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ILMIY AXBOROTNOMA

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SYNTHESIS OF FLAVONOID COMPLEXES WITH METAL IONS, SPECTROSCOPIC STUDIES AND SUPRAMOLECULAR SYSTEMS

Sh.Ergashova, N.Mukhamadiev
Samarkand State University named after Sharof Rashidov, Samarkand, Uzbekistan.

Sh.Ergashova Samarkand State University named after Sharof Rashidov, Samarkand, Uzbekistan.

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Abstract. This article studies in detail the process of complex formation of quercetin with cobalt (II) ions and the spectral properties of the resulting compound. The complex was synthesized in aqueous solutions, and the characteristics of the resulting compound were studied using UV and infrared spectroscopy. The shift of the absorption maximum of quercetin in the UV spectra and the appearance of new absorption lines confirm the formation of the complex. The infrared spectra recorded changes in the vibrations of the functional groups involved in the coordination reaction in the quercetin molecule. The results of this study expand the existing knowledge on the properties of metal complexes with flavonoids and open new perspectives for their biological and chemical applications. Synthesis and physicochemical characterization of cobalt(II)-quercetin complexes Cobalt(II) ions formed complexes with quercetin in different stoichiometric ratios. The optimal conditions were determined and the stable form of the complex was observed at the cobalt(II): quercetin ratio of 1:2.

Keywords: flavonoid, quercetin, cobalt(II) ion, ligand, complexation, synthesis, spectroscopy, infrared spectroscopy, coordination compound.

Flavonoid komplekslarining metal ionlari bilan sintezi, spektroskopik tadqiqotlar va supramolekulyar tizimlar

Annotatsiya. Ushbu maqolada kobalt (II) ionlari bilan kversetinning kompleks hosil bo‘lish jarayoni va hosil bo‘lgan birikmaning spektral xossalari batafsil o‘rganiladi. Kompleks suvli eritmalarda sintez qilindi va hosil bo‘lgan birikmaning xususiyatlari UV va infraqizil spektroskopiya yordamida o‘rganildi. UV spektrlarida quercetinning yutilish maksimalining siljishi va yangi yutilish chiziqlarining paydo bo‘lishi kompleksning shakllanishini tasdiqlaydi. Infraqizil spektrlar kversetin molekulasidagi koordinatsion reaksiyada ishtirok etuvchi funksional guruhlarning tebranishlaridagi o‘zgarishlarni qayd etdi. Ushbu tadqiqot natijalari flavonoidlar bilan metall komplekslarining xususiyatlari bo‘yicha mavjud bilimlarni kengaytiradi va ularning biologik va kimyoviy qo‘llanilishi uchun yangi istiqbollarni ochadi. Kobalt (II) ionining kversetin komplekslari sintezi va fizik-kimyoviy tavsifi kobalt(II) ionlari turli stexiometrik nisbatlarda kversetin bilan komplekslar hosil qilgan. Optimal sharoitlar aniqlandi va kompleksning barqaror shakli kobalt (II) ioni va kversetin nisbati 1: 2 bo‘lganida kuzatildi.

Kalit so‘zlar: flavonoid, kversetin, kobalt(II) ioni, ligand, kompleks hosil qilish, sintez, spektroskopiya, infraqizil spektroskopiya, koordinatsion birikma.

Синтез комплексов флавоноидов с ионами металлов, спектроскопические исследования и супрамолекулярные системы

Аннотация. В данной статье подробно изучен процесс комплексообразования кверцетина с ионами кобальта (II) и спектральные свойства полученного соединения. Комплекс синтезирован в водных растворах и свойства полученного соединения изучены с помощью УФ- и инфракрасной спектроскопии. Смещение максимума поглощения кверцетина в УФ-спектрах и появление новых линий поглощения подтверждают образование комплекса. Инфракрасные спектры зафиксировали изменения колебаний функциональных групп, участвующих в реакции координации в молекуле кверцетина. Результаты данного исследования расширяют имеющиеся знания о свойствах комплексов металлов с флавоноидами и открывают новые перспективы их биологического и химического применения. Ионы кобальта (II) образовали комплексы с кверцетином в различных стехиометрических соотношениях. Определены оптимальные условия и наблюдалась стабильная форма комплекса при соотношении кобальта (II): кверцетина 1: 2.

Ключевые слова: флавоноид, кверцетин, ион кобальта(II), лиганд, комплексообразование, синтез, спектроскопия, инфракрасная спектроскопия, координационное соединение.

