

Treatment the Contamination of Real Samples and Herbal Extracts Using Paroxetine Drug in Thi-Qar province, Iraq

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Abstract. This study presented a simple, novel, and cost-effective method that has become the focus of numerous studies for the removal of heavy metals from real samples (water, plants, and soil) and herbal extracts (black tea, fenugreek, and anise). Copper oxide nanoparticles (CuO NPs) were prepared and analyzed using various techniques, including UV-Visible, FT-IR, XRD, SEM, and AFM, allowing for the investigation of the nanomaterial's physical and chemical properties. These nanomaterials were used as catalysts for amines. Paroxetine was used as the pharmaceutical amine, as it is classified as an amine due to its active amine group. The nano-catalyzed pharmaceutical amine was used to enhance the efficiency of heavy metal removal from both real and herbal samples. Optimal reaction conditions, including pH, temperature, nanomaterial concentration, and time, were determined to ensure the production of stable and effective particles. This method is characterized by its high efficiency and environmental compatibility, offering an alternative to chemical methods.

Keywords: CuO NPs, Paroxetine drug, Heavy metal, Adsorption

Introduction

Pollution is one of the most prominent problems facing humanity and nature, especially after the technological advancements that have accompanied modern life. Pollution occurs in various forms (water pollution, air pollution, soil pollution) as a result of the presence of harmful organic and inorganic materials, or as a result of the deficiency or excess of certain essential elements in the environment beyond their natural levels. Pollution also arises from human activities or natural phenomena[1]. Water pollution is considered one of the most serious environmental problems. In 1961, the World Health Organization defined water pollution as any change that occurs in the physical, chemical, and biological properties of water, leading to a change in its condition, directly or indirectly, rendering the water unsuitable for its intended uses, whether for drinking, domestic consumption, agriculture, or other purposes[2] One of the methods used to treat heavy metal pollution is adsorption, which is one of the oldest, most common, and most effective physical and chemical processes. In this process, pollutant particles or ions adhere to the surface of a solid material called the adsorbent[3]. This method is characterized by its ability to remove pollutants even at very low concentrations and its ease of application. Adsorption is classified into two types based on the type of bonding forces between the surface of the adsorbent and the adsorbed material: physical adsorption, which occurs as a result of van der Waals forces between molecules and the surface and is reversible; and chemical adsorption, which occurs when strong chemical bonds form between the pollutant and the surface of the adsorbent and is often irreversible. Several models also describe adsorption, such as the Langmuir and Freundlich models, which help researchers understand the adsorption process and evaluate its efficiency[4]. In this context, Kowalski et al. conducted a study in Poland in 2021 entitled "Pharmacological Effects of Paroxetine as a Selective Serotonin Reuptake Inhibitor." This study elucidated the mechanism of action of paroxetine, a drug belonging to the class of selective serotonin

reuptake inhibitors (SSRIs). These drugs increase serotonin levels in the brain, a neurotransmitter responsible for improving mood and reducing depression[5]. Ibtihaj also conducted a study in 2016 in Al-Shatra, Iraq, on the evaluation of the concentrations of some heavy elements in soils selected from the city of Al-Shatra. The results showed a significant increase in the percentages of lead, cadmium, and nickel in all the studied areas. This indicates clear soil pollution[6].

Materials and Methods

1. Materials Used

Copper Sulfate Penta hydrate ($\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$) (BDH), Hydrochloric acid (BDH), Perchloric acid (Sigma Aldrich), Ethanol (BDE), Chloroform (Sigma Aldrich), Sodium hydroxide (Merck).

2. Preparation of extract from the fruit of the Berberis plant

Fresh Berberis Vulgaris fruits were collected from their natural habitat. The samples were collected and thoroughly washed with deionized water to remove dirt and dust. They were left to air dry for two weeks at room temperature, then thoroughly ground using an electric grinder. An aqueous extract of Berberis Vulgaris was then prepared using 18gm of the plant powder, placed in a 1000mL conical flask, and 600mL of deionized water was added. The mixture was heated for 30 minutes at 70°C with continuous stirring. The heater was turned off after 30 minutes, and the mixture was stirred for one hour. The mixture was then given some time to settle. Filter paper No. 1 waltman was used to filter the stabilized extract. It was stored in the refrigerator at 4°C . The preparation was then used to synthesize nanoparticles[7].

3. Preparation of Copper Oxide Nanoparticles

pentahydrate salts using Berberis fruit extract as a plant source rich in active compounds such as alkaloids, flavonoids, bacilli, and vitamin C, which contribute to the reduction.

Converting metal ions into nanoparticles (Reducing agents)

It Prevents Particle aggregation and maintains its Nano scale Size (Capping agents)

Steps: An aqueous solution of copper(II) sulfate pentahydrate (0.2M) was prepared by adding 4.98 g of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ to a 250 mL flask, then adding 100 mL of deionized water. The mixture was then shaken to obtain a homogeneous solution. Then CuO nanoparticles were prepared by mixing 200ml of copper(II) sulfate pentahydrate solution at a concentration of (0.2) with 200ml of Berberis plant extract with continuous stirring at a temperature of 70°C for two hours. NaOH was added in droplets to the solution in order to adjust the acidity function (pH 9). The mixture was then left to settle at room temperature for 24 hours and then centrifuged for 20 minutes at 2000 rpm. After that, the precipitate formed was separated and washed with deionized water and ethanol. The precipitate was then dried in an oven at a temperature of $100\text{--}110^\circ\text{C}$, and then the product was kept in an airtight container until use.

4. Promoted Catalysis of pharmaceutical amines with copper oxide nanoparticles

One gram of copper oxide (CuO NPs) was placed in a 100 ml flask, and 10 ml of deionized water was added. The suspension was placed in an ultrasonic device for a sufficient time to ensure homogeneous particle distribution. An amine solution was also prepared by dissolving one gram of amines paroxetine drug in an appropriate amount of deionized water. The nanosuspension was then mixed with the amine solution at a 1:1 ratio, and the pH was adjusted (pH = 7) using a buffer solution. The amine solution was gradually added to the CuO NPs, suspension while stirring with a magnetic stirrer to ensure a good reaction at $40\text{--}45^\circ\text{C}$ for 30 minutes. The precipitate was then filtered and washed twice with deionized water and once with ethanol. Finally, it was dried in an oven at 60°C . The resulting nano-catalyzed amine was obtained[8].

5. Preparation of stander Solution of Heavy metal (V+5, Ni +2, Co+2)

For the purpose of conducting an analytical study, both (V+5, Ni+2, CO+2) were prepared at a concentration of 1000 ppm, by dissolving (0.0426) gm, (0.049) gm and (0.047)gm, of vanadium (IV) sulfate trihydrate and nickel(II) nitrate hexahydrate and Cobalt (II) Sulfate heptahydrate, respectively, using deionized water in a 100 ml volumetric flask. The volume was then topped up to the mark with deionized water. From these concentrations, a series of other dilute solutions of vanadium, nickel and cobalt were prepared[9].

6. Determining the optimal conditions for heavy metal removal using a nano-catalyst amine

To determine the optimal conditions, 10 ml of a standard solution containing known concentrations of the heavy metals Ni, V and CO was taken and placed in a 15 ml centrifuge tube. 0.5 g of plant-extract nano-catalyzed amines were added, and the mixture was shaken manually or by agitating for two minutes to obtain a homogeneous solution. The pH of the solution was then adjusted to the desired value (pH = 6). The tube was then placed in an ultrasonic device for 10 minutes. The ultrasonic vibrations equilibrated the two phases, allowing ion adsorption onto the surface of the nanomaterial. The solid phase was separated from the liquid phase by centrifuging the tube at 4000 rpm for 10 minutes, and the results were then measured using a spectrophotometer[10].

Effect of PH

In three 15 mL volumetric bottles, each containing 10 mL of vanadium or nickel, Cobalt solution at a concentration of 1 ppm, 0.5 g of nano-catalyzed amines were added, and the pH was adjusted to different values (pH = 3, 7, 9). The solution was then mixed and diluted to the mark with deionized water. The mixture was then centrifuged at 5000 rpm for 10 minutes, and the result was measured using a spectrophotometer.

Effect of Temperature

Three 15 mL volumetric bottles, each containing 10 mL of vanadium or nickel, Cobalt solution at a concentration of 1 ppm, were prepared. Then, 0.5 g of nano-catalyzed amines were added, and the pH was adjusted to optimum values. The bottles were then left at different temperatures (5, 25, and 60 °C), mixed, and diluted to the mark with deionized water. The mixture was then centrifuged at 5000 rpm for 10 minutes, and the resulting mixture was measured using a spectrophotometer.

Effect of different Concentration

In three 15 mL volumetric bottles, each containing 10 mL of vanadium or nickel, Cobalt solution at a concentration of 1 ppm, different concentrations (1 g, 0.1 g, 0.5 g) of nano-catalyzed amines were added, maintaining all optimal conditions. The mixture was then centrifuged at 5000 rpm for 10 minutes, and measurements were taken using a spectrophotometer.

Effect of time

In three 15 mL volumetric bottles, each containing 10 mL of heavy metal solutions, 0.5 g of nano-catalyzed amine was added while maintaining optimal conditions of pH, temperature, and substance concentration. Different time intervals (10 min, 30 min, 120 min) were selected to determine the optimal time, and the contents were centrifuged at 5000 rpm for 10 min.

7. Preparation of Herbal Extracts

Commercially available herbal extracts including(fenugreek, anise, and black tea) were used. These extracts were finely ground using an electric grinder to obtain a homogeneous, fine powder. 10 g of each herbal extract was weighed and dissolved in 100 mL of deionized water with continuous stirring to ensure complete dissolution. This solution was divided into two 50mL portions. The first served as an untreated control sample, While the second was treated by adding 1g of the nano-catalytic active ingredients . Both vials were held steady for 30 minutes under optimal conditions. They were then centrifuged for 10 minutes at 5000 rpm, filtered to remove suspended particles, concentrated using a rotary evaporator, dried to obtain a solid precipitate, and then reconstituted with distilled water for measurement.

8. The Area of The Study

The Dhi-Qar Governorate is located in southern Iraq, approximately 360 km southeast of Baghdad, between latitudes 31°23' N and longitudes 46°15' E, and covers an area of about 12,900 km². To ensure the reduction of several administrative issues such as photography, favors, and reforms, the region is characterized by a hot, dry climate in summer and a mild climate in winter with limited rainfall. The Euphrates River flows through the area, providing water resources for agriculture and domestic use. Due to its industrial and agricultural impact, the region faces challenges in its green spaces, including water and soil enrichment with minerals, making it a suitable model for small plants[11].

9. The Collection of Samples

Samples were collected from different areas in Dhi-Qar Governorate, Iraq (Al-Gharraf, Al-Fadhiliya, and Nasiriyah) during the same growing season in November 2025 to ensure uniformity of

environmental conditions. Okra plant samples were collected and placed in clean, tightly sealed bags, each labeled with information regarding the collection site, plant type, and time. Soil samples were also collected from the same site as the plant samples. This selection of the same location aimed to compare heavy metal accumulation. Water samples were also collected from the same site. Water samples used for soil analysis were placed in tightly sealed plastic bottles to prevent external contamination until use.

