

# **Annexures**



# Spectroscopic overview of quercetin and its Cu(II) complex interaction with serum albumins

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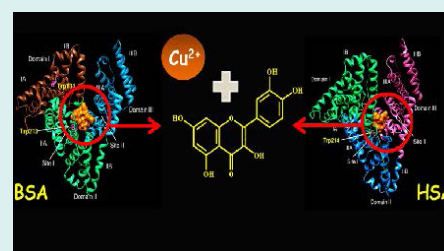
## Abstract

**Introduction:** Flavonoids are widely used as dietary supplements, and thus, play a significant role in the research field. In recent time, the interaction of flavonoid-metal complexes with serum albumin (SA) has widely been studied since the complexation poses a significant impact on biological activities. Additionally, the binding nature of flavonoids with SA gets modified in the presence of metal ions.

**Methods:** In the present review, we studied the interaction of quercetin (Qu), a well-known flavonoid, and its Cu<sup>2+</sup> complexes with SA to provide sufficient information about the beneficial role of metal-flavonoid complexes over free flavonoids.

**Results:** Complexation with Cu(II) ion may alter the mode of binding of Qu with SAs. The strength of binding might be increased in the presence of Cu(II) as evidenced by the binding constant calculation. However, the drug binding site in bovine serum albumin (BSA) and human serum albumin (HSA) are not altered during the complexation process.

**Conclusion:** To enhance the pharmaceutical outcomes of Qu molecules, one may use Qu-Cu(II) complex for the development and delivery of the small molecules.



## Introduction

Flavonoids, a subgroup of polyphenolic compounds, are generated in plants, common fruits, vegetables, tea, wine, etc. In recent decades, flavonoids have widely been used in many biological activities, including cardiovascular diseases, cancers or age-related disorders.<sup>1</sup> Due to the variety of activities, the impacts of flavonoids have widely been considered on various biological processes.<sup>2,3</sup> Further, flavonoids can form chelates with the metal ions, which may change their antioxidant activity and biological effects.<sup>4</sup>

Quercetin (Qu), as shown in Fig. 1, is one of the most common bioactive and dietary flavonoids, which can be found in the flowers, leaves, and fruits of many plants.<sup>5</sup> Qu can form complexes with transition metal ions, such as Cu<sup>2+</sup>, Mn<sup>2+</sup>, Fe<sup>2+</sup>, etc. Among them, the stability of Qu-Cu(II) complex is reported to be the highest.<sup>5</sup>

Cu(II) is one of the most abundant trace minerals in the human body. In the blood, it can often act as a

cofactor for angiogenesis.<sup>6</sup> In some recent researches, it has been established that naturally occurring polyphenols can prevent the emergence of angiogenesis. Further, the catalytic role of transition metal ions such as Fe(III) and Cu(II) is well-known in the formation of hydroxyl radical ( $\bullet$ OH) via metal-catalyzed Haber-Weiss reaction or Fenton reaction. Metal ion chelation by flavonoids is known to inhibit the aforementioned oxidative damage caused by metal ions. Also, the biological activities such as anti-oxidant effect, anti-bacterial and various kinds of enzymatic functions of free flavonoids get affected as a result of the complex formation.<sup>7,8</sup> Therefore, it is important to understand the effect of Cu(II) on the interactions between flavonoids and SAs. According to available literature, Qu-metal complexes seem to produce better biological activities than the bare Qu itself.<sup>8,9</sup>

In keeping with the above facts, in this review, we have studied the ultimate behavior of Qu and Qu-Cu(II) complex with SAs. SAs are the most abundant transport

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## Biophysical and theoretical studies of the interaction between a bioactive compound 3,5-dimethoxy-4-hydroxycinnamic acid with calf thymus DNA

