic properties. To assess the biological activity of the systems, we focused on pesticide tests on compound 2, which showed an inhibitory effect in plant growth of *Agrostis tenuis* Higland. © 2017 Elsevier B.V.

Characterization

DFT

Pyridazinone

Synthesis

Bioactivity

Characterization

Chemical compounds

Chlorine compounds

Nitrogen compounds

Nuclear magnetic resonance spectroscopy

Pesticides

Quantum chemistry

Synthesis (chemical)

X ray diffraction

¹³C NMR spectroscopy

Inhibition activity

Pharmacological properties

Pyridazinone

Quantum chemical calculations

Spectroscopic property

Synthesis of new compound

X-rays diffraction

Bromine compounds