10. Digestion of Samples

The digestion method is used to analyze soil and plant samples, using a mixture of nitric acid (HNO₃) and per chloric acid (HClO₂). This mixture is effective in breaking down organic and mineral matter. 1g of each sample is placed in a 50 mL crucible. Initial digestion is performed by adding 10 mL of concentrated nitric acid to the sample. The crucible is then placed on a hot plate for 30 minutes to allow initial oxidation. After cooling, 5 mL of perchloric acid (70%) is added to the crucible, and it is reheated until the solution becomes clear and almost dry, indicating complete digestion. The sample is then cooled and filtered using Whatman filter paper (No. 42). The filtered solution is transferred to a 25 mL volumetric flask, and the volume is then filled to the mark with deionized water. Finally, the solution is analyzed using flame atomic absorption spectroscopy.

Results and Discussion

1. Chemical analysis of Prepared nanoparticles

1.1. FT-IR Spectra of CuO NPs

The Fourier transform infrared (FT-IR) spectrum of the plant extract shows major absorption peaks at (3427) cm⁻¹, (2877) cm⁻¹, and (1730) cm⁻¹, attributed to the vibrations of O–H, C–H, and C=O groups, respectively, indicating the presence of active organic compounds such as phenols and amines. The spectrum of the CuO nanoparticles showed peaks at (3741–3444) cm⁻¹, (2920) cm⁻¹, and (1622) cm⁻¹, indicating the presence of O–H, C–H, and C=O bonds, along with the characteristic peak of the Cu–O bond in the range of (455–617) cm⁻¹, confirming the formation of copper oxide nanoparticles and their association with the plant extract. These results indicate the success of the nano-catalytic process and the interaction of functional groups between the plant extract and the CuO NPs particles to form a composite material effective in heavy metal removal, as shown in **Figure 1 to 2 and Table 1**[12].

Table 1. Represents the most important bands appearing in the FT-IR Plant extract and the nanomaterial

Material	μ(O-H)	μ(C-H)	μ(C=O)	μ(C-O)	μ(C=C)	μ(C=C)	μ(CuO)
Plant Extract	3427	2877	1730	1219-1080	1454	1647	-----
CuO NPs	3741-3444	2920	1622	1050	1516	1592	617-455

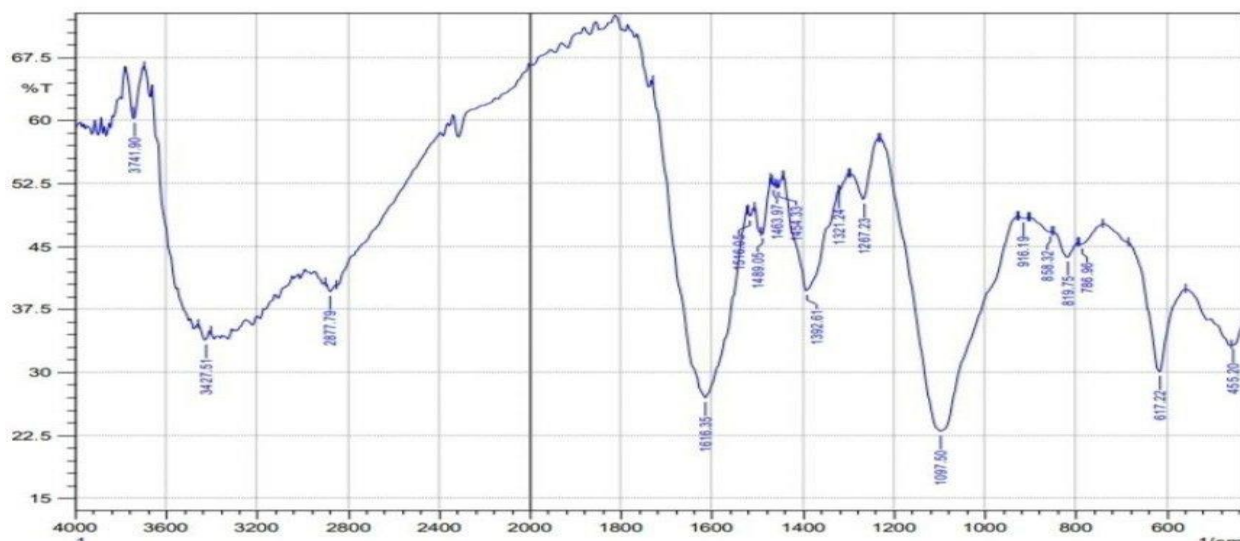


Figure 1. FT-IR of CuO NPs

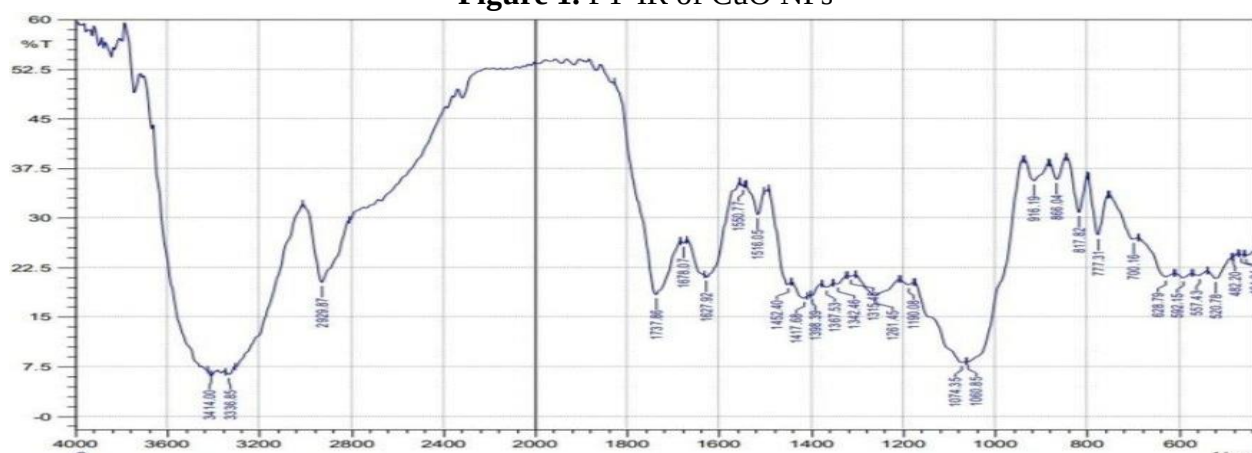


Figure 2. FT-IR of Berberis plant extract

1.2. UV-Vis Spectrum of Nano-CuO NPs

The absorption spectrum of the prepared copper oxide nanoparticles was measured using UV-Vis spectroscopy at different wavelengths within the range of (200–800) nm. The UV-Vis spectrum of CuO NPs showed absorption peaks at (270–295) nm, representing electron transfer from oxygen (O₂) to copper(II) (Cu) within the copper oxide lattice. This absorption indicates the presence of strong Cu–O bonds and is evidence of the formation of a CuO crystalline structure. Two absorption peaks were also observed: a primary peak at 281 nm and a smaller peak at (372) nm, indicating the presence of CuO nanoparticles. This is consistent with previous studies, as shown in **Figure 3** [13].

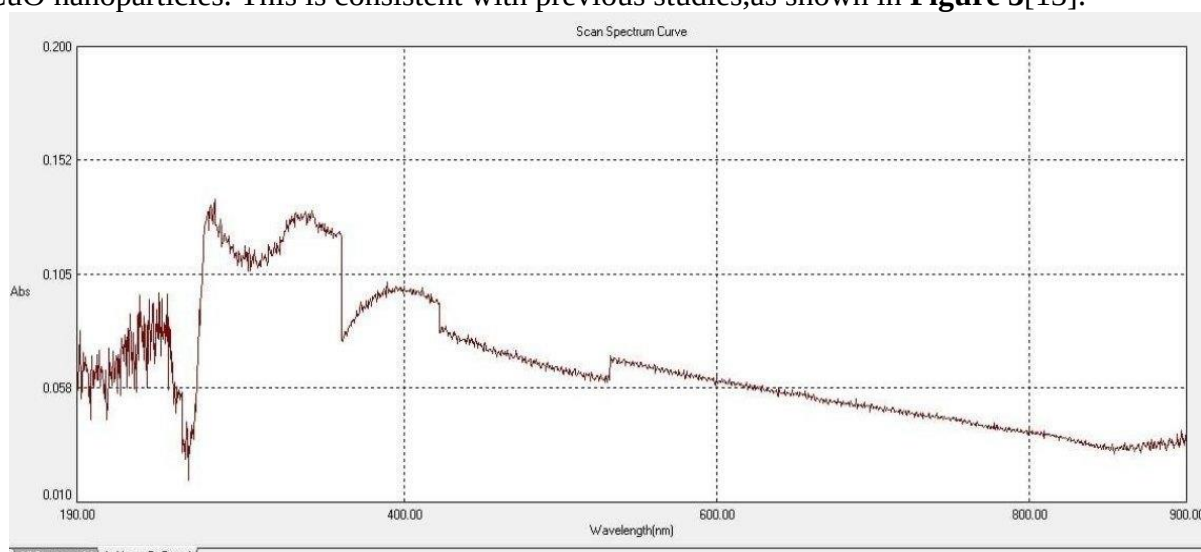


Figure 3. UV-Vis Spectrum of CuO NPs

1.3. X-Ray Diffraction (XRD)

Copper oxide nanoparticles CuO NPs were analyzed using X-ray diffraction (XRD) to determine their crystal structure and crystal size. The spectrum showed diffraction peaks at (2θ) angles of 32.10° , 35.40° , 38.20° , 41.48° , 53.50° , and 61.20° , which correspond to the (110), (002), (111), (131), (123), and (002) crystal planes, respectively. These peaks indicate the formation of a highly crystalline material with a characteristic crystalline quality. The average crystal size was calculated using the Scherrer equation and was found to be (21.4) nm, confirming the stable nanoscale nature of the prepared particles, as shown in **Figure 4**[14].

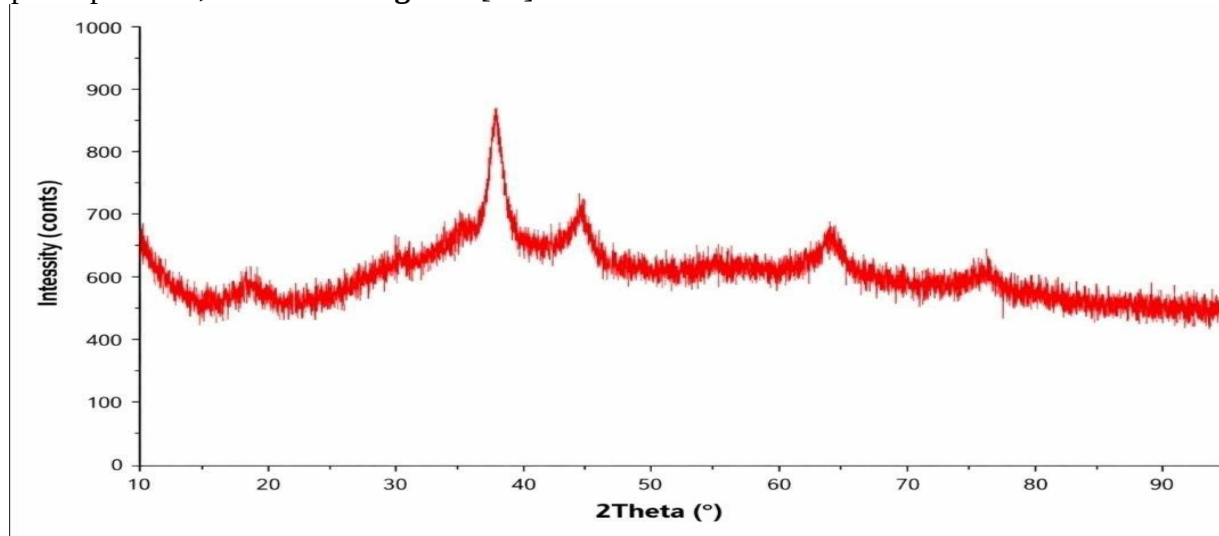


Figure 4. X-Ray diffraction of Prepared CuO NPs

1.4. FE-Scanning Electron Microscopy (FE-SEM)

Scanning electron microscopy (SEM) was used to study the surface structure and size of copper oxide nanoparticles CuO NPs. Images showed that the particle size ranged from (36 to 56) nm, with a rough, heterogeneous surface structure and the presence of agglomerates and cracks—a common phenomenon in nanomaterial fabrication. The plant extract used in the preparation is believed to have contributed to the formation of these agglomerates through its influence on the shaping process. At high magnification, irregular, quasi-spherical particles were observed, confirming the nanoscale nature of the material and reflecting an increased specific surface area, which enhances its suitability for surface-interacting applications, as shown in **Figure 5**[15].

