

VALORISATION OF WALNUT SHELL AS A SOURCE OF BIOACTIVE DERIVATIVES: IN SILICO POLYPHENOL OXIDASE INHIBITION AND TOXICITY PREDICTION

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Waste valorisation has been identified as key component of global sustainability, UN sustainable development goals and the bioeconomy [1, 2]. In this context, walnut shell (WNS), an agro-waste which accounts for more than half of the total weight of the nut and potentially could be explored as a source of bioactive ingredients in food processing/packaging technologies. In this study, phenolic-rich methanolic extract was obtained from WNS via microwave assisted extraction [3] and its bioactivity was assessed. The antioxidant activity assays demonstrated that extract has IC₅₀ of 203.91 mg/mL, 102.48 mg/mL and 71.52 µg/mL, against ABTS•+, DPPH• and O₂•- radicals, respectively, as well as FRAP value of 629.33 µmol Fe (II)/g. In addition, the IC₅₀ of extract against mushroom tyrosinase was found to be 512.46 µg/mL. LC-MS and GC-MS analyses revealed a total of 53 phenolic and non-phenolic compounds in the WNS extract which were docked against mushroom tyrosinase. Molecular docking analysis indicated better binding interactions between the WNS compounds, chlorogenic acid (-9.3 kcal/mol), 3-O-p-coumaroylquinic acid (-9 kcal/mol), betulin (-8.9 kcal/mol) when compared to epigallocatechin gallate (-8.2 kcal/mol) and butylated hydroxytoluene (-6.5 kcal/mol), which are well known food preservatives. Furthermore, the WNS compounds evaluated were observed to be relatively non-toxic based on their predicted LD₅₀, pLC₅₀ and pIGC₅₀ values as well as their predicted pharmacokinetic properties. These results underscore the significance of WNS as a renewable bioresource for high-value applications, however, more work is required to demonstrate its potential within food related applications.

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[2] B. Segers et al. *RSC Sustain.* vol. 2, pp 3730-3749, (2024).
[3] A. A. B. Mokaizh, et al., *J. Ind. Eng. Chem.* vol. 142, pp. 321-328, (2025).