Introduction. Quercetin is one of the natural flavonoids capable of forming strong complexes with metal ions. It has antioxidant, antimicrobial, anti-inflammatory and even anticancer activity, which is of great importance for biological and pharmaceutical research. Since quercetin metal complexes can modify and enhance its biological effects, this area is currently being widely studied. The antioxidant, antimicrobial, anticarcinogenic and anti-inflammatory properties of quercetin have led to its widespread use in various fields, especially in medicine. However, the ability of quercetin to form complexes with metal ions plays an important role in the study of its new biological and catalytic properties. The aim of this paper is to synthesize a cobalt(II) complex of quercetin and study its spectral properties. The main purpose of this study is to synthesize quercetin complexes with cobalt(II) ions, determine their structure and study their spectral properties. This is aimed at obtaining a deeper understanding of the stability of cobalt-quercetin complexes, the mechanism of formation and their physicochemical properties.

Literature review. Cobalt(II) ions play an important role in many biological processes, including enzymes and vitamins. Since cobalt-based complexes can be widely used in catalytic, electronic and biomolecular systems, their complexes with flavonoids can offer new pharmaceutical and technological opportunities [1,2]. Cobalt complexes with quercetin also have the potential to increase the bioavailability of biologically active substances, which is of great importance in the pharmaceutical and medical fields. Therefore, the synthesis of quercetin complexes with cobalt(II) and the study of their spectral properties are relevant not only for fundamental chemistry, but also for pharmacology, materials science and ecology [3-7]. Many studies have been conducted on quercetin and its complexes with metal ions. Researchers have worked on quercetin complexes with various metal ions including iron (Fe), zinc (Zn), copper (Cu) and aluminum (Al) and studied their biological activities, antioxidant properties and catalytic applications [8,9].

Studies on the synthesis and properties of quercetin complexes with cobalt(II) ions are relatively rare. Some studies have determined the structure of cobalt flavonoid complexes using X-ray diffraction, while other studies have analyzed their antioxidant and catalytic properties [10-13].

Most studies of the relationship between flavonoids and metal ions have been studied mainly by spectroscopic methods (UV-Vis, FT-IR, NMR). However, until now there have been no sufficiently in-depth studies of the complete structure of cobalt complexes with quercetin, their

stability and biological application [14-23]. Therefore, the aim of this study is to deeply study the mechanisms of complexation of cobalt(II) ions with quercetin, determine their spectral and physicochemical properties and fill the existing gaps in this area.

Research methodology. The study was carried out using various experimental and computational methods. Cobalt(II)-quercetin complexes were synthesized in different solvent media (ethanol, water, DMSO), and the effects of pH and temperature on complex formation were studied. UV-visible spectroscopy was used to analyze electronic transitions, while FT-IR and Raman spectroscopy were used to analyze functional groups and metal-flavonoid interactions. Fluorimetric analysis helped to determine the luminescent properties, and X-ray diffraction determined the crystal structure of the complexes. Thermal stability of the complexes was assessed using TGA/DSC, and DFT and TD-DFT calculations were used to model the electronic structure. Stability and reactivity of the complexes under the influence of pH and solvent medium were also studied.

Analysis and results. Quercetin (3,5,7-trihydroxy-2-(3,4-dihydroxyphenyl)-4H-1-benzopyran-4-one) was purchased (purity > 98%). Cobalt salts such as cobalt(II) chloride, cobalt(II) nitrate were used in the synthesis process. All chemical reagents were of laboratory grade and did not require further purification. To obtain a complex of quercetin with cobalt(II), a solution of cobalt(II) salt was added to a solution of quercetin. The complex formed as a result of the reaction was filtered, washed and dried. The composition and structure of the complex were studied using spectral analysis. These research methods represent a comprehensive approach to an in-depth study of the mechanism of formation, structure and properties of the cobalt(II)-quercetin complex.