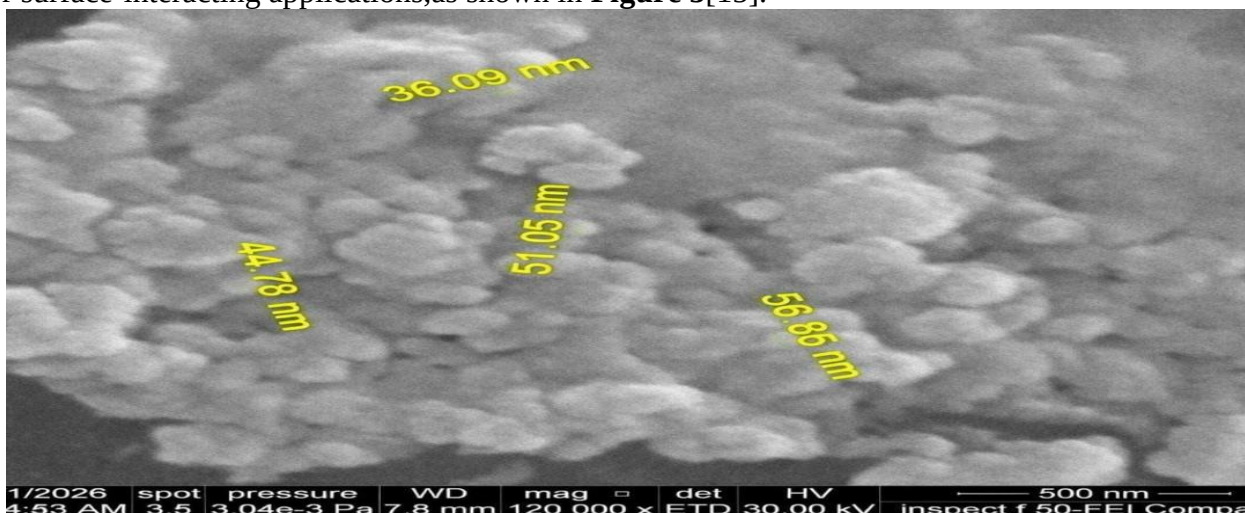


Figure 5. Scanning electron microscopy of Prepared CuO NPs

1.5. Atomic Force Microscopy (AFM)

Copper oxide nanoparticles CuO NPs were analyzed using atomic force microscopy (AFM). Threshold detection revealed 668 particles with a surface coverage of 51.15%, an average diameter of (66.49) nm, and a maximum height of 322.5 nm, indicating a dense and homogeneous distribution and a high effective surface area. Roughness parameters showed that the average surface height (S_a) = 16.59 nm and standard deviation (S_q) = 23.19 nm indicate moderate nano-roughness, with

maximum values of $S_p = 200.8$ nm and $S_v = 57.58$ nm, and a maximum height range of $S_z = 258.3$ nm. Positive values for the standard deviation (S_{sk}) = 1.895 and the kurrhagia (S_{ku}) = 11.87 indicate that the surface has more ridges than pits, with sharp peaks, which supports the surface activity of the nanomaterial, as shown in **Figure 6**[16].

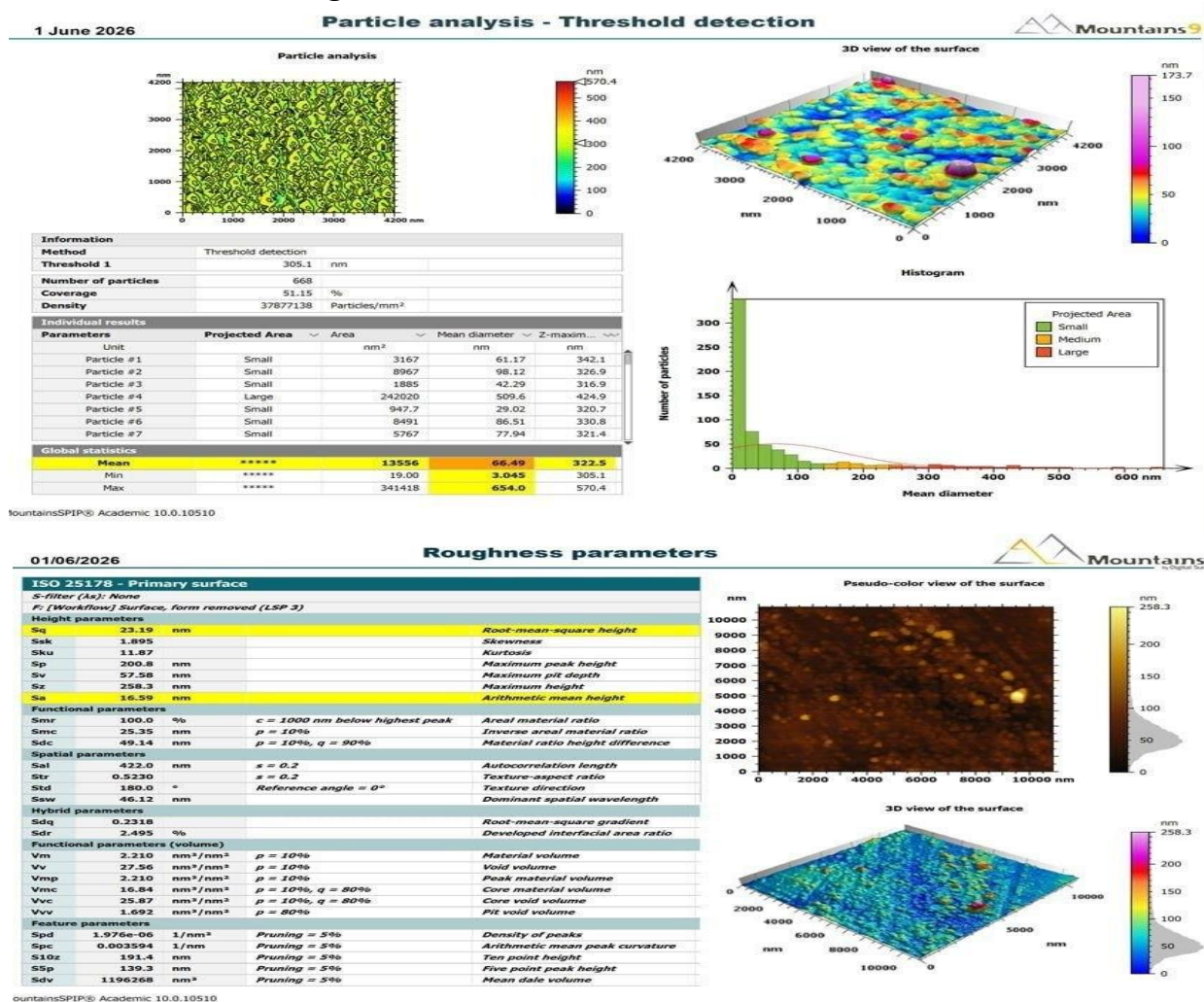


Figure 6. Atomic Force Microscopy of Prepared CuO NPs

2. Chemical analyses of The paroxetine drug

2.1. UV-Vis Spectrum

The visible and ultraviolet (UV-visible) spectrum of paroxetine appears within the range of 200-800 nm. The spectrum, as shown in Figure, exhibits a single major absorption peak that begins to rise at a wavelength of 210 nm and continues to rise to a wavelength of 293 nm. The absorption coefficient (Abs) is 0.8. The appearance of this peak is attributed to the presence of the amine in the drug. The sharp shape of the peak reflects the purity of the compound, as shown in **Figure 7**[17].

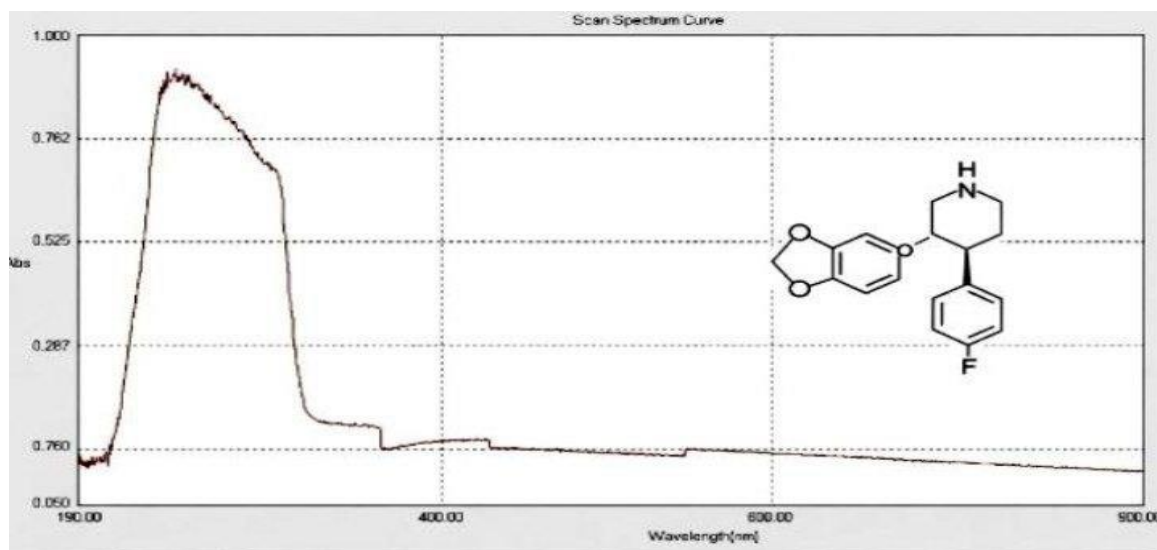


Figure 7. UV-Vis of Paroxetine drug

2.2. Infrared Spectrum

The visible and ultraviolet (UV-visible) spectrum of paroxetine appears within the range of 200-800 nm. The spectrum, as shown in Figure (), exhibits a single major absorption peak that begins to rise at a wavelength of 210 nm and continues to rise to a wavelength of 293 nm. The absorption coefficient (Abs) is 0.8. The appearance of this peak is attributed to the presence of the amine in the drug. The sharp shape of the peak reflects the purity of the compound, as shown in **Figure 8 and Table2**[18].

