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## Title

### ***Synthesis and theoretical study of a new family of pyrazole derivative***

## Abstract

Pyrazole-containing molecules are key in the development of new pharmaceuticals or pesticides. Thus, we synthesize a new series of pyrazole derivatives using the cycloaddition methods. The synthesized compounds present a (E)-4-((4-iodophenyl)diazanyl)-3,5-dimethyl-1-(R-phenyl)-1H-pyrazole structure. The compounds were characterized by UV-vis, FTIR, <sup>1</sup>H-NMR, and <sup>13</sup>C-NMR. Also, DFT and Hammett correlation calculations were performed over the whole family of derivatives. Our results demonstrate that the synthesized compound was obtained with an overall yield of 50 %. UV/Vis spectroscopic characterization shows that all compounds present three absorption bands related to the pyrazole ring, the -N=N- bond and benzene rings. Additionally, theoretical calculation shows that the dihedral angle decreases when the electron-attractive nature of the substituent of the pyrazole ring increases. Finally, Hammett correlation studied shows a good fit in some of the measured properties. © 2023 Elsevier B.V.

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