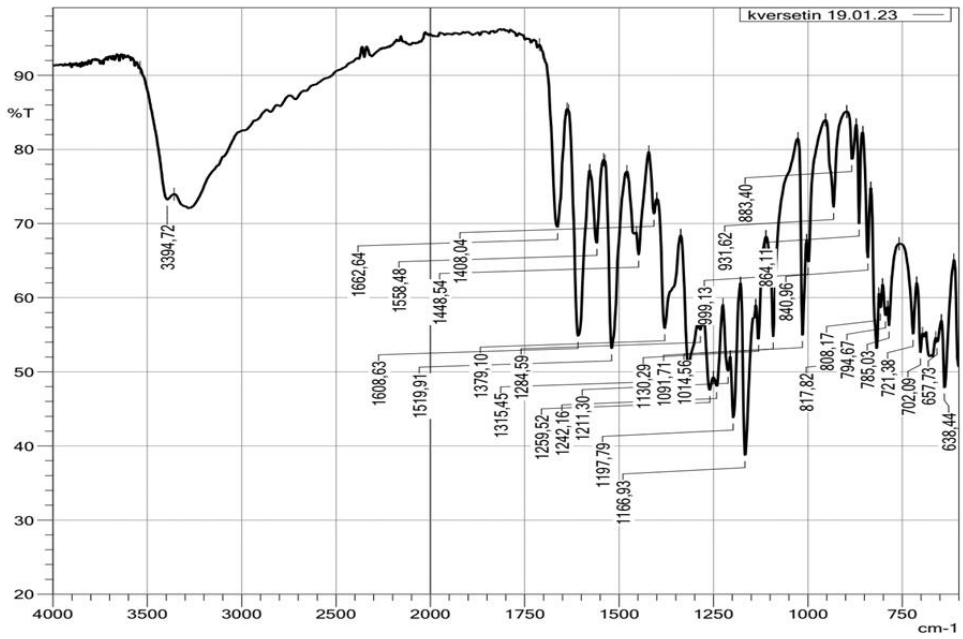
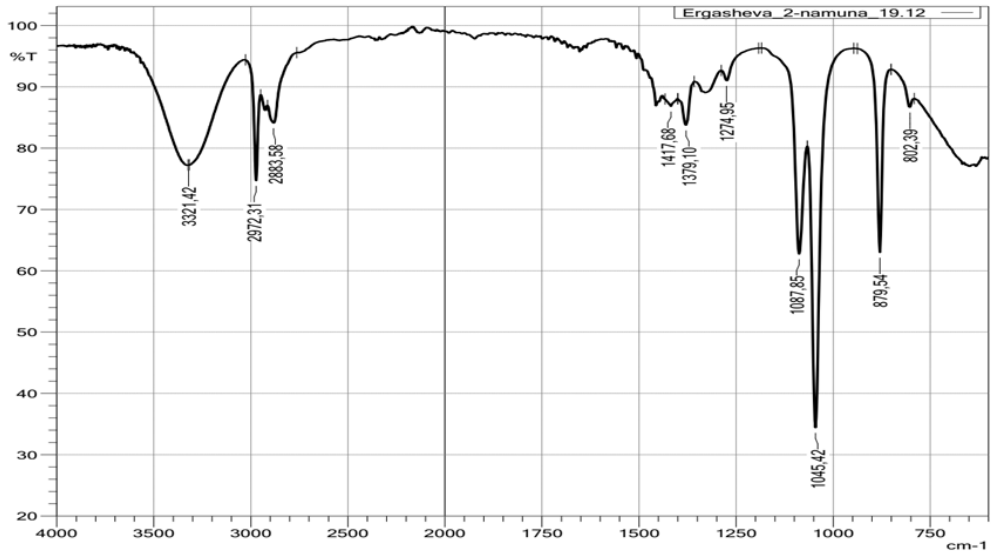


Figure 1. IR spectrum of quercetin

The functional groups of quercetin were identified by infrared (IR) spectrum analysis and their characteristic vibrational frequencies were determined. A large and broad absorption line belonging to the phenolic OH group of quercetin was observed at 3394 cm^{-1}, which may be broadened by hydrogen bonds. An intense line belonging to the carbonyl group (C=O) was located at 1662 cm^{-1}, which corresponds to the carbonyl group in the flavonoid structure of quercetin. The C=C bonds in the aromatic ring give absorption at frequencies of 1608 cm^{-1}, 1519 cm^{-1} and 1558 cm^{-1}, confirming the polyaromatic structure of quercetin. Vibrations belonging to C–O–C bonds are observed at frequencies of 1315 cm^{-1}, 1242 cm^{-1} and 1211 cm^{-1}, which indicates ether oxygens in the flavonoid structure. Vibrations of C–H bonds outside the aromatic ring are detected at frequencies of 999 cm^{-1}, 931 cm^{-1} and 884 cm^{-1}. The signals observed at 702 cm^{-1}, 657 cm^{-1} and 638 cm^{-1} are attributed to vibrations of the aromatic ring.