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### ABSTRACT

3,5-Dimethoxy-4-hydroxycinnamic acid commonly known as Sinapic acid is a well-known derivative of hydroxycinnamic acids, is commonly present in human diet. Due to its wide variety of pharmacological activities like antioxidant, antimicrobial, anti-inflammatory, anticancer, and anti-anxiety, it has attracted much attention for the researchers. In our previous published work we have already analyzed the interaction between sinapic acid (SA) with a model transport protein. In this work our aim is to demonstrate a detailed investigation of the binding interaction between sinapic acid with another carrier of genetic information in a living cell, the DNA. Here we have used calf thymus DNA (ct-DNA) as a model. The binding characteristic of SA with ct-DNA was investigated by different spectroscopic and theoretical tools. The spectroscopic investigation revealed that quenching of intrinsic fluorescence of SA by ct-DNA occurs through dynamic quenching mechanism. The thermodynamic parameters established the involvement of hydrogen bonding and weak van der Waals forces in the interaction. Further, the circular dichroism, competitive binding experiment with ethidium bromide and potassium iodide quenching experiment suggested that SA possibly binds to the groove position of the ct-DNA. Finally, molecular docking analysis established the SA binds to minor groove position of ct-DNA in G-C rich region through hydrogen bonding interaction. Additionally, gel electrophoresis analysis has been performed to determine the protective efficacy of SA against UVB induced DNA damage and 50  $\mu\text{M}$  of SA was found to protect the DNA from UVB induced damage. We hope that our study could provide the validation of SA on behalf of therapeutics and development of next generation therapeutic drug as well as designing new efficient drug molecule and methodology for the interaction study of the drug with DNA.

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### 1. Introduction

Study of the interaction of deoxyribonucleic acid (DNA) with small molecules is of immense interest in the arena of pharmaceutical chemistry [1]. DNA controls heredity of life in the living organism and involved in essential biological process such as mutagenesis, gene transcription, gene expression, carcinogenesis and cell death, that makes them interesting to many researchers [1–6]. According to literature the binding affinity and sequence specificity of small molecules with DNA depends on the various structural and electronic factors [1,7]. In this respect it is important to understand the binding affinities and binding mechanism between small molecules and DNA in modern clinical research.

Being a naturally occurring biologically significant molecule, phenolic acids are elaborately studied in the field of small molecule-DNA interaction. Phenolic acid contains a phenolic ring and organic carboxylic acid functionalities. Classes of naturally occurring phenolic acids are hydroxybenzoic acid and hydroxycinnamic acid, which are extensively found in nature, especially in vegetables, fruits and a variety of beverages like tea, coffee etc. The schematic diagram of phenolic acids and their application are summarized in Fig. 1. Due to a wide variety of pharmacological activity and availability of hydroxycinnamic acids, the primary interest of researchers is to study the nature and dynamics for DNA-drug binding, which can lead to the design and construction of new and more efficient drugs targeted to DNA. Very few researchers have investigated the interaction of DNA with hydroxycinnamic acids and its derivatives. The interaction of caffeic acid with ct-DNA was investigated by Sarwar et al. and they concluded that caffeic acid interacted with ct-DNA through groove binding [8]. Zhang et al. investigated the interaction of ferulic acid with calf thymus DNA and according

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## Evaluation of Sinapic Acid to Ameliorate Ionizing Radiation Induced Peripheral Blood Mononuclear Cell Death

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### Abstract

**Introduction:** The UV radiation is known as a potential environmental carcinogen which causes damages of macromolecules like DNA, RNA, lipid, and protein inside the cell and eventually causes cell death. Persons who chronically exposed to UV radiation due to occupational or environmental exposure have a potential risk to develop cancer of the skin and internal organs. Polyphenols have a promising role in scavenging reactive oxygen species developed in our body due to a variety of exposure including radiation. In the present study, we are therefore evaluating the role of sinapic acid (SA), a polyphenol, in scavenging UV radiation-induced generation of reactive oxygen species and eventual cell death. We have studied the biological activity of SA as a potential antioxidant on human peripheral blood mononuclear cells taken from human volunteers.

**Methods :** Graded concentration of SA in different solvent mediums was applied to UV exposed peripheral blood mononuclear cells for evaluating the best effective delivery system and concentration against UV radiation.

**Result:** After series of experiments, we have observed that even at 10  $\mu$ M concentration, SA is effective against UV induced cellular death.

**Conclusion:** Finally, from this work we are inviting lots of works in this field to establish this molecule as a medicine to reduce radiation-induced cellular death.

**Keywords:** Sinapic Acid, UVB Radiation, Antioxidant, Cytotoxicity, Peripheral Blood Mononuclear Cell.

### Introduction

Ultraviolet radiation is a potent environmental carcinogen, induces oxidative and inflammatory skin damage and eventually cancer. Naturally occurring polyphenols are potent antioxidants and anti-inflammatory agents which can potentially reduce the damaging effects of ultraviolet (UV) rays on the human body. Reduction in the ozone layer in the atmosphere promotes considerable UV radiation to enter into the earth surface which may cause damages to the biological systems. Although both UVA and UVB are potentially harmful, the effect of UVB is more severe as it causes burn to the absorbing tissues. UV ray can penetrate the skin and contributes its damaging effects mostly on the keratinocyte and fibroblast. Most of the UVB is absorbed in the epidermis layer of the skin leaving little to enter into the dermis layer.

