

USING ARTIFICIAL INTELLIGENCE FOR SELECTION OF ANALYTICAL REAGENTS, EXEMPLIFIED BY DETERMINATION OF IRON CONTENT IN WATER SAMPLES

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Currently, education and science in Ukraine are facing many new challenges, including war. These challenges determine new priority areas of science and technology development, which in turn affects scientists and students of higher education institutions. The significant pollution of natural resources (marine environment, surface waters and soils) caused by active military operations is the reason for the emergence of many new research projects. Students of higher education institutions, especially chemical, environmental, and technical majors, often face the problem of choosing the analysis methods they will use in the experimental part of their coursework or thesis. Also students often engage in scientific research, sometimes even within the framework of various projects, including those related to monitoring the marine environment of Ukraine. Traditionally, the selection process is accompanied by a lengthy and laborious literature search. But in recent years, the rapid development of artificial intelligence has made it possible to significantly simplify this process. The article is devoted to studying the relevance of information that ChatGPT-4o mini provided in response to different formulations of prompts. The search concerned the selection of analytical reagents for determining the iron content in water samples. By improving the prompts step by step, recommendations for reagents for simultaneous determining of Fe(II) and Fe(III) in water was received from ChatGPT-4o mini. The prompts were gradually made more complicated by introducing limitations on application and reaction conditions. It was found that currently ChatGPT-4o mini did not always effectively cope with the selection of reagents, but it can somewhat simplify the literature search. However, it's possible that future versions of ChatGPT will feature a more efficient reagent selection process.

Keywords: artificial intelligence, ChatGPT-4o mini, chromogenic compounds, iron detection, reagents selection

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1. Introduction

Currently, education and science in Ukraine are facing many new challenges, including war. These challenges determine new priority areas of science and technology development, which in turn affects students of higher education institutions. The significant pollution of natural resources (marine

environment, surface waters and soils) caused by active military operations is the reason for the emergence of many new research projects (Kyrii et al., 2024; Litynska & Pelekhata, 2024). Such projects, especially those under the auspices of the Ministry of Education and Science, often involve undergraduate, graduate, and postgraduate students to assist in conducting research. The results of their

work later become the basis for their coursework and thesis. For example, in the first year of the project “The novel selective indicator systems for assessing the state of the marine environment in Ukraine” 6 graduate students and 2 master's students were involved. One of the tasks of these students was to find analytical methods for detecting different metal ions in water. Traditionally, this process is accompanied by a lengthy and laborious literature search (Bolaños et al., 2024). But in recent years, the rapid development of artificial intelligence has made it possible to significantly simplify this process (Bolaños et al., 2024; Wagner et al., 2021). Although the complexity of the search

process using artificial intelligence is usually imperceptible to the consumer due to the high speed of the processes, in reality this search is very multi-stage (Figure 1).

Often the search can be based on the use of methods such as a natural language processing (NLP)-based keyword augmentation and screening (NKAS) (Ma et al., 2022). Upon using the NKAS, the quantity of pertinent papers decreased compared to the original search. However, the precision significantly increased (73.83% vs. 34.6%) and the recall also improved (98.4% vs. 59.93%) when compared to the results from the original search (Ma et al., 2022).