Table 2. Represents the most important bands appearing in the FT-IR of The Paroxetine drug

Material	$\mu(\text{C-H})$	$\mu(\text{C-H})$	$\mu(\text{C=N})$	$\mu(\text{C=C})$	$\mu(\text{C-N})$
Drug	3334	2891	1674	1616	1319-
Paroxetine					1510

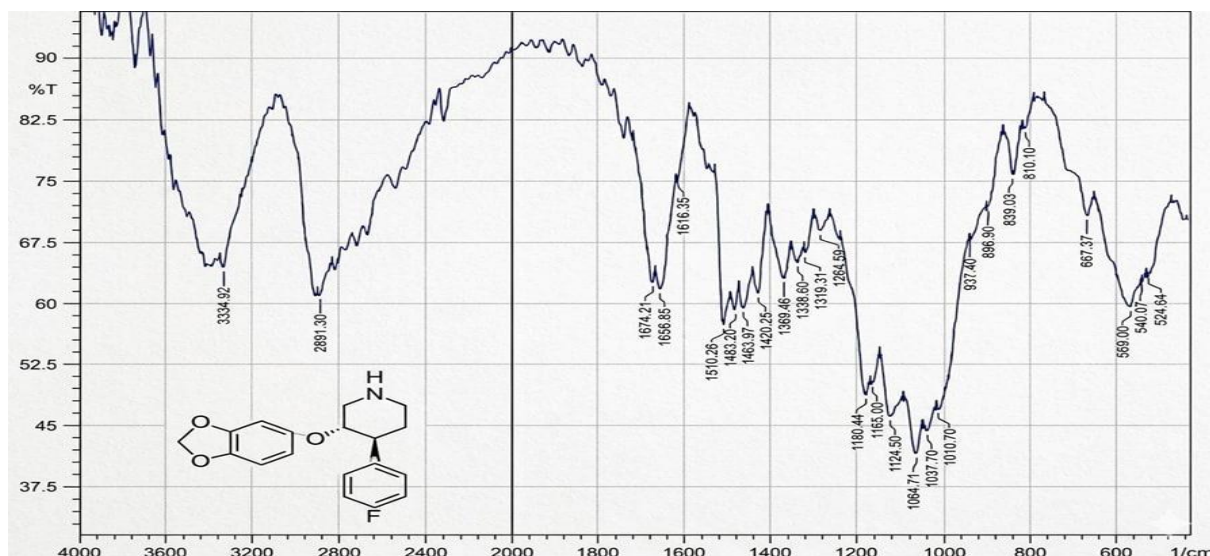
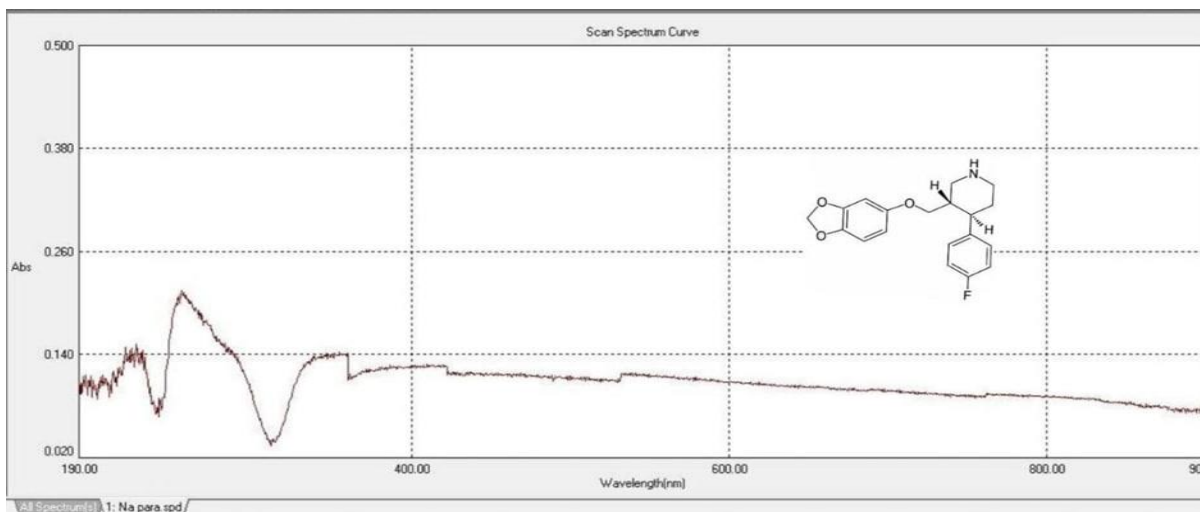


Figure 8. FT-IR of paroxetine drug

3. Chemical analysis of The nano- activation paroxetine drug

3.1. UV-Vis Spectrum

The visible and ultraviolet (UV-Visible) spectrum of nano-activation paroxetine appears within the 200-400 nm range. A clear change in the spectrum is observed in the position and intensity of the peaks. The peaks begin to rise at a wavelength of 190 nm and extend to 340 nm. The absorption intensity (Abs = 0.14) is also noteworthy. This indicates the formation of a new compound, compared to the spectrum of the drug paroxetine and the nanoscale spectrum alone, as shown in **Figure 9**[19].



Figure(9): UV-Vis for The nano-activation paroxetine drug

3.2. Infrared Spectrum

Infrared spectroscopy is an important analytical tool for identifying functional groups in organic compounds. We observe distinct peaks in the IR spectrum of nano-activation paroxetine. A peak at 3360 nm is attributed to N-H vibrations, and another at 2891 nm is attributed to C-H vibrations. Additionally, C=N bands appear at 1699 nm, and bands between 4899 and 896 nm are attributed to Cu-O vibrations. The appearance of these bands indicates an interaction between the nanoparticles and the drug, as shown in **Figure 10 and Table 3**[20].

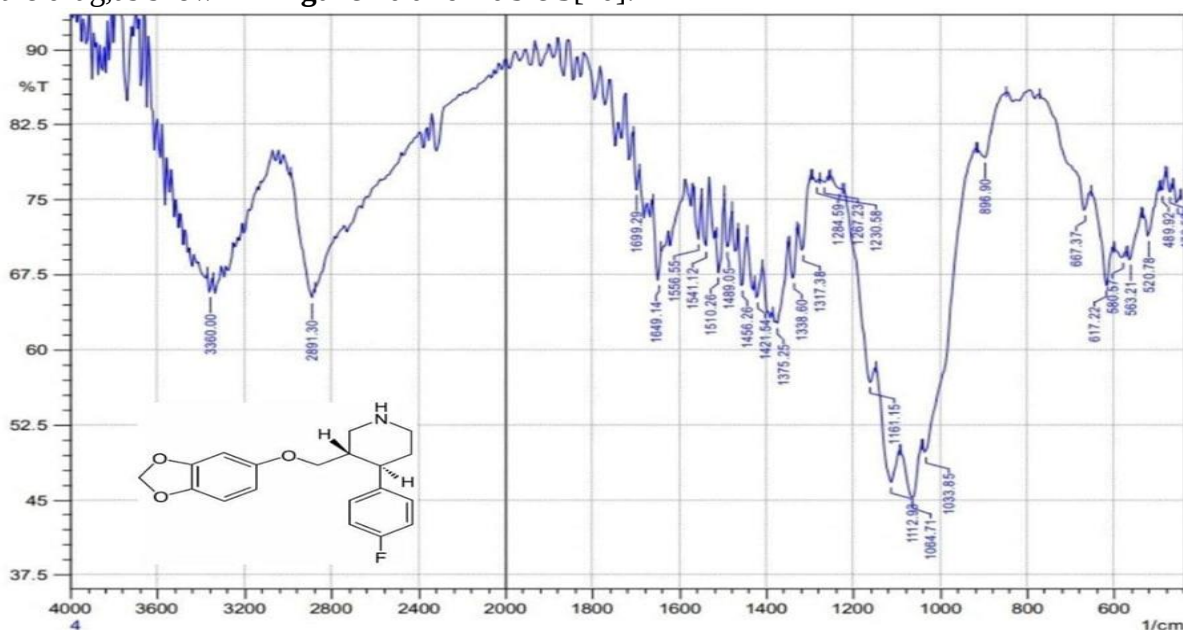


Figure 10. FT-IR of nano-activation paroxetine drug

Table 3. Spectral bands of FT-IR nano- activation paroxetine drug

Material	$\mu(\text{N-H})$	$\mu(\text{C=N})$	$\mu(\text{C=C})$	$\mu(\text{C-O})$	$\mu(\text{Cu-O})$
Nano-activation drug paroxetine	3360	1649-1699	1458-1510	1033-1284	896-489

4. Determination of Calibration Curve for Vanadium and Nickel Ions

To establish the standard calibration curve for vanadium and nickel ions, several solutions with concentrations ranging from 2 to 12 mg/L for each ion were prepared. The absorbance values of these solutions were then recorded at the maximum wavelength of 760 nm for vanadium and 398 nm for nickel.

