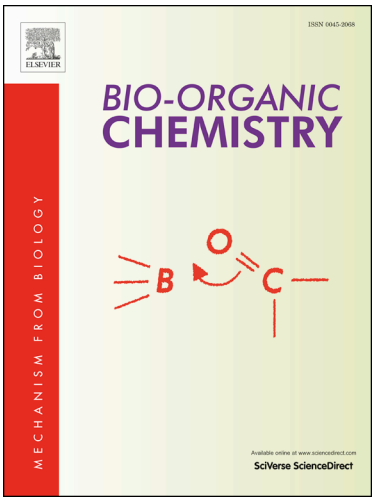

Inhibitory properties of aromatic thiosemicarbazones on mushroom tyrosinase: Synthesis, kinetic studies, molecular docking and effectiveness in melanogenesis inhibition

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Inhibitory properties of aromatic thiosemicarbazones on mushroom tyrosinase: Synthesis, kinetic studies, molecular docking and effectiveness in melanogenesis inhibition

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Abstract

The group of 19 thiosemicarbazones (TSCs) were synthesized and its inhibitory activity toward mushroom tyrosinase and ability to inhibition of melanogenesis in B16 cells were investigated. Moreover, molecular docking of these compounds to the active site of the enzyme was performed. The obtained results allowed to make the structure-activity relationship (SAR) analysis. Kinetic studies revealed that TSCs 1, 2, 11 and 18 have better inhibitory properties than kojic acid, a reference compound, with the best inhibitory constant (K_i) value of 0,38 µM for TSC 2. According to SAR analysis, the smaller and less branched molecules exhibit higher affinity to the enzyme. Melanin production in B16 cells was inhibited by all investigated compounds at micromolar level. Most of compounds studied in this work can be considered as potent inhibitors of tyrosinase and melanogenesis. They may have broad application in food preservatives and cosmetics. Combined results of molecular docking and SAR analysis can be helpful in designing novel tyrosinase inhibitors of desired properties.

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