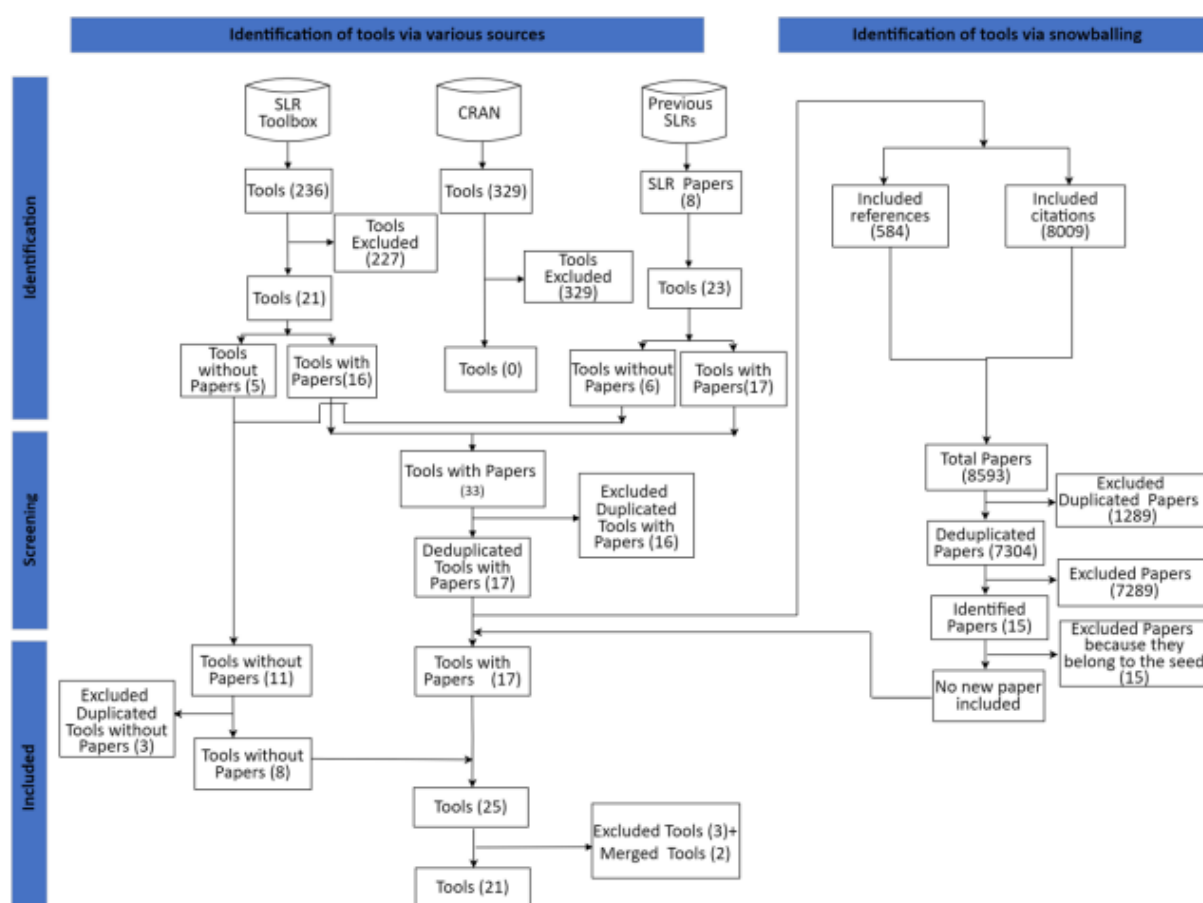


Fig. 1. Main phases of the search process (Bolaños et al., 2024)

ChatGPT is one of the large language models. Accordingly, it can also be used for literary search (Wang et al., 2023;

Mostafapour et al., 2024). Although large language models such as ChatGPT show potential for a range of tasks, their use in

systematic reviews presents considerable challenges at the moment. These challenges restrict ChatGPT's ability to create thorough and dependable search strategies, which are essential in the systematic review process (Parisi & Sutton, 2024).

But usage of ChatGPT also has certain disadvantages. The most frequently mentioned limitation of this large language model is ChatGPT's propensity to "hallucinate." Although ChatGPT can theoretically create a search string, it encounters difficulties with database-specific syntax, often inventing index terms like MeSH headings, and it cannot perform the search once the string is created (Parisi & Sutton, 2024; Alshami et al., 2023). In work (Mostafapour et al., 2024) GPT-4 initially identified 6 relational factors by utilizing iterative prompts, starting with a broad request. However, after being prompted for additional factors multiple times, it became clear that GPT-4 started to generate unrelated factors after reaching 21, likely due to hallucinations. In total, GPT-4 produced a list of 21 relational factors and compiled 54 references. Among these 21 factors, 14% were deemed irrelevant. Approximately 24% of the references were classified as somewhat related to the topic but lacking in strong relevance, and 7.5% were identified as irrelevant (Mostafapour et al., 2024).

The effectiveness of using ChatGPT depends very much on the version (Bayer et al., 2024; O'Leary, 2024). According to the work (O'Leary, 2024), the versions 4o and 4 give more accurate results than the version 3.5. It is important that ChatGPT-4o is capable of swiftly executing real-time translations across various languages, creating interactive content, simulating human-like speech, and generating personalized material.

Given these key functionalities, it is anticipated that ChatGPT-4o will see extensive use in personal learning settings. Additionally, with further developments in the model's background, it could yield more meaningful and realistic responses (Bayer et al., 2024).