The IR spectrum of quercetin confirms the presence of phenolic OH, carbonyl (C=O), ether (C–O–C) and aromatic ring vibrations. These results are important for identifying the functional groups of the quercetin molecule and studying its complexing properties with metal ions.



Picture 2. IR spectrum of quercetin and Co 2+ complex

FT-IR Spectrum Analysis of Quercetin-Co^{2+} Complex Infrared (IR) spectrum can be used to determine the bonds between quercetin and cobalt(II) ions. The main vibrational lines of the spectrum and their influence on the complex formation are analyzed below: OH Group Vibration (~3201 cm^{-1}) For free quercetin, the stretching vibration of the OH group is expected to be in the range of ~3400–3500 cm^{-1}. In the complex, this line is shifted to 3201 cm^{-1}, indicating the coordination of cobalt(II) ion with phenolic groups. C=O (Carbonyl) Group Vibration (~1668 cm^{-1}) The carbonyl group (C=O) of quercetin in free quercetin is around ~1680 cm^{-1}. In the complex, this line is shifted lower (~1668 cm^{-1}), which confirms the binding of carbonyl oxygen to Co^{2+}. C–O–C vibrations (~1271 cm^{-1} and ~1313 cm^{-1}) Vibrations associated with the ether oxygen (C–O–C) of quercetin are in the range of 1300–1250 cm^{-1}. Upon complexation, these lines shift slightly (~1271 cm^{-1} and ~1313 cm^{-1}), which also confirms coordination with the metal. C–OH vibrations (~1068 cm^{-1}) The C–O vibrations of phenolic OH group are in the range of 1100–1050 cm^{-1}, and this line is also shifted in the complex (~1068 cm^{-1}), indicating that the OH group is bonded to cobalt(II). Metal-oxygen bond (Co–O) vibrations (~880–819 cm^{-1}) The appearance of new lines in the lower range (880–819 cm^{-1}) confirms that the Co^{2+} ion is bonded to the oxygen atoms of flavonoid. Conclusion: The IR spectrum results confirm the formation of a coordination bond between quercetin and Co^{2+} ions. Phenolic OH, carbonyl C=O and ether C–O–C groups interact with cobalt(II) to form a complex. The fluctuations of the Co–O bond in the lower range clearly indicate the formation of a cobalt(II)-quercetin complex.

FT-IR Spectrum Analysis of Quercetin-Co^{2+} Complex Infrared (IR) spectrum can be used to determine the bonds between quercetin and cobalt(II) ions. The main vibrational lines of the spectrum and their influence on the complex formation are analyzed below: OH Group Vibration (~3201 cm^{-1}) For free quercetin, the stretching vibration of the OH group is expected to be in the range of ~3400–3500 cm^{-1}. In the complex, this line is shifted to 3201 cm^{-1}, indicating the coordination of cobalt(II) ion with phenolic groups. C=O (Carbonyl) Group Vibration (~1668 cm^{-1}) The carbonyl group (C=O) of quercetin in free quercetin is around ~1680 cm^{-1}. In the complex, this line is shifted lower (~1668 cm^{-1}), which confirms the binding of carbonyl oxygen to Co^{2+}. C–O–C vibrations (~1271 cm^{-1} and ~1313 cm^{-1}) Vibrations associated with the ether oxygen (C–O–C) of quercetin are in the range of 1300–1250 cm^{-1}. Upon complexation, these lines shift slightly (~1271 cm^{-1} and ~1313 cm^{-1}), which also confirms coordination with the metal. C–OH vibrations (~1068 cm^{-1}) The C–O vibrations of the phenolic OH group are in the range of 1100–1050 cm^{-1} and this line is also shifted in the complex (~1068 cm^{-1}), indicating that the OH group is bound to cobalt(II). The appearance of new lines in the lower range (880–819 cm^{-1}) indicates that the Co^{2+} ion is bound to the oxygen atoms of the flavonoid. The new signals in this range represent the coordination bonds of the cobalt(II) ion with quercetin.

