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BOOK OF ABSTRACTS

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C-YPP21. IN VITRO ASSESMENT OF ANTIOXIDANT ACTIVITY OF NEW BENZIMIDAZOLE-2-THIONE HYDRAZONE DERIVATIVES AND DFT STUDY OF THEIR MECHANISM OF ACTION

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Benzimidazole-2-thione derivatives containing hydrazone moieties designed as melatonin analogues were effective in inhibiting induced oxidative stress and acted as potent hepatoprotectors.^{1, 2} As a continuation from our previous work we have synthesized new derivatives of the benzimidazole-2-thione containing residues of vanillin, syringaldehyde and veratral.

For the estimation of the antioxidant potential of the tested compounds have been chosen two model systems containing stable free radicals (ABTS and DPPH) and one evaluating protection effect against ferrous iron induced oxidative damage of lecithin. The studied compounds demonstrated different extent of scavenging effect against both stable free radicals which could be attributed to their structural dissimilarity and to the different mechanism of radical neutralization (HAT for DPPH and SET for ABTS).

All compounds demonstrated capability to diminish the concentration of the ABTS radical. Comparison of the estimated using linear regression analysis C-50 values for the vanillin and syringaldehyde containing compounds denoted stronger activity than the reference Trolox at the same experimental conditions. The third compound containing veratral had weaker antiradical capacity against.

In the DPPH model system no statistically significant decrease of the absorbance of the samples containing veratral residue compared to the control ones was observed. Again we witnessed better antiradical effectiveness of the hydrazones with vanillin and syringaldehyde moiety compared to the Trolox.

All the tested compounds decreased ferrous iron induced oxidative molecular damage. For all the hydrazones the observed protection effect was in the same concentration range like the one of strong reference antioxidants as Trolox and Quercetin.

Different possible mechanisms such as hydrogen atom transfer (HAT), single-electron transfer (SET-PT), sequential proton loss electron transfer (SPLET) were studied by DFT computations of the respective reaction enthalpies in polar and nonpolar solvents. The reactivity against various free radicals was accounted by analyzing the thermodynamic data of reactions with hydroxyl, hydroxyperoxyl, alkoxyl and alkoxyperoxyl radicals.

Keywords: benzimidazoles, antioxidants, ABTS, DPPH, DFT

References

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