2. Materials and methods

ChatGPT-4o mini (OpenAI, 2024a) was used to select methods and reagents for determining iron content in water samples. ChatGPT-4o mini is a version of ChatGPT that has a reduced amount of parameters compared to the full version of ChatGPT-4. This model is designed to optimize speed and reduce resource requirements, making it convenient for use on devices with limited capabilities. The GPT-4o mini outperforms GPT-3.5 Turbo and other smaller models on academic benchmarks, excelling in both textual intelligence and multimodal reasoning. It also supports the same range of languages as GPT-4o (OpenAI, 2024b).

We analyzed the results of search and compared them with the data we found personally. Then, the search results were checked for consistency by comparing the properties and costs of different reagents. All prices in the comparison were indicated as of January 2025.

3. Results and Discussion

Since there are a very large number of very expensive reagents for determining iron content, which are inaccessible to most Ukrainian scientists and students, the prompts included the word "cheap".

Prompt 1. Find the names of cheap reagents for determining the iron content in water.

Answer. There are several inexpensive reagents commonly used for determining iron content in water. Here are a few:

1. 1,10-Phenanthroline
 - A colorimetric reagent that forms a complex with iron, allowing for measurement.
2. Ferrozine
 - Another colorimetric reagent that selectively binds to ferrous ions, providing a visual indication that can be measured.
3. Potassium thiocyanate (KSCN)
 - Forms a red complex with iron ions, which can be used in titrations and colorimetric assays.
4. Calcium hydroxide (Ca(OH)₂)
 - Used to adjust pH in some tests, making detection of iron more effective.
5. Sodium bicarbonate (NaHCO₃)
 - Commonly used for adjusting the pH in a sample solution, which can enhance iron solubility.

Make sure to follow safety guidelines when handling any chemicals, and consult specific protocols for the most accurate results.

As can be seen from the answer to prompt 1, ChatGPT-4o mini included in the list some compounds (calcium hydroxide and sodium bicarbonate) that are not directly related to the determination of iron content. Therefore, in the next prompt, we replaced “reagents” with the term “chromogenic compounds” to exclude such reagents from being included in the list.

Prompt 2. Find the names of cheap chromogenic compounds for determining iron content in water.

Answer. Here are some inexpensive chromogenic compounds that can be used for determining iron content in water:

1. 1,10-Phenanthroline
 - Forms a colored complex with ferrous ions, allowing for spectrophotometric measurement.
2. Ferrozine
 - A popular reagent that forms a highly stable complex with ferrous ions, yielding a measurable color change.
3. Benzene-1,2-diol (Catechol)
 - Can react with iron, producing a colored product that can be quantified.
4. Sulfoquinoline
 - Forms a colored complex with iron and can be used in colorimetric assays.
5. 2,4-Dihydroxyacetophenone
 - Reacts with iron, generating a colored solution that can be analyzed.

These chromogenic compounds are typically easy to obtain and economical, making them suitable for laboratory analyses of iron in water. Always refer to specific procedures for preparation and measurement.

All of the compounds listed in the answer to prompt 2, excluding sulfoquinoline, are indeed directly related to the determination of content of different iron species. Among compounds with a similar name, 5-sulfoquinoline-8-ol can be used to detect iron. The next prompt narrowed this list down to one item.

Prompt 3. Find the name of the cheapest chromogenic compound for determining iron content in water.

Answer. The cheapest chromogenic compound commonly used for determining iron content in water is 1,10-Phenanthroline.

This compound is cost-effective and forms a colored complex with ferrous ions, making it a popular choice for

spectrophotometric analyses in various laboratories.

1,10-phenanthroline is indeed a chromogenic component, but it forms a colored compound only in Fe(II) (Komadel & Stucki, 1988), while in surface waters the main form is Fe(III), which creates some difficulties in analysis.

Prompt 4. Find the name of the cheapest chromogenic compound for determining total iron content in water.

Answer. The cheapest chromogenic compound for determining total iron content in water is ferrozine. Ferrozine forms a stable, intensely colored complex with iron(II), which can be quantified spectrophotometrically. It is widely used in analytical methods due to its affordability and sensitivity for measuring total iron (both Fe(II) and Fe(III)) after reduction.

But ferrozine, like 1,10-phenanthroline, forms a colored compound only with Fe(II). That is, the determination process requires an additional reduction stage, which complicates the determination. Therefore, in the next prompt, "determining total iron content" was replaced with "simultaneous determining of Fe(II) and Fe(III) without additional reduction step".