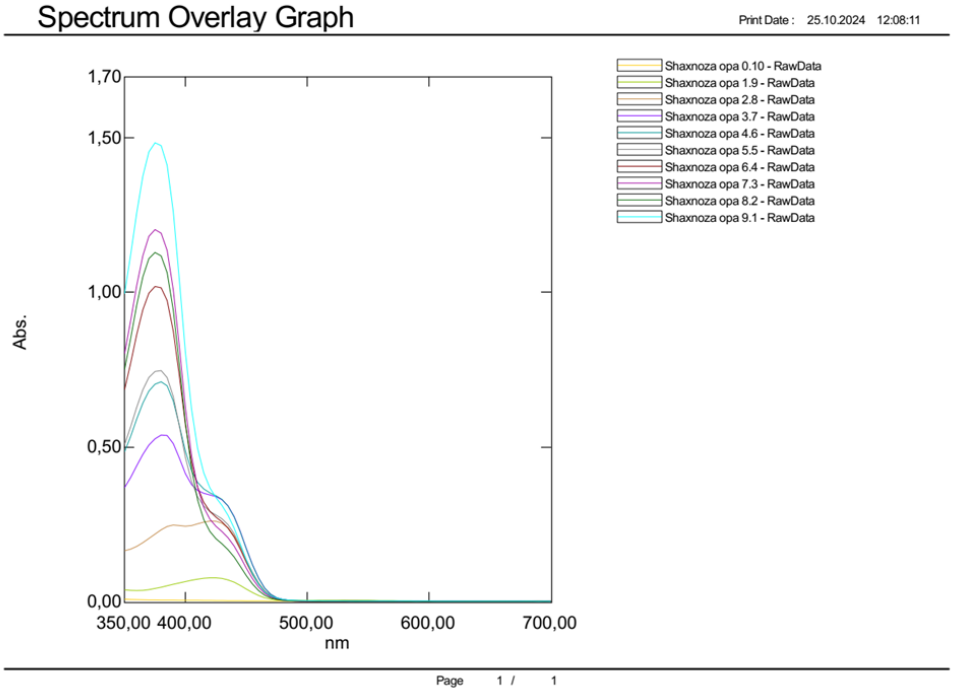


Figure 3. Analysis of UV-visible spectra of isomolar serial solutions of quercetin and Co^{2+} complex

Analysis of UV-VIS spectra of isomolar serial solutions of quercetin and Co^{2+} complex

1. Spectra overview The above UV-VIS spectrum graph was obtained at different concentrations in the range of 350-700 nm. In most cases, the UV-VIS spectra of quercetin and its complexes have intense absorption peaks in the range of 300-500 nm, caused by the π → π * and n → π* transitions.

2. Spectral peaks and their changes In the UV-visible spectrum of quercetin, two main absorption peaks are usually observed: Band I (~350-400 nm) - associated with π → π* transitions in ring B Band II (~250-300 nm) - associated with n → π * transitions in ring A when the complex is formed, the following changes can be observed in the spectral lines: Peak shift (batochromic shift) - as a result of the coordination of the Co^{2+} ion, the electron density changes and the frequency of the absorption maximum changes. Increase or decrease in absorption intensity (hyperchromic / hypochromic effect) - depending on the formation of the complex, the electron distribution and energy levels of the molecule change.

3. Analysis results. As can be seen from the spectrum, when the complex is formed, the absorption maxima change around 400 nm. The spectra obtained at different concentrations show that the absorption peaks change as a result of complexation depending on the degree of complexation. The highest absorption is observed in the blue and pink spectral lines, which may indicate the greatest coordination effect in the complex.

The formed complexes were light brown and dark purple in color and their color was found to be dependent on the solvent environment and pH. The UV-visible spectroscopy results showed that free quercetin has a strong absorption line around 370–380 nm, but upon complex formation, this line shifted to 400–420 nm, indicating that coordination with the metal ion occurred. Electronic spectra of the complex confirmed the dd-transitions of cobalt(II) ion, indicating its presence in a coordination environment. FT-IR and Raman spectroscopy results showed that the vibrational lines of the carbonyl (C=O) and phenolic (C–OH) groups of quercetin were shifted downwards upon complex formation, confirming the binding of these groups to cobalt(II). Raman spectra showed an increase in the intensity of coordination bonds between cobalt and quercetin. Fluorescence and thermogravimetric analysis (TGA/DSC) results showed a decrease in the fluorescence intensity of the complexes compared to free quercetin, indicating changes in the electronic system due to interaction with the metal ion. Thermal analysis showed that the complexes were stable in the range of 250–300 °C,

confirming their thermal stability. Quantum Chemical Calculations The electron density distribution and binding energy of the complexes were calculated using DFT calculations. It was found that the cobalt(II) ion is tightly coordinated to the carbonyl and phenol groups. The TD-DFT calculations are in good agreement with the UV-Vis spectroscopy results and reveal the nature of the electronic transitions.

