Green Electrochemical Nitration of Bioactive Compounds: Biological Evaluation with Molecular Modelling

Authors : Sara Torabi, Sadegh Khazalpour, Mahdi Jamshidi

Abstract : Nitro aromatic compounds are valuable materials because of their applications in the preparation of chemical intermediates for the synthesis of dyes, plastics, perfumes, energetic materials, and pharmaceuticals. Chemical and electrochemical procedures are reported for nitration of aromatic compounds. Flavonoid derivatives are present in many vegetables and fruits and are constituent of many common pharmaceuticals and dietary supplements. Electrochemistry provides very versatile means for the electrosynthesis, mechanistic and kinetic studies. To the best of our knowledge, and despite the importance of these compounds in numerous scientific fields, there are no reports on the electrochemical nitration of Quercetin derivatives. Herein, we describe a green electrochemical synthesis of a nitro compound. In this work, electrochemical oxidation of Quercetin has been studied in the presence of nitrite ion as a nucleophile in acetate buffer solution (c = 0.2 M, pH = 6.0), by means of cyclic voltammetry and controlled-potential coulometry. The results indicate the participation of produced o-benzoquinones in Michael reaction with nitrite ion (in the divided cell) to form the corresponding nitro diol (EC mechanism). The purity of product and characterization was done using ^{1}H NMR, ^{13}C NMR, FTIR spectroscopic techniques. The presented strategies use a water/ethanol mixture as solvent. Ethanol as cosolvent was also used in the previous studies because of its low cost, safety, easy availability, recyclability, bioproductability, and biodegradability. These strategies represent a one-pot and facile process for the synthesis of nitro compound in high yield and purity under green conditions.

Keywords : electrochemical synthesis, green chemistry, cyclic voltammetry, molecular docking
Conference Title : ICECE 2021 : International Conference on Electrochemical Cells and Electrochemistry
Conference Location : Bangkok, Thailand
Conference Dates : January 18-19, 2021