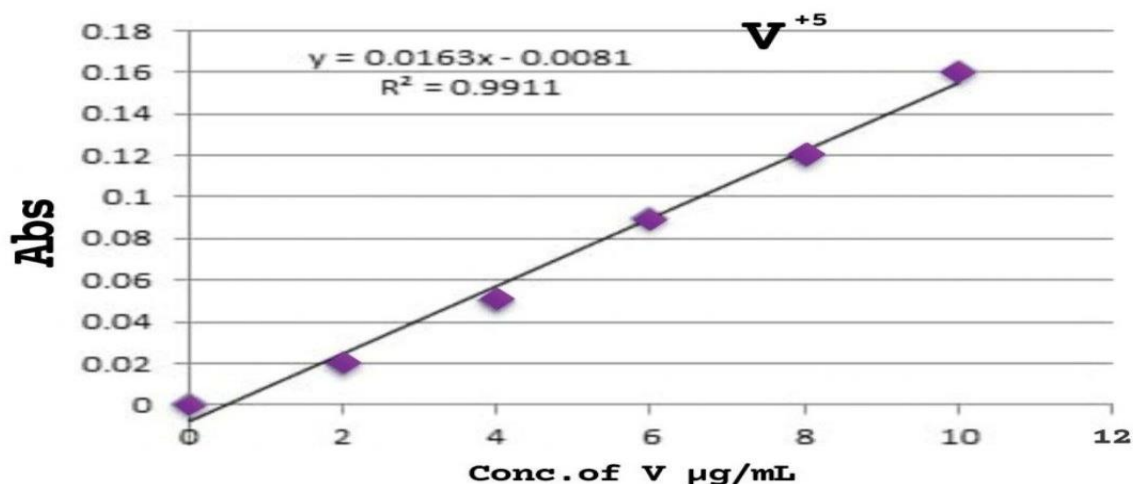


Figure 11. Stander titration curve for vanadium ion

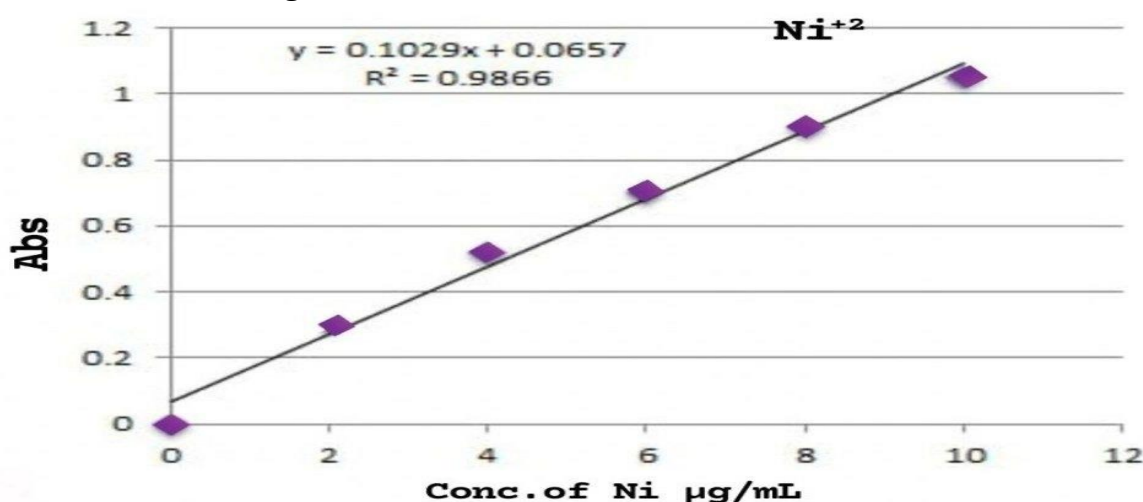


Figure 12. Stander titration curve for Nickel ion

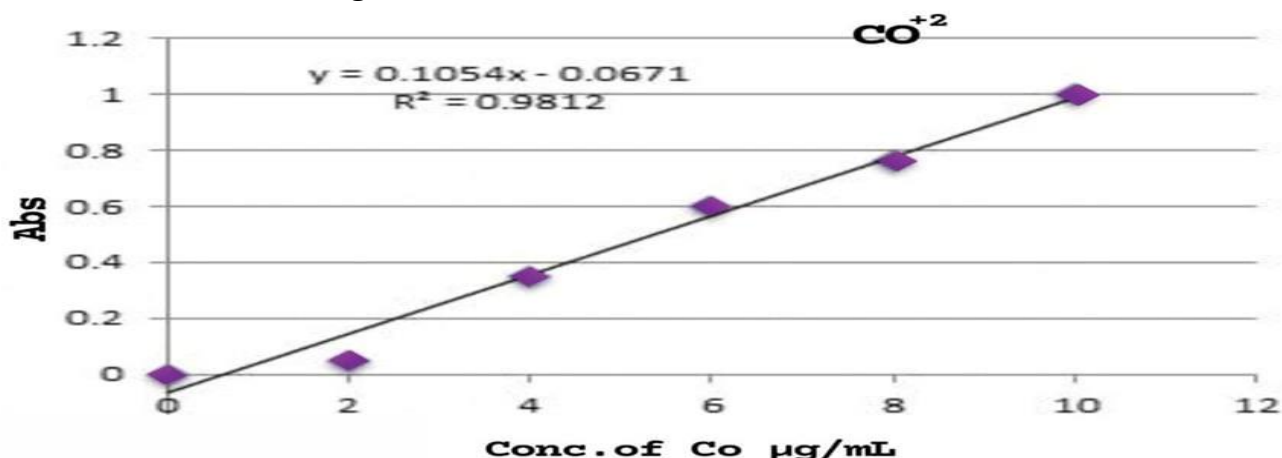


Figure 13. Stander titration curve for Cobalt ion

5. Determining the optimal condition for heavy metal removal using nano-catalyzed amine

Effect of PH

The pH of the sample solution is a critical factor influencing the removal efficiency of heavy metals from aqueous media. The effect of pH on the removal of vanadium and nickel ions was investigated at values of 3, 7, and 9, adjusted using NaOH and HCl, and monitored with a pH meter. The objective was to determine the optimal pH for maximum removal efficiency. The results demonstrated that removal efficiency increased with rising pH, reaching its highest value at pH 9, where the most favorable state for adsorption[21].

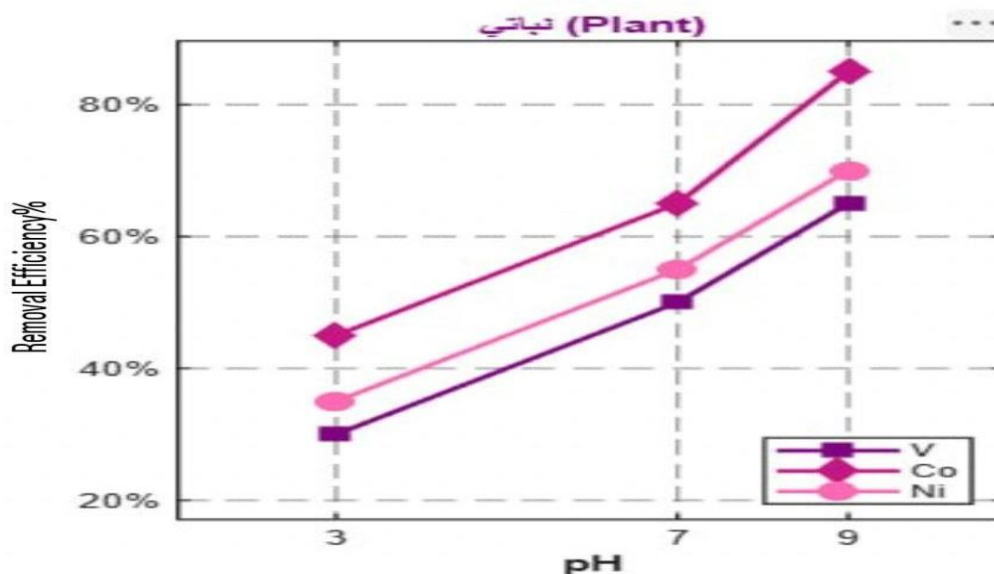


Figure 14. Effect of pH on element removal efficiency

Effect of Temperature

The effect of temperature on the removal process was studied at 5, 25, and 60 °C to determine the optimal condition. Results indicated that removal efficiency increased with rising temperature, confirming an endothermic adsorption process. The enhancement is attributed to higher ion kinetic energy and activation of surface functional groups, which facilitate coordination bonding. Therefore, 60 °C was identified as the optimal temperature for maximum removal efficiency[22].

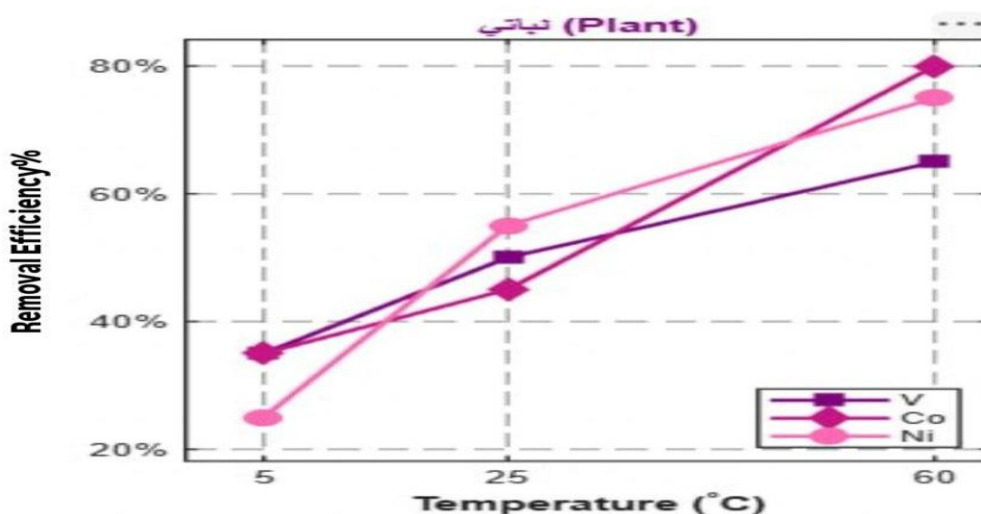


Figure 15. Effect of temperature on element removal efficiency

Effect of different Concentration

The effect of nanomaterial concentration on the adsorption efficiency of Ni^{2+} , V^{5+} , Co^{2+} ions was investigated at different dosages (0.1, 0.5, and 1 g). Increasing the nanomaterial amount enhanced removal efficiency due to the availability of more active binding sites and the large surface area. The highest removal efficiency was achieved at 1 g, indicating this dosage as the optimal concentration[23].

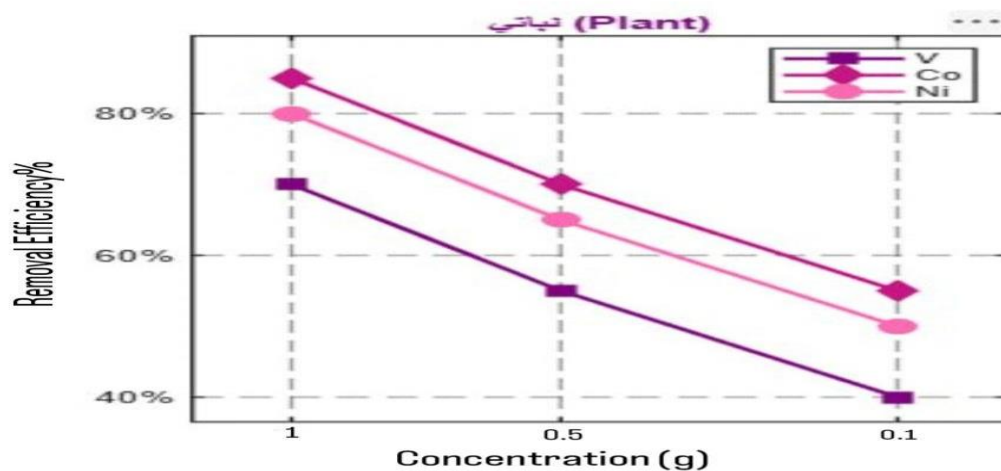


Figure 16. Effect of concentration on element removal efficiency

Effect of time

The results showed that increasing the contact time between the ions and the nanomaterial provides a greater opportunity for the ions to cross into the active sites on the particle surface. The results indicated that a time of (30 min) is optimal, at which the removal rate is relatively high[24].

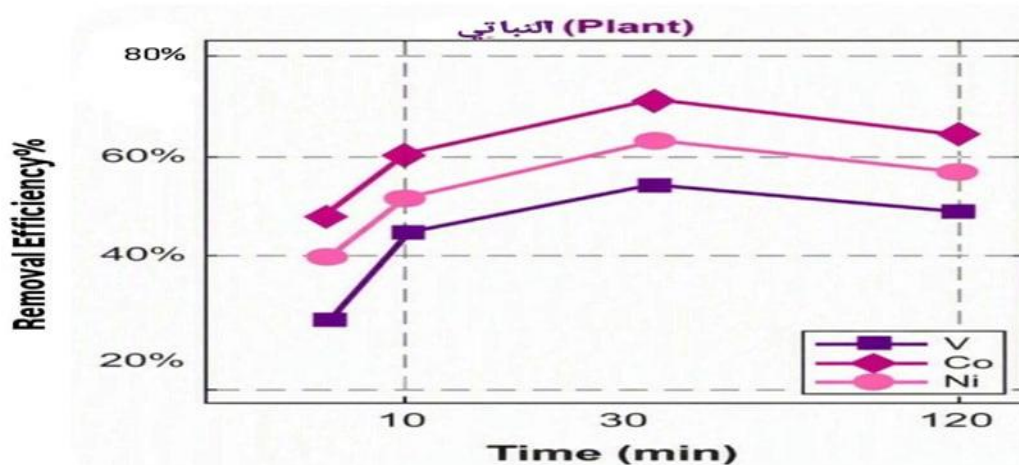


Figure 17. Effect of time on element removal efficiency

6. Real Samples

6.1. Removal of Heavy metals from water samples using amine pharmaceutical nano-activation

The results of water sample analysis using the nano-catalyzed pharmaceutical amine showed a clear difference in both the removal percentage and adsorption capacity of the studied elements (nickel, cobalt, and vanadium) in the Al-Gharraf, Al-Fadhiliya, and Al-Nasiriyah regions. This difference indicates the influence of varying environmental conditions in each region. Nickel recorded the highest removal percentage in Al-Nasiriyah at 99.1% and the lowest in Al-Gharraf at 92.0%. Cobalt also recorded the highest percentage in Al-Nasiriyah at 98.7% and the lowest in Al-Gharraf at 94.1%. Vanadium also recorded the highest percentage in Al-Nasiriyah at 96.6% and the lowest in Al-Gharraf at 95.4%. This indicates that the nano-catalyzed pharmaceutical amine possesses high chemical purity and uniformity in its active (amine) group, as shown in **Figure 18 and Table 4**