Prompt 5. Find the name of the cheapest chromogenic compound for simultaneous determining of Fe(II) and Fe(III) in water without additional reduction step.

Answer. The cheapest chromogenic compound for the simultaneous determination of Fe(II) and Fe(III) in water, without the need for an additional reduction step, is

3,3',5,5'-tetramethylbenzidine (TMB). TMB reacts with both Fe(II) and Fe(III), producing a color change that can be measured spectrophotometrically, allowing for the simultaneous determination of both iron forms. It's a commonly used reagent due to its cost-effectiveness and ease of use in colorimetric assays.

But according to the work (Yang et al., 2018), 3,3',5,5'-tetramethylbenzidine does not form colored compounds with Fe(II). That is, the use of this compound requires an additional oxidation step for Fe(II) in the case of the simultaneous presence of both species. Therefore, the word "oxidation" was added to the next prompt.

Prompt 6. Find the name of the cheapest chromogenic compound for simultaneous determining of Fe(II) and Fe(III) in water without additional reduction or oxidation step.

Answer. The cheapest chromogenic compound for the simultaneous determination of Fe(II) and Fe(III) in water, without requiring additional reduction or oxidation steps, is 1,10-phenanthroline. This compound forms stable, colored complexes with both Fe(II) and Fe(III), allowing for their simultaneous measurement in water. It's widely used because it's affordable, simple to apply, and sensitive enough to distinguish between the two oxidation states without needing extra chemical treatments.

Since the complex of phenanthroline with Fe(III) is colorless, the mandatory stage of the analysis is the reduction of Fe(III) to Fe(II) (Komadel & Stucki, 1988). That is, in this case, a typical case of ChatGPT's "hallucination" was observed.

Table 1 reviewed all chromogenic compounds suggested by ChatGPT-4o mini.

Table 1. Comparison of chromogenic compounds suggested by ChatGPT-4o mini

Chromogenic compound	Iron species detection (ChatGPT-4o mini)	Iron species detection (literature)	Price, UAH/kg
1,10-Phenanthroline	Fe(II) and Fe(III)	Fe(II), Fe(III) after reduction	24000.0-712950.0
Ferrozine	Fe(II)	Fe(II), Fe(III) after reduction	Not available for sale
Potassium thiocyanate	Without specification	Fe(III), Fe(II) after oxidation	806.4-17144.9
Catechol	Without specification	Fe(III), Fe(II) after oxidation	26934.3-30240.0
Sulfoquinoline	Without specification	-	-
2,4-Dihydroxyacetophenone	Without specification	Fe(III)	Not available for sale
3,3',5,5'-Tetramethylbenzidine	Fe(II) and Fe(III)	Fe(III), Fe(II) after oxidation	54000.0-2437304.4

Table 1 showed that all the reagents suggested by ChatGPT-4o mini are unsuitable for simultaneous determining of Fe(II) and Fe(III) in water without additional reduction or oxidation step. In addition, most of the proposed reagents were very expensive, meaning the result clearly did not meet the requirement of cheapness that was specified in the prompts. Sulfosalicylic acid never appeared in the responses to the prompts, even though it perfectly met the requirements. This is an inexpensive compound (836.0-870.0 UAH/kg) that is suitable for determining total iron. Fe(III) forms different colored complexes with sulfosalicylic acid depending on the pH. At pH 1.8-2.5, the formed complex has a red-violet color with maximum absorbance at a wavelength of 510 nm (Laboratory Work No. 2, 2024). When the pH increases to 4-8, a red-brown bis-complex is formed. But this complex is not used for analytical purposes due to its low stability (Salvadó et al., 1990). In an alkaline medium at pH 9.0-11.5, a yellow trisulfosalicylate complex is formed with

maximum absorbance at a wavelength of 416 nm, but at pH > 12, the complex decomposes with precipitation of iron hydroxide (Laboratory Work No. 2, 2024). Although the yellow complex is somewhat less stable than the purple complex, it is characterized by higher absorbance values at the same iron concentrations (Laboratory Work No. 2, 2024; Salvadó et al., 1990). In an alkaline medium, due to the easy oxidation of Fe (II) to Fe (III) with sulfosalicylic acid, the total iron content can be determined (Laboratory Work No. 2, 2024).

Since ChatGPT-4o mini never gave sulfosalicylic acid in its response, it is advisable to check whether this information is among the data available to ChatGPT-4o mini.

