

# Utilizing Metal Chelating Flavonols as Metal Ion Filter and Hydroxyl Detector in Aqueous System

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## Abstract

Flavonols are the group of compounds with conjugated structure having at least one hydroxyl and one keto group on adjacent C on ring C of flavone within planner structure. This particular arrangement provides flavonols with excellent radical scavenging potencies metal chelating properties and DNA intercalating ability at the same time. Apart from determining the pharmaceutical benefits of flavonols, they can be explored for brilliant environmental applications such as ROS detectors and water purifiers. In the current study, we are exploring the typical pharmaceutical benefits for engineering selective electrochemical ROS detector and metal trapping filters for water purification. Three Hydroxy flavones (HF); 2'PHF, 3'PHF and 5HF were subjected to metal complexation (M-HF) with Mn and Ni followed by RSA and DNA binding analysis of bare flavonol (HFs) and their metal complexes (M-HFs). The antioxidant potencies of M-HF, Ni-HF and Mn-HF were described in terms of RSA (radical scavenging activity) against 1,1-diphenyl-2-picrylhydrazyl radicals (DPPH<sup>•</sup>), hydroxyl radicals (OH<sup>•</sup>), tetramethyl-piperidiny radicals (TEMPO<sup>•</sup>) and superoxide radicals (O<sub>2</sub><sup>•-</sup>). The quantity required to scavenge the 50% of radicals IC<sub>50</sub> were estimated from RSA vs concentration plots in physiological conditions. The computed ionization potential (IP) and ΔE<sub>HOMO</sub> were complementary with IC<sub>50</sub> trend. The comparative investigations indicated M-HF to be stronger scavenger then corresponding HF. So, metal complex were also used for OH<sup>•</sup> sensor fabrication. The flavonols (HF) and their metal complexes (M-HF) were deposited over APTES-FTO (3-aminopropyl triethoxy saline-fluorine doped TiO<sub>2</sub>) to fabricate (M-)HF-APTES-FTO electrode leading to stable sensor formation. This sensor responded to nano-molar concentrations of ROS through decrease in peak current. The anodic wave signal decayed upon incremental addition of OH<sup>•</sup> at a concentration as low as 5nM leading to good sensitivity towards OH<sup>•</sup> detection. The OH<sup>•</sup> brought significant current decay when compared with higher concentrations of other ROS suggesting reasonable sensitivity and selectivity of HF/M-HF-APTES-FTO for OH<sup>•</sup>

The DNA binding constant for HF, Mn-HF and Ni-HF were in the range of 10<sup>2</sup>-10<sup>4</sup> (M<sup>-1</sup>) with negative ΔG depicting stable and spontaneous DNA binding. The variation patterns of absorption spectra and voltammograms were explored to assign modes of binding such as intercalation, groove binding, electrostatic binding or mixed ones. The M-HF were found to be stronger DNA binders than respective HF which reveals that after metal chelation the DNA bound molecule will remain bound with it which can be utilized for engineering a DNA binding based filter for chelation of heavy metal ions from aqueous solutions. Three different assemblies were comparatively studied for their efficiency towards metal ion capture. There patterns of chelation and immobilization were tested for relative success towards ion capture which included (i) immobilization of DNA intercalated metal-flavonol, (ii) intercalation of M-HF on APTES pre-immobilized DNA (iii) chelating metal ion over pre-intercalated Flavonol over DNA-APTES matrix. The M-HF-DNA immobilization over APTES captured around 65% ions from solution. The M-HF have intercalated into DNA-APTES films up to 82%. However, M chelation over HF-DNA-APTES matrix was effective in ion capture from the solution phase up to 99%. Our results depicted that the DNA intercalation/interaction can be utilized to successfully remove hazardous ions from the solution up to safer limits.

**Keywords:** Radical Scavenger, Hydroxyl Radical Detection, Metal ion removal, DNA intercalator

## Short biography



Dr. Erum Jabeen is currently working as a Lecturer at Department of Chemistry, Allama Iqbal Open University, Islamabad Pakistan. She got her PhD with specialization in Physical Chemistry from Quaid-i-Azam University Islamabad Pakistan in 2017. She got her MPhil in physical chemistry (2012) and MSc in physical chemistry (2010) from Quaid-i-Azam University Pakistan. During her stay at Quaid-i-Azam University Islamabad, she won QAU merit scholarship 2008-2010, 1st position award 2010 and HEC indigenous scholarship 2012-2017. Currently her research focuses on biosensor fabrication for hydroxyl radical sensing, electrode modifications for electrochemical enzyme kinetic assays, electrochemical enantioseparation techniques, biomedical DNA biomarkers, adsorption of inorganic pollutants such as CO<sub>2</sub> and toxic metals such as As, Pb, organic pollutants such as phenols. She is also focusing on DNA binding and antioxidant investigations for versatile applications, electrochemical water treatment, photo-electrochemical oxidation and reactor/systems for waste water treatment. She has won "AIOU research publication grant 2020-2021" at Allama Iqbal Open University Islamabad Pakistan.