A novel series of pyrazole derivatives toward biological applications: experimental and conceptual DFT characterization

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Abstract

Abstract: A new series of 13 pyrazole-derivative compounds with potential antifungal activity were synthetized with good yields. The series have the (E)-2-((1-(R)-3,5-dimethyl-1H-pyrazol-4-yl)diazenyl)phenol general structure and were characterized by means of X-ray diffraction, UV–Vis, FTIR, ^{1}H-NMR, ^{13}C-NMR, and two-dimensional NMR experiments. This experimental characterization was complemented by DFT simulations. A deep insight regarding molecular reactivity was accomplished employing a conceptual DFT approach. In this sense, dual descriptors were calculated at HF and DFT level of theory and GGV spin-density Fukui functions. The main reactive region within the molecules was mapped through isosurface and condensed representations. Finally, chemical descriptors that have previously shown to be close related to biological activity were compared within the series. Thus, higher values of chemical potential ω and electrophilicity χ obtained for compounds 10, 9, 8, 6 and 7, in this order, suggest that these molecules are the better candidates as biological agents. Graphic abstract: [Figure not available: see fulltext.]

Author keywords

DFT; Pyrazoles library of new compounds; Synthesis of new compounds; TDDFT