Prompt 7. Is it possible to determine the total iron content in water using sulfosalicylic acid?

Answer. Yes, it is possible to determine the total iron content in water using sulfosalicylic acid. This method involves

adding sulfosalicylic acid to a water sample containing iron, which forms a colored complex with iron ions. The intensity of the color produced is proportional to the concentration of iron present. You can measure the absorbance of the solution using a spectrophotometer to quantify the iron content. This method is often used for its sensitivity and simplicity in environmental water analysis.

Therefore, the neural network has information about the possibility of using sulfosalicylic acid to determine the content of total iron, but it did not indicate this reagent among the list of reagents in the responses to the previous prompts. Therefore, the effectiveness of using ChatGPT-4o mini in selection of analytical methods was still quite low. But perhaps in future versions of ChatGPT, reagent selection will become more efficient.

6. Conclusions

Currently, education and science in Ukraine are facing many new challenges, including war. These challenges determine new priority areas of science and technology development, which in turn affects students of higher education institutions. The significant pollution of natural resources (marine environment, surface waters and soils) caused by active military operations is the reason for the emergence of many new research projects. Traditionally, this process is accompanied by a lengthy and laborious literature search. But in recent years, the rapid development of artificial intelligence has made it possible to significantly simplify this process. ChatGPT is one of the large language models and can be used for search of analytical methods and reagents.

By improving the prompts step by step, we received from ChatGPT-4o mini recommendations for reagents for simultaneous determining of Fe(II) and Fe(III) in water. All the reagents suggested by ChatGPT-4o mini are unsuitable for the simultaneous determination of Fe(II) and Fe(III) in water without additional reduction or oxidation steps. In addition, there were typical cases of ChatGPT's "hallucination", when ChatGPT-4o mini provided non-existent information. Furthermore, many of the proposed reagents were costly, failing to meet the affordability criteria specified in the prompts. Sulfosalicylic acid was never mentioned, despite being a perfect match for the requirements. It is an inexpensive compound that works well for determining total iron under alkaline conditions. As a result, the effectiveness of ChatGPT-4o mini in selecting appropriate analytical methods remains quite low. However, it's possible that future versions of ChatGPT will feature a more efficient reagent selection process.

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ВИКОРИСТАННЯ ШТУЧНОГО ІНТЕЛЕКТУ ДЛЯ ВИБОРУ АНАЛІТИЧНИХ РЕАГЕНТІВ, НА ПРИКЛАДІ ВИЗНАЧЕННЯ ВМІСТУ ФЕРУМУ У ЗРАЗКАХ ВОДИ

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Наразі освіта та наука в Україні стикаються з багатьма новими викликами, зокрема війною. Ці виклики визначають нові пріоритетні напрямки розвитку науки і техніки, що, у свою чергу, впливає на науковців та студентів вищих навчальних закладів. Значне забруднення природних ресурсів (морського середовища, поверхневих вод та ґрунтів), спричинене активними військовими діями, є причиною появи багатьох нових дослідницьких проєктів. Студенти вищих навчальних закладів, особливо хімічних, екологічних та технічних спеціальностей, часто стикаються з проблемою вибору методів аналізу, які вони використовуватимуть в експериментальній частині своєї курсової роботи чи дипломної роботи. Також студенти часто займаються науковими дослідженнями, іноді навіть у рамках різних проєктів, зокрема тих, що пов'язані з моніторингом морського середовища України. Традиційно процес вибору супроводжується тривалим та трудомістким пошуком літератури. Але в останні роки швидкий розвиток штучного інтелекту дозволив значно спростити цей процес. Стаття присвячена вивченню актуальності інформації, яку ChatGPT-4o міні надавав у відповідь на різні формулювання запитів. Пошук стосувався вибору аналітичних реагентів для визначення вмісту феруму у зразках води. Шляхом поетапного вдосконалення запитів, від ChatGPT-4o міні були отримані рекомендації щодо реагентів для одночасного визначення Fe(II) та Fe(III) у воді. Запити поступово ускладнювалися шляхом введення обмежень на застосування та умов реакції. Було виявлено, що наразі ChatGPT-4o міні не завжди ефективно справляється з вибором реагентів, але це може децю спростити пошук літератури. Однак, можливо, що майбутні версії ChatGPT матимуть ефективніший процес вибору реагентів.

Ключові слова: вибір реагентів, виявлення феруму, ChatGPT-4o міні, хромогенні сполуки, штучний інтелект