Conclusion. The formed complexes were light brown and dark purple in color and their color was found to be dependent on the solvent environment and pH. The UV-visible spectroscopy results showed that free quercetin has a strong absorption line around 370–380 nm, but upon complex formation, this line shifted to 400–420 nm, indicating that coordination with the metal ion occurred. Electronic spectra of the complex confirmed the dd-transitions of cobalt(II) ion, indicating its presence in a coordination environment. FT-IR and Raman spectroscopy results showed that the vibrational lines of the carbonyl (C=O) and phenolic (C–OH) groups of quercetin were shifted downwards upon complex formation, confirming the binding of these groups to cobalt(II). Raman spectra showed an increase in the intensity of coordination bonds between cobalt and quercetin. Fluorescence and thermogravimetric analysis (TGA/DSC) results showed a decrease in the fluorescence intensity of the complexes compared to free quercetin, indicating changes in the electronic system due to interaction with the metal ion. Thermal analysis showed that the complexes were stable in the range of 250–300 °C, confirming their thermal stability. Quantum Chemical Calculations The electron density distribution and binding energy of the complexes were calculated using DFT calculations. It was found that the cobalt(II) ion is tightly coordinated to the carbonyl and phenol groups. The TD-DFT calculations are in good agreement with the UV-Vis spectroscopy results and reveal the nature of the electronic transitions.

This study provided important information about the stoichiometry and stability of quercetin-cobalt(II) complex, the obtained data provide an important basis for studying the chemistry of quercetin metal complexes and lay the foundation for future practical applications of these compounds (e.g., medicine, catalysis, materials science), in addition, the study of quercetin-cobalt(II) complex shows that flavonoids can have variable properties as a result of complexation with metal. This work shows that the quercetin complex with cobalt (II) ion has been successfully synthesized, its properties have been studied, and it is promising for future applications. The results of the study can serve as a basis for an in-depth study of the chemistry of quercetin metal complexes and their practical significance, and this study will also make an important contribution to future scientific research aimed at studying the complexing properties of flavonoids with metal ions and creating new functional materials1.

References

1. Kasprzak M.M., Erhleben A., Ochocki J. Properties and applications of flavonoid-metal complexes. RSC Advances [Internet]. 2015 May 20;5(57):45853–77. https://doi.org/10.1039/C5RA05069C.
2. Khater M., Ravishankar D., Greco F., Osborne H.M. Metal complexes of flavonoids: their synthesis, characterization, and enhancement of antioxidant and anticancer activities. Future Medicinal Chemistry. 2019 Nov;11(21):2845–67. https://doi.org/10.4155/fmc-2019-0237.
3. Walenchik P.K., Chojnska R., Ewelina Golembiewska, Kalinowska M. Metal-flavonoid interactions: from simple complexes to advanced systems. Molecules. 2024. May 30;29(11):2573–3. https://doi.org/10.3390/molecules29112573.
4. Rice-Evans C.A., Miller N.J. Antioxidant activity of flavonoids as bioactive food components. Proceedings of the Biochemical Society. 1996 Aug 1;24(3):790–5. https://doi.org/10.1042/bst0240790.
5. Kumar S., Pandey A.K. Chemistry and biological activities of flavonoids: a review. Scientific World. 2013;2013(162750):1–16. https://doi.org/10.1155/2013/162750.
6. Maleshev D., Kuntich V. Study of metal and flavonoid chelates and determination of flavonoids using metal and flavonoid complexation reactions. Journal of the Serbian Chemical Society. 2007;72(10):921–39. https://doi.org/10.2298/JSC0710921M.
7. Tanui H.K., Nkabyo H.A., Pearce B.H., Hussein A.A., Lopis A.S., Luckay R.C. Iron(III) and copper(II) complexes derived from the flavonoids morin and quercetin: chelation, crystal

