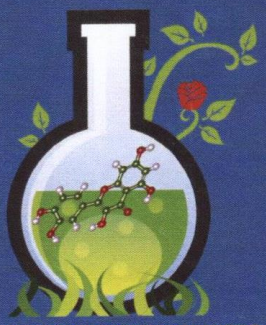


BIO-ANTIOXIDANTS
2018

2nd International Conference on Bio-antioxidants

2nd Young Scientists School on Bio-antioxidants

BOOK OF ABSTRACTS

07—10 September 2018
Varna, Bulgaria

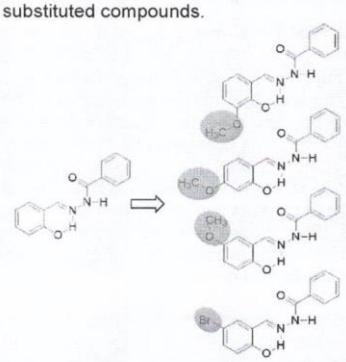
www.bio-antioxidants2018.com

F-PP29. SELECTED AROYLHYDRAZONES AS POTENTIAL FREE RADICAL SCAVENGERS: A DFT STUDY

Neda O. ANASTASSOVA,[a] Denitsa Y. YANCHEVA,[a] Boryana I. NIKOLOVA-MLADENOVA,[b] Vera A. HADJIMITOVA,[c] Nadya G. HRISTOVA-AVAKUMOVA,[c] Silvia E. ANGELOVA[a]

[a] Institute of Organic Chemistry with Centre of Phytochemistry, Bulgarian Academy of Sciences, 1113 Sofia, BULGARIA
[b] Department of Chemistry, Faculty of Pharmacy, Medical University of Sofia, Sofia, BULGARIA
[c] Department of Medical Physics and Biophysics, Faculty of Medicine, Medical University of Sofia, BULGARIA

Hydrazones derived by condensation of salicylaldehyde and acid hydrazides (aroylhydrazones) constitute a wide class of biologically active molecules. Aroylhydrazones are tridentate iron chelators that possess antioxidant and/or antineoplastic activities.[1,2] A hydrogen atom abstraction (Hydrogen Atom Transfer, HAT) from the hydroxyl and amide groups in their molecular structure is also possible. In polar medium, the aroylhydrazones could undergo ionization and the formed ionic species to be stabilized by the polar medium. Thus Single-Electron Transfer (SET) and Sequential Proton Loss-Electron Transfer (SPLET) mechanisms might became more favorable than the HAT mechanism. A set of selected aroylhydrazones is designed in order to study the structure – radical scavenging activity relationship for the parent and substituted compounds.



DFT calculations at B3LYP/6-31+G** level are carried out in order to identify the stable isomers and conformers of the studied aroylhydrazones in the gas phase and in water. A full geometry optimization of the corresponding radical and ionic species that can be generated from the studied compounds is performed at the same level of theory. The possible mechanisms for free-radicals scavenging are analyzed here by quantum chemical calculations and the results are compared with the available experimental data. The roles of the molecular geometry and of the substituents are rationalized. Identifying the exact mechanism and accurately evaluating the structure – radical scavenging activity relationship is of fundamental importance to understand antioxidant behavior and to assess the potential of these compounds.

Keywords: aroylhydrazones, free radical scavengers, DFT calculations

References

1. K. Hrušková, E. Potůčková, T. Hergeselová, L. Liptáková, P. Hašková, P. Mingas, P. Kovaříková, T. Šimůnek, K. Vávrová, *Eur. J. Med. Chem.* **2016**, *120*, 97-110.
2. D. R. Richardson, *Crit. Rev. Oncol. Hematol.* **2002**, *42(3)*, 267-281.