Table 4. Estimation of Adsorption Capacity and Removal Efficiency of Heavy Metals in Water Samples Using Amine pharmaceutical nano-activation

Element	Region	Co	Ce	Qm	Removal Efficiency
Ni	Al-Gharraf	1.207	0.096	11.11	92.0
	Al-Fadhliyya	1.378	0.035	13.43	97.5
	Al-Nasiriyah	1.467	0.013	14.54	99.1
CO	Al-Gharraf	1.054	0.063	9.91	94.1
	Al-Fadhliyya	1.296	0.055	12.41	95.8
	Al-Nasiriyah	1.398	0.018	13.80	98.7

V	Al-Gharraf	1.336	0.062	12.68	95.4
	Al-Fadhliyya	1.352	0.053	12.72	96.1
	Al-Nasiriyah	1.253	0.042	12.97	96.6

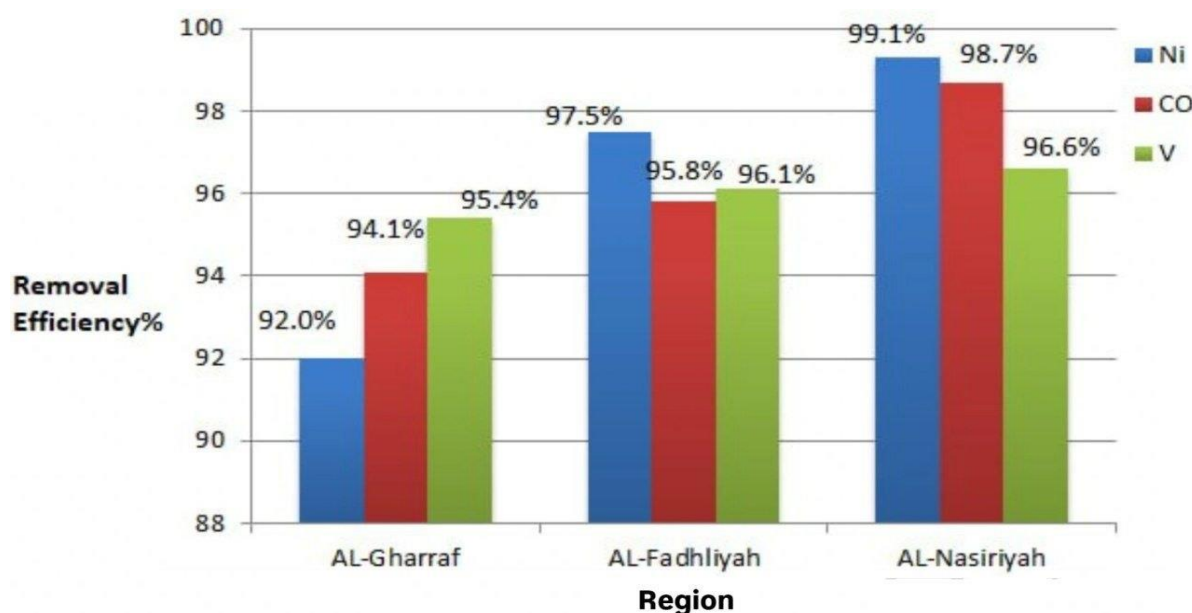


Figure 18. Shows the Percentage of heavy metal removal in water samples

6.2. Removal of Heavy metals from Soil samples using amine pharmaceutical nano-activation

The results of soil sample analysis using the nano-catalyzed pharmaceutical amine showed a clear difference in both the removal percentage and adsorption capacity of the studied elements (nickel, cobalt, vanadium) in the Al-Gharraf, Al-Fadhiliya, and Al-Nasiriyah regions. This difference reflects the effect of the physical and chemical properties of the soil. Nickel recorded the highest removal percentage in the Al-Nasiriyah region at 98.5% and the lowest percentage in the Al-Gharraf region at 97.2%. Cobalt recorded the highest percentage in the Al-Fadhiliya region at 98.2% and the lowest percentage in Al-Gharraf at 96.4%. As for vanadium, it recorded the highest percentage in the Al-Fadhiliya region at 99.2% and the lowest percentage in the Al-Gharraf region at 92.3%. This indicates that the nano-catalyzed pharmaceutical amine possesses high chemical purity and regularity in the active (amine) group, as shown in **Figure 19** and **Table 5**

Table 5. Estimation of Adsorption Capacity and Removal Efficiency of Heavy Metals in Soil Samples Using Amine pharmaceutical nano-activation

Element	Region	Co	Ce	Qm	Removal Efficiency
Ni	Al-Gharraf	1.245	0.034	12.11	97.2
	Al-Fadhliyya	1.219	0.025	11.94	97.9
	Al-Nasiriyah	1.280	0.018	12.62	98.5
CO	Al-Gharraf	1.280	0.045	12.35	96.4
	Al-Fadhliyya	1.102	0.019	10.83	98.2
	Al-Nasiriyah	1.229	0.033	11.96	97.2
V	Al-Gharraf	1.200	0.093	11.07	92.3
	Al-Fadhliyya	1.260	0.010	12.50	99.2
	Al-Nasiriyah	1.354	0.064	12.90	95.3

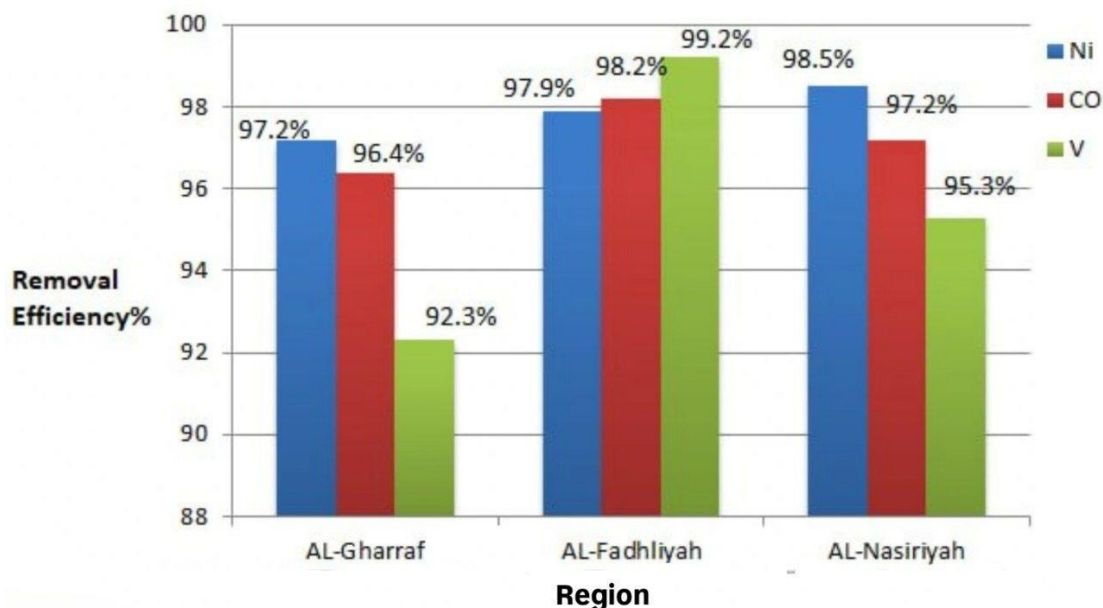


Figure 19. Shows the Percentage of heavy metal remove in soil samples

6.3. Removal of Heavy metals from Plant samples using Amine pharmaceutical nano-activation

Analysis of plant samples using nano-catalyzed pharmaceutical amines revealed significant differences in both the removal percentage and adsorption capacity of the studied elements (nickel, cobalt, and vanadium) in the Al-Gharraf, Al-Fadhliya, and Al-Nasiriyah regions. This variation reflects the environmental conditions, plant characteristics, and soil types in each region. Nickel recorded the highest removal percentage in Al-Nasiriyah at 99.8% and the lowest in Al-Gharraf at 97.9%. Cobalt also recorded its highest percentage in Al-Nasiriyah at 98.8% and its lowest in Al-Gharraf at 94.8%. Similarly, vanadium recorded its highest percentage in Al-Nasiriyah at 97.9% and its lowest in Al-Gharraf at 94.8%. This indicates that the nano-catalyzed pharmaceutical amine possesses high chemical purity and uniformity in its active (amine) group, as shown in **Figure 20 and Table 6**

Table 6. Estimation of Adsorption Capacity and Removal Efficiency of Heavy Metals in Plant Samples Using Amine pharmaceutical nano-activation

Element	Region	Co	Ce	Qm	Removal Efficiency
Ni	Al-Gharraf	1.423	0.029	13.93	97.9
	Al-Fadhliyya	1.387	0.014	13.73	98.9
	Al-Nasiriyah	1.422	0.002	14.20	99.8
CO	Al-Gharraf	1.386	0.068	13.18	95.1
	Al-Fadhliyya	1.163	0.046	11.17	96.0
	Al-Nasiriyah	1.247	0.014	12.33	98.8
V	Al-Gharraf	1.288	0.062	12.26	94.8
	Al-Fadhliyya	1.367	0.061	13.06	95.5
	Al-Nasiriyah	1.256	0.026	12.30	97.9

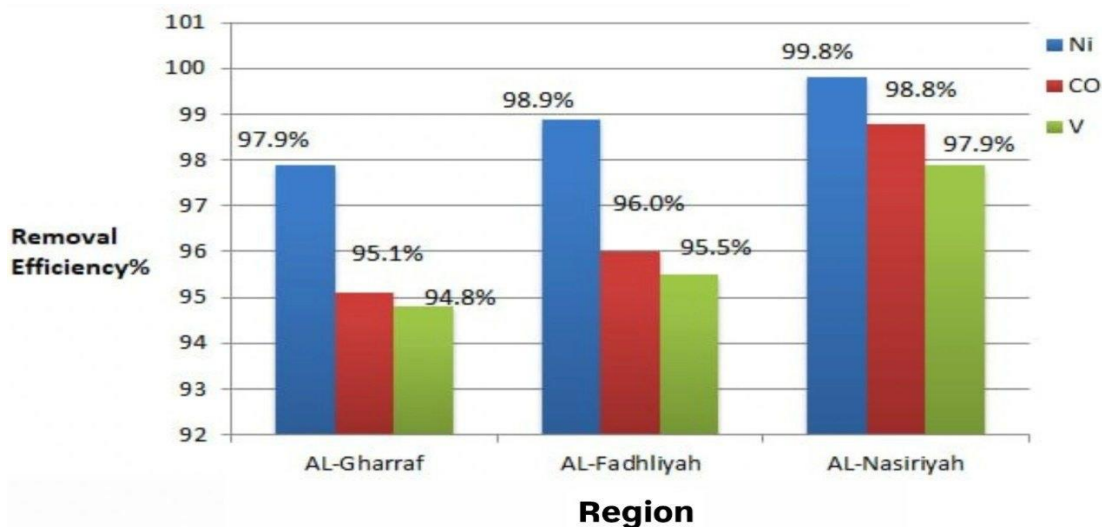


Figure 20. Shows the Percentage of heavy metal remove in Soil samples

6.4. Removal of Heavy Metals from Herbal Extract Samples Using Amine pharmaceutical nano-activation

The results for the herbal samples (tea, fenugreek, and anise) using the nano-activated pharmaceutical amine showed a clear difference in both the removal percentages and adsorption capacities of the studied elements (nickel, cobalt, and vanadium). This difference reflects the nature of the active compounds present in each herbal type. Tea extract recorded the highest percentages for nickel (99.0%), cobalt (99.1%), and vanadium (98.8%), while anise had the lowest percentages for all elements, at nickel (97.1%), cobalt (93.7%), and vanadium (95.8%). Although the values were lower, they were still high, indicating the effectiveness of the adsorbent, as shown in **Figure 21** and **Table 7**. Estimation of Adsorption Capacity and Removal Efficiency of Heavy Metals in Her Samples Using Amine pharmaceutical nano-activation