UVB induced damages most precisely causes cell death and apop-

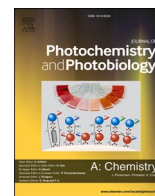
toxis although not known to us that whether it may induce cell necrosis or not. Exposure to UVB causes formation of reactive oxygen species (ROS), cell cycle arrest, activation of various genes and cell markers [1]. Among all three types of UV rays, UVA and UVB rays can penetrate in human body. The UVA rays possessing the longest wavelength can reach deeper into the human skin, beneath the dermis layer, while, comparatively little UVB rays can penetrate into the dermis layer. UVC rays are fully absorbed by ozone layer and cannot reach the Earth surface. UVB is potentially the more dangerous than UVA rays and it causes burning of the cells and responsible for producing skin cancer.

The carcinogenicity of UVB is well established and has been understood as a potential damaging agent to DNA from which gene mutation arises. On the other hand, UVA is generally far more abundant on earth surface, and goes deeper into the skin surface,



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## Ni-sinapic acid nanocomposite in the selective sensing of permanganate ions

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## ABSTRACT

A polyphenolic acid assisted synthesis of Ni nano particles for absorption spectrophotometric sensing of MnO<sub>4</sub> ions in micro molar range is reported here. The synthesis was carried out using a green approach where sinapic acid acts as a capping agent. The synthesized nano particle was then characterized using UV-Vis spectroscopy, Fourier transform infrared spectroscopy, transmission electron microscopy, powder X-ray diffraction analysis, X-ray photoelectron spectroscopy. The particle size is around 5 to 10 nm with the presence of both porosity and nano crystallinity as obtained from the transmission electron microscopic analysis. This nano particle can selectively sense permanganate ions in presence of different co-existing ions with the limit of detection (LOD) 0.413 μM. The sensing mechanism was examined with the isothermal titration calorimetry (ITC) and X-ray photoelectron spectroscopy (XPS). Isothermal titration calorimetric data suggests that the interaction between permanganate and the nano particle is enthalpy driven process with ΔH and ΔG values are -80 kcal/mol and -5.72 kcal/mol respectively. XPS data confirmed the presence of Ni(II) ions in the Ni-SA NPs and the atomic percentage of the same differed in presence of KMnO<sub>4</sub>. There was no significant interference from the contemporary ions and even in the presence of Mn<sup>2+</sup> ion. The method has also been applied for the natural water samples and for vegetable. ~ 88 to 108 % of the added KMnO<sub>4</sub> could be recovered from the tap water sample using our prepared methodology. The limit of detection and the present technique are compared with the previously reported literature and have been found to be comparable, even in solvent-free conditions and using simple instrumentation.

## 1. Introduction

Nanotechnology has become one of vastly growing research fields in the modern science community. In recent years, metals like Fe, Co and Ni have received an immense interest as nanoparticles for their beneficial applications in different fields. Nano-structured materials have found applications in chemical sensing [1,2], magnetic resonance imaging [3,4], memory storage devices [5], catalysis [3,6–8], drug delivery [9,10], and very recently in the treatment of cancer cells [11]. One of such metal nanoparticles is Ni-based nanoparticles that can be a good semiconductor with their band gap energy in the range 3.6 to 4 eV [12]. Additionally, Ni nanoparticles have a great potential for application in various pharmaceutical synthesis [13,14], like magnetic biocatalysis [15], biomolecular separation [16], biosensor, [17] etc. They have different applications in several other fields

[18,19,20,21,22,23–25]. Various processes have been utilized to prepare the Ni nanoparticles of different shape and size, which include sol-gel method [26], electrodeposition [27], thermal decomposition of organic complexes [28], chemical reduction [29], co-precipitation [30], solvothermal methods [31,32], etc. In order to avoid the tedious protocol and the sophisticated instrumentation associated with such methods, green synthesis can be a better option to reduce the use of toxic chemicals and make the process economically more viable [33,34]. One such green methodology to synthesis metal-based nanoparticles is to use plant extract or naturally occurring substances that can act both as capping and reducing agents. Gebretinsae et al., reported the synthesis of nickel oxide nanoparticles using cactus plant extract [12]. Whereas, Karpagavinayagam et al., used *Avicennia Marine* leaf extract [35] for this purpose. NiO nanoparticles can also be synthesized using egg white [36].

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