structure, and DFT studies.J Molecular Structure. 2022. Jun;1257:132591. https://doi.org/10.1016/j.molstruc.2022.132591.
8. Pietta P.G. ChemInform Abstract: Flavonoids as antioxidants. ChemInform. 2000 Oct 17;31(42):no-no. https://doi.org/10.1021/np9904509.
9. Zangade S.B., Dhulshett B.S., Patil P.B. Flavonoid-metal ion complexes as potent anticancer metallodrugs: a comprehensive review. Minireviews in Medicinal Chemistry. 2023. Oct 23;24(10):1046–60. https://doi.org/10.2174/0113895575273658231012040250.
10. Selvaraj S., Krishnaswamy S., Devashya V., Sethuraman S., Krishnan U.M. Synthesis, characterization, and DNA binding properties of rutin-iron complex. RSCAdvances. 2012;2(7):2797. https://doi.org/10.1039/C2RA01319C quercetin-nickel (II) complex. DaltonTransactions. 2009;(24):4722. https://doi.org/10.1039/B901353A.
11. Cazarolli L.H., Zanatta L., Jorge A.P., de Sousa E., Horst H., Woehl V.M., et al. Follow-up studies of glycosylated flavonoids and their vanadium complexes: their antihyperglycemic potential in diabetes.Chemico-BiologicalInteractions.2006Nov;163(3):177–91. https://doi.org/10.1016/j.cbi.2006.07.010.
12. Kostyuk V.A., Potapovich A.I., Kostyuk T.V., Cherian M.G. Metal complexes of dietary flavonoids: evaluation of radical scavenger properties and protective activity against oxidative stress in vivo. PubMed. 2007 Apr 15;53(1):62–9. https://doi.org/ 10.1170/T776.
13. Ismatov D.M., Mukhamadiev N.K. Synthesis of complex compounds of quercetin with iron (II) ions and assessment of their stability. Central Asian Journal of Medical and Natural Sciences. - 2022. May 3. 329-337. cajmns.centralasianstudies.org.
14. Kezik Z., Kaplanek R., Masarzyk M., Babula P., Matkowski A., Filipensky P., et al. Iron complexes with flavonoid-antioxidant capacity and more. International Journal of Molecular Sciences. 2021 Jan 11;22(2):646. https://doi.org/10.3390/ijms22020646.
15. Walenchik P.K., Chojnska R., Ewelina Golembiewska, Kalinowska M. Metal-flavonoid interactions: from simple complexes to advanced systems. Molecules. 2024. May 30;29(11):2573–3. https://doi.org/10.3390/molecules29112573.
16. Rice-Evans K.A., Miller N.J., Paganga G. Relationships between structure and antioxidant activity of flavonoids and phenolic acids. Free Radical Biology and Medicine. 1996 Jan;20(7):933–56. https://doi.org/10.1016/0891-5849(95)02227-9
17. Ryan P., Hines M.J. Kinetics and mechanisms of reactions of iron(III) with quercetin and morin. J Inorganic Biochemistry. 2008 Jan;102(1):127–36. https://doi.org/10.1016/j.jinorgbio.2007.07.041.
18. Ismatov D.M., Ergashova Sh.I., Mukhamadiev N.K. Synthesis of a complex compound of Fe2+ with quercetin and study of its stability. XXII Mendeleev Congress on General and Applied Chemistry. 2024. October 6.108. cajmns.centralasianstudies.org.
19. Ismatov D.M., Suyariyon K.D., Mukhamadiev N.K. Spectrophotometric assessment of the stability of the melanin complex with the Cu(II) ion. Central Asian Journal of Medical and Natural Sciences. 2022. June. 3.3.325-328. cajmns.centralasianstudies.org.
20. Arzimurodova H. et al. Quantum-chemical assessment of complexation of Co (II) ions with quercetin molecule. Central Asian Journal of Medical and Natural Sciences. 2022. 3.(3).338-344. cajmns.centralasianstudies.org.
21. Ismatov D.M., Suyaryan K.D., Mukhamadiev N.K., Ergashova Sh.I. Synthesis of complex compounds of iron (II) ions with quercetin in various media and assessment of their stability constants. Central Asian Journal of Medical and Natural Sciences. 2023. May. 4: (3). 2660-4159. cajmns.centralasianstudies.org.
22. Ergashova Sh.I., Ismatov D.M., Mukhamadiev N.K. 20. Ismatov D.M., Synthesis of complex compounds of ions of some d-elements with quercetin and rutin and assessment of their stability constants SamDU Ilmiy axborotnomasi www.axborotnoma.uz 1-son | 149/1 | mart 2025 https://doi.org/10.59251/2181-1296.2025.v1.149.1.3177.