Element	Herbal Extract	Co	Ce	Qm	Removal Efficiency
Ni	Blacktea	2.42	0.024	23.96	99.0
	Fenugreek	2.08	0.029	20.51	98.6
	Anise	2.19	0.063	21.27	97.1
CO	Black tea	3.00	0.027	29.73	99.1
	Fenugreek	2.55	0.100	24.50	96.1
	Ainse	2.78	0.174	26.06	93.7
V	Black tea	3.46	0.041	34.19	98.8
	Fenugreek	2.14	0.067	20.73	96.9
	Ainse	2.28	0.109	24.71	95.8

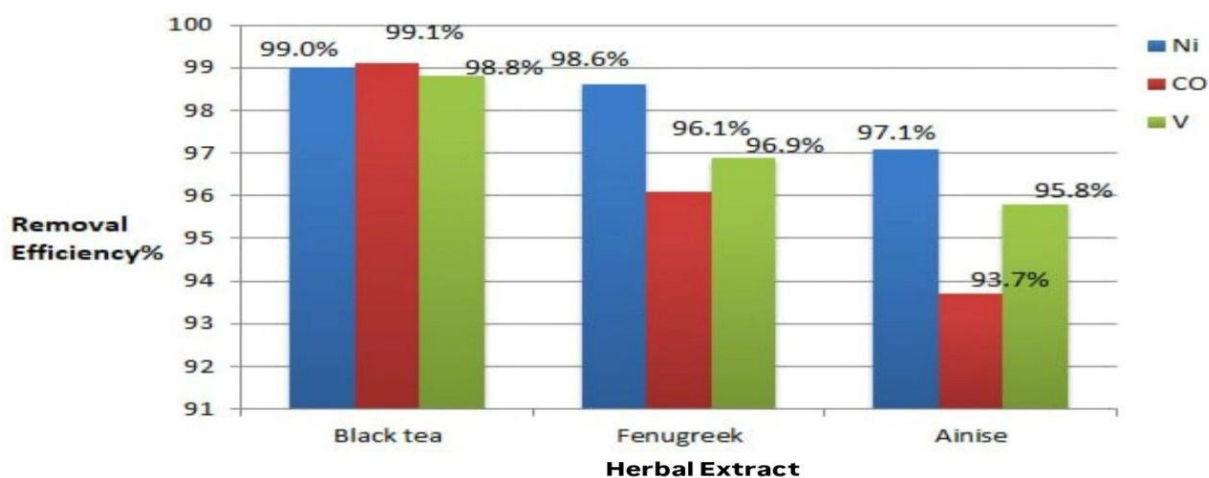


Figure 21. Shows the Percentage of heavy metal remove in Plant samples

7. Adsorption Isotherms

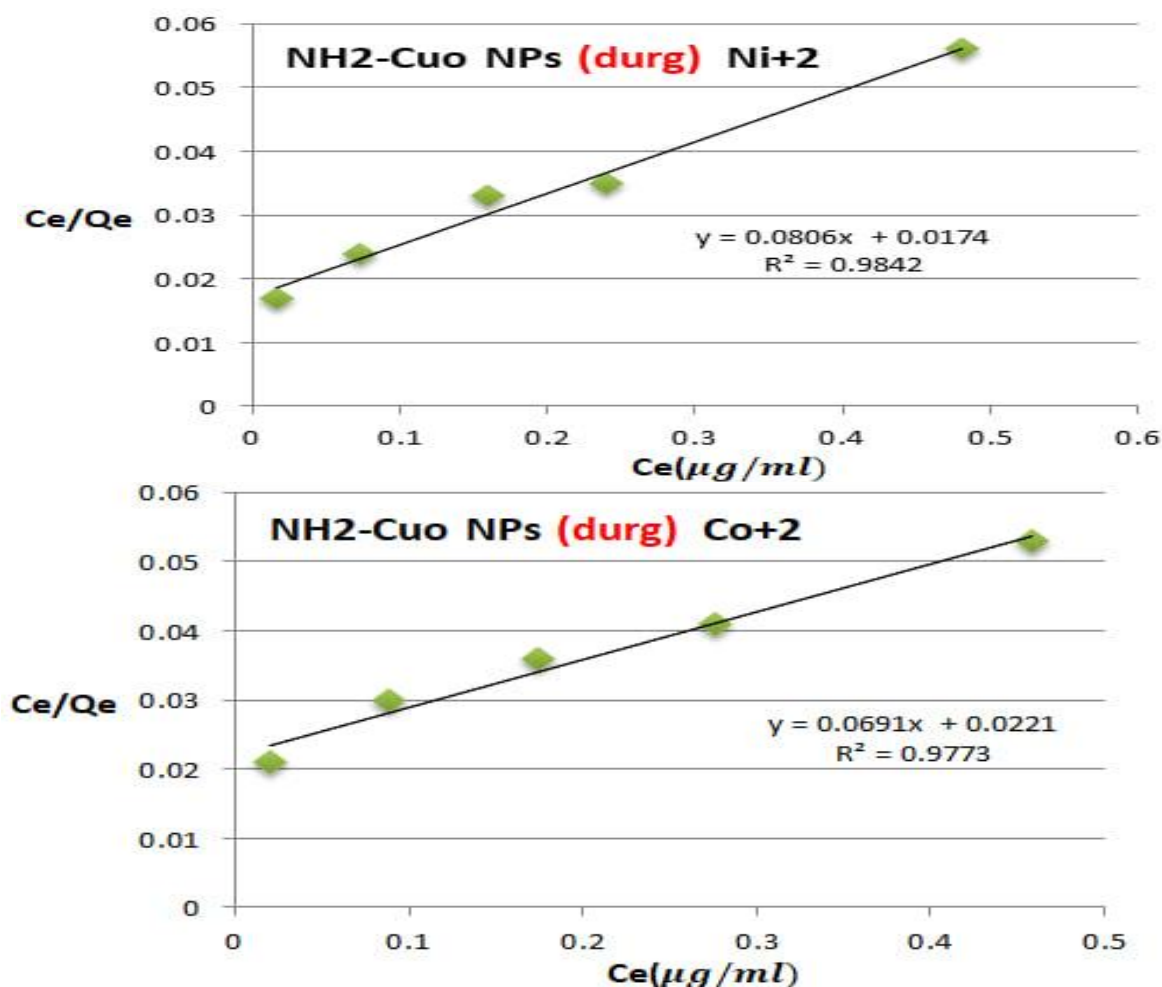
7.1. Adsorption of nickel and cobalt and vanadium ions to nano-catalyzed amines according to the Langmuir equation

In this study, the Langmuir equation, considered the simplest and most widely used model, was employed to explain the adsorption of nickel, cobalt, and vanadium ions using a pharmaceutical amine activation with nanotechnology. The Langmuir equation assumes that adsorption occurs on a homogeneous, single-layer surface and that all effective adsorption sites are equivalent in energy[25]. The study was conducted according to the Fedandlich equation:

$$\frac{Ce}{Qe} = \frac{1}{Qm \cdot b} + \frac{Ce}{Qm}$$

Table 8. Values for the adsorption of nickel, cobalt, vanadium ions by amine pharmaceutical nano-activation according to the Langmuir equation

Adsorbent	Co	Ni			Co			V		
		Ce	Qe	Ce/Qe	Ce	Qe	Ce/Qe	Ce	Qe	Ce/Qe
NH ₂ -CuO NPs	1	0.016	0.984	0.163	0.020	0.098	0.059	0.012	0.988	0.013
	3	0.073	0.299	0.249	0.089	0.291	0.204	0.056	2.944	0.019
	5	0.160	0.484	0.331	0.175	0.482	0.306	0.199	4.801	0.042
	7	0.240	0.676	0.355	0.276	0.672	0.410	0.263	6.737	0.039
	9	0.481	0.852	0.565	0.458	0.852	0.536	0.458	8.542	0.054



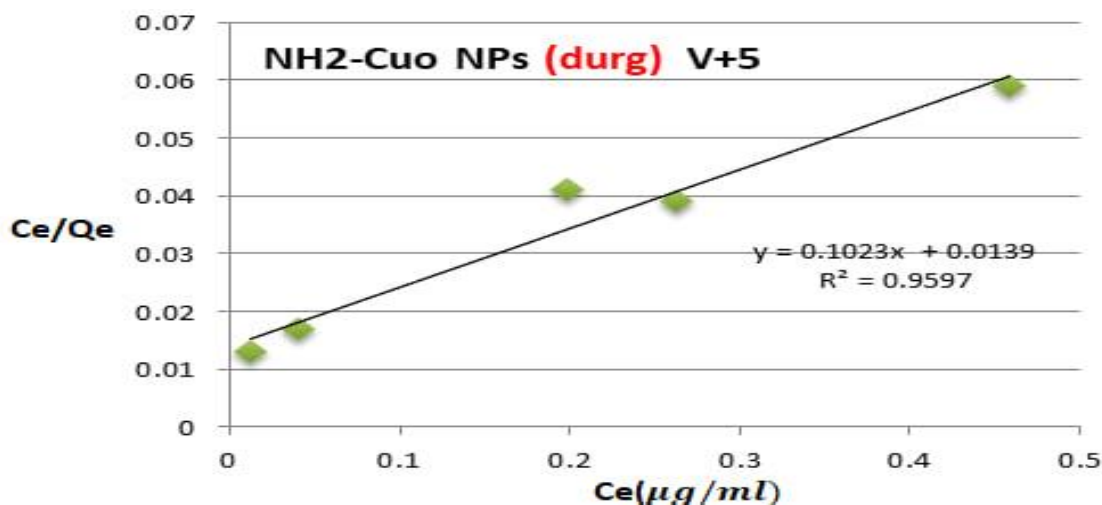


Figure 22.Shows the equation of straight line and Langmuir constant

Table 9. Langmuir Constant values

Element	Adsorbent	Qm	b	R2
Ni	NH2-CuO NPs	12.41	4.63	0.9842
Co	NH2-CuO NPs	14.74	3.14	0.9773
V	NH2-CuO NPs	9.78	7.36	0.9597

7.2. Adsorption of nickel and cobalt and vanadium ions to nano-catalyzed amines according to the freundlich equation

The Freundlich equation assumes that adsorption occurs on a heterogeneous surface and is affected by layering and energy variations at the adsorption sites[26]. The study was conducted according to the Freundlich equation.

$$\text{Log } Q_e = \text{Log } k_f + \frac{1}{n} * \text{Log } C_e$$

Table 10.Values for the adsorption of nickel, cobalt,vanadium ions by amine pharmaceutical nano-activation according to the freundlich equation

Adsorbent	Co	Ni		Co		V	
		Log Ce	Log Qe	Log Ce	Log Qe	Log Ce	Log Qe
NH2-CuO NPs	1	-1.796	-0.007	-1.699	-0.009	-1.920	-0.005
	3	-1.137	0.466	-1.051	0.464	-1.252	0.469
	5	-0.796	0.685	-0.757	0.683	-0.701	0.681
	7	-0.620	0.830	-0.559	0.827	-0.580	0.829
	9	-0.318	0.930	-0.339	0.931	-0.339	0.931

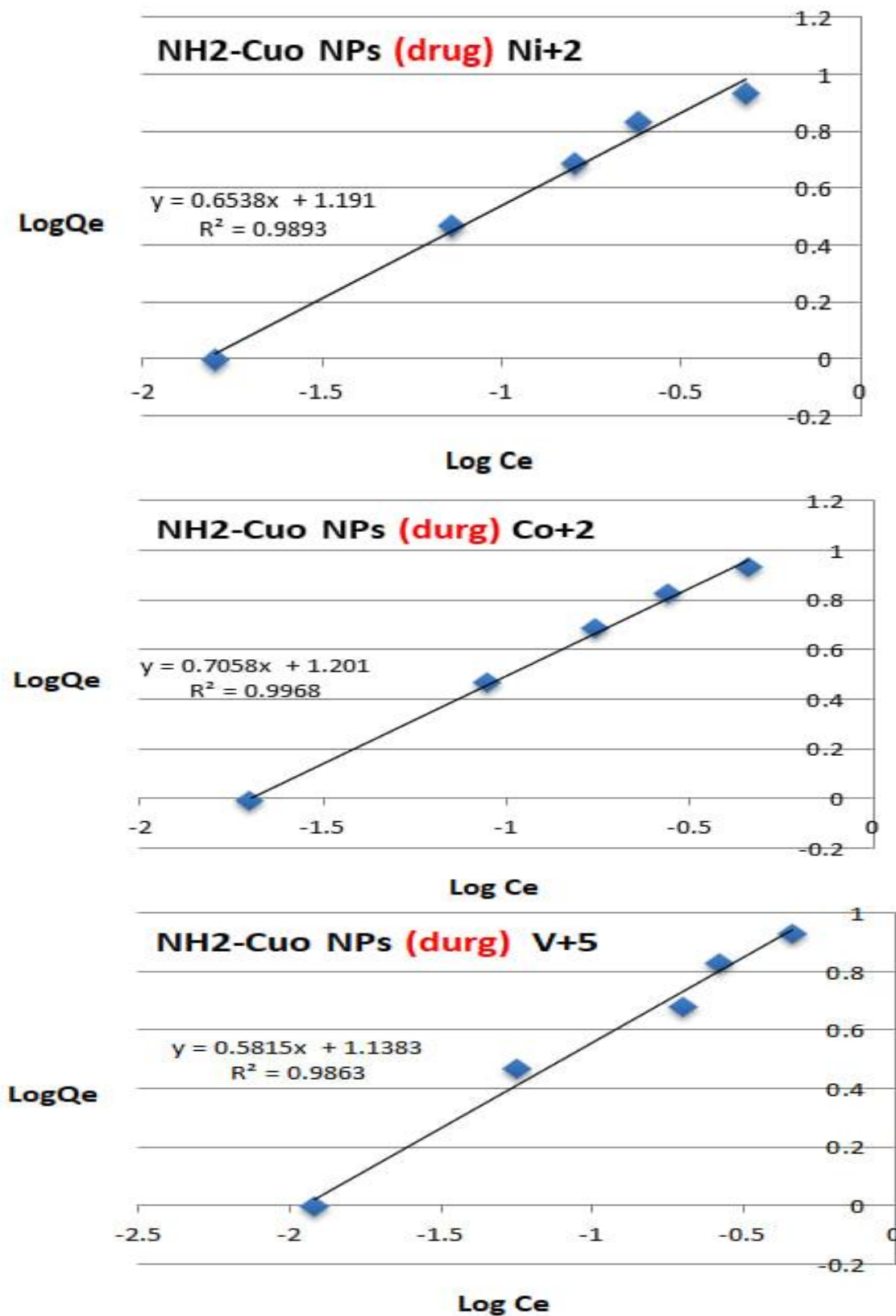


Figure 23. shows the equation of straight line and freundlich constant
Table 11.Freundlich constant values

Element	Adsorbent	Qm	b	R2
Ni	NH2-CuO NPs	1.53	15.5	0.9893
Co	NH2-CuO NPs	1.42	15.9	0.9968
V	NH2-CuO NPs	1.72	13.7	0.9863

Conclusion

In this work, an efficient and environmentally friendly method was developed for preparing copper oxide nanoparticles to catalyze the paroxetine amine, aiming to improve its removal efficiency. The results showed that the nano-catalyzed pharmaceutical amine exhibited high efficiency in removing heavy metals (nickel, cobalt, and vanadium) in real samples (black tea, fenugreek, and anise). This method is not only efficient but also environmentally friendly, safe, and cost-effective.

References

- [1] R. R. Appannagari, "Environmental pollution causes and consequences: A study," *International Research Journal of Social Sciences and Humanities*, vol. 3, no. 8, pp. 151–161, 2017.
- [2] H. M. Aieshan, "Studies on some heavy metals removal in industrial and drinking water: A review," *University of Thi-Qar Journal of Science (UTJsc)*, vol. 12, no. 2, pp. 34–42, Dec. 2025, doi: 10.32792/utq/utjsci/v12/2/1404.
- [3] N. M. Aljamali, R. A. Aldujaili, and I. O. Alfaltawi, "Physical and chemical adsorption and its applications," *International Journal of Thermodynamics and Chemical Kinetics*, vol. 7, no. 2, 2021.
- [4] K. S. Baidya and U. Kumar, "Adsorption of brilliant green dye from aqueous solution onto chemically modified areca nut husk," *South African Journal of Chemical Engineering*, vol. 35, pp. 33–43, 2021.
- [5] M. Kowalska, J. Nowaczyk, T. Fijatkowski, and A. Nowaczyk, "Paroxetine—Overview of the molecular mechanisms of action," *International Journal of Molecular Sciences*, vol. 22, no. 4, Art. no. 1662, Feb. 2021.
- [6] S. T. Jawad and E. J. A. Kadhem, "Assessment of the concentration of some heavy metals of selected soils from Shattrah city," *University of Thi-Qar Journal of Science (UTsci)*, vol. 6, no. 1, pp. 45–52, Dec. 2016.
- [7] F. W. Alterm and T. D. Zeldek, "Green synthesis of silver and cobalt oxide nanoparticles using plant extract and evaluation of their antibacterial activity," *Nanomed Journal*, vol. 11, no. 1, pp. 8–22, Winter 2024.
- [8] J. J. Sephra, P. Barneechdaram, M. Sivakumar, T. D. Thangadurai, and K. Nehru, "CuO/SiO₂ modified amine-functionalized reduced graphene oxide with enhanced photocatalytic and electrochemical properties," *SN Applied Sciences*, Springer Nature, 2024.
- [9] M. A. Al-Kazareji, D. T. Al-Heremi, and A. A. Hiridan, "Adsorption of 4-chlorophenol from aqueous solution onto Iraqi bauxite: Equilibrium, kinetic, and thermodynamic studies," *Oriental Journal of Chemistry*, vol. 33, no. 6, p. 2083, 2017.
- [10] S. Shintre, S. Kolhe, S. Vidhate, and S. Padmanabhan, "A simple and novel method to reduce heavy metal contamination from aqueous solutions and herbal extracts," *Med Discoveries*, vol. 3, no. 7, pp. 1–10, Jul. 2024.
- [11] A. Salem, "Assessment of heavy metals contamination of agricultural soils using pollution indicators in Thi-Qar governorate, Southern Iraq," *University of Thi-Qar Journal of Science (UTsci)*, vol. 11, no. 2, Dec. 2023.
- [12] K. R. Patil, K. Shirsat, and R. Kumbhar, "Synthesis of bimetallic nanoparticles and their photocatalytic performance," *Proceedings of Acta Materialia*, vol. 26, Art. no. 120202, 2022.
- [13] O. P. Keseadika and A. O. Akanni, "Comparative study on synthesis and characterization of copper oxide nanoparticles," *Journal of Chemical Sciences*, vol. 18, no. 2, pp. 125–132, 2020.
- [14] M. M. Chikkaman, S. Neelagund, and M. B. Hiremath, "Biological synthesis, characterization, and photocatalytic activity of copper oxide nanoparticles (CuO NPs)," *Journal of Biomolecular Structure and Dynamics*, vol. 12, no. 1, pp. 92–99, 2018.
- [15] A. Yasin *et al.*, "Fabrication of copper oxide nanoparticles using *Passiflora edulis* extract for the estimation of antioxidant potential and photocatalytic methylene blue dye degradation," *Agronomy*, vol. 12, no. 10, Art. no. 2315, 2022.
- [16] R. Chandrasekaran, S. A. Yadav, and S. Sivaperumal, "Phytosynthesis and characterization of copper oxide nanoparticles using *Trigonella foenum-graecum* extract and evaluation of their antibacterial and antioxidant activities," *Agronomy*, vol. 12, Art. no. 230, 2020.

- [17] I. Darwish, H. Abidin, S. Amer, and L. Al-Reis, "Simple spectrophotometric method for determination of paroxetine in tablets using 1,2-naphthoquinone-4-sulfonate," *International Journal of Analytical Chemistry*, vol. 2009, Art. no. 237601, 2009.
- [18] V. Chis *et al.*, "IR, Raman, SERS and DFT study of paroxetine," *Journal of Molecular Structure*, vol. 993, pp. 243–248, 2011.
- [19] P. Ravisankar, Ch. Roja, G. K. Babu, and K. S. Rahul, "Validated UV spectrophotometric method for quantitative analysis of paroxetine in bulk and pharmaceutical dosage form," *Der Pharmacia Lettre*, vol. 8, no. 3, pp. 254–260, 2016.
- [20] V. Chis, "IR, Raman, SERS and DFT study of paroxetine," *Journal of Molecular Structure*, vol. 993, pp. 243–248, 2011.
- [21] M. Malik, K. H. Chan, and G. Azimi, "Quantification of nickel, cobalt, and manganese concentration using ultraviolet–visible spectroscopy," *RSC Advances*, vol. 11, pp. 28014–28028, 2021.
- [22] M. Hassan, R. Ahmed, and L. Zhou, "Temperature-dependent adsorption of Ni(II) and Co(II) ions using plant-based nanoadsorbents," *Journal of Environmental Chemical Engineering*, vol. 9, no. 5, pp. 106–118, 2021.
- [23] J. Liu, Y. Zhang, and M. Chen, "Effect of SiC nanoparticles size and concentration on the partial discharge behavior of synthetic ester oil," in *Proc. IEEE Industry Applications Society Annual Meeting (IAS)*, Jun. 2025, pp. 1–6.
- [24] S. A. Ali, M. Rahman, and E. H. Khan, "Thermodynamic and kinetic studies of heavy metal adsorption on amino-functionalized nanomaterials," *Environmental Nanotechnology, Monitoring & Management*, vol. 18, pp. 100–112, 2022.
- [25] G. Hanbali, S. Jodeh, O. Hamed, R. Bol, B. Khalaf, A. Qdemat, and S. Samhan, "Enhanced ibuprofen adsorption and desorption on synthesized functionalized magnetic multiwall carbon nanotubes from aqueous solution," *Materials*, vol. 13, no. 15, Art. no. 3329, 2020.
- [26] N. K. Mondal, A. Samanta, S. Chakraborty, and W. A. Shaikh, "Enhanced chromium(VI) removal using banana peel dust: Isotherms, kinetics and thermodynamics study," *Sustainable Water Resources Management*, vol. 4, no. 3, pp. 489–497, 2017.