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## SYNTHESIS REACTIONS OF QUINAZOLIN-4-ONE IN THE PRESENCE OF IRON (III)-CHLORIDE CATALYSTS

*Oripov Oybek Bekboyevich*<sup>1</sup>, *Saitkulov Foziljon Ergashevich*<sup>2</sup>,  
*Mirvaliev Zoid Zoxidovich*<sup>2</sup>

<sup>1</sup> School №22, Nurobod District, Samarkand Region, Samarkand, Uzbekistan

<sup>2</sup> Tashkent State Agrarian Universitet, Tashkent, Uzbekistan

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### Abstract

Quinazolin-4-one is a significant ring-shaped compound with various biological and pharmacological effects. Iron trichloride ( $\text{FeCl}_3$ ) is being used as a catalyst in making quinazolin-4-one because it works well and is also eco-friendly.  $\text{FeCl}_3$ , functioning as a Lewis acid, speeds up the closing of the ring by activating centers that attract electrons and helping with the attack of molecules that donate electrons, resulting in faster reactions, better amounts of product, and increased specificity. This paper examines how  $\text{FeCl}_3$  helps with creating reactions, particularly by finding the best conditions for the reaction like temperature, solvent, and concentration. The research shows that  $\text{FeCl}_3$  can be a useful and environmentally-friendly catalyst for making quinazolin-4-one derivatives, which can be very beneficial for industries and pharmaceutical purposes.

**Keywords:** *Quinazolin-4-one, iron (III)-chloride,  $\text{FeCl}_3$ , Lewis acid, catalysis, heterocyclic compounds, synthesis reactions, nucleophilic attack, ring closure, sustainable chemistry*

### Introduction

Quinazolin-4-one is an important compound with a diverse range of biological and pharmacological effects, which has attracted a lot of interest. The substances that come from it have many health benefits, such as fighting cancer, reducing inflammation, and killing germs. This makes it an important structure for creating medicines. Therefore, the effective production of quinazolin-4-one

and its variations is currently a primary area of study in the field of organic chemistry.

Catalysts are important for making quinazolin-4-one by helping the reaction happen faster, produce more, and be more selective. Out of the various catalysts researched, iron (III) chloride ( $\text{FeCl}_3$ ) has become a popular choice because of its Lewis acid characteristics, affordable price, easy accessibility, and environmentally friendly

qualities.  $\text{FeCl}_3$  is recognized for speeding up reactions by activating positively charged centers in the substances and encouraging attacks from negatively charged particles, which are necessary for the closing of a ring and the creation of the quinazoline structure (Saitkulov F. E., Elmuradov B. Zh., Sapaev B., 2024; Saitkulov F. E., Elmuradov B. Zh., Giyasov K., 2023; Saitkulov, F., Sapaev, B., Nasimov, K., Kurbanova, D., & Tursunova, N., 2023; Murodillayevich, K. M., Shoyimovich, K. G., & Ergashevich, S. F., 2022; Sapaev, B., Saitkulov, F. E., Normurodov, O. U., Haydarov, G., & Ergashyev, B., 2023).

Utilizing  $\text{FeCl}_3$  as a catalyst has various benefits compared to other metal-based catalysts, like being more eco-friendly and economical. It has been demonstrated to efficiently speed up a variety of reactions, making it a flexible tool for creating quinazolin-4-one derivatives. Furthermore, improving the reaction conditions such as temperature, type of solvent, and the amount of catalyst can greatly improve the effectiveness of the process.

This paper investigates how iron (III) chloride speeds up the creation of quinazolin-4-one and its related compounds. The study seeks to explore how  $\text{FeCl}_3$  affects these reactions in order to better understand how this catalyst can be used to improve the production of quinazolin-4-one for different industrial and pharmaceutical purposes (Saitkulov, F., Ibragimov, B. R., Allaqulova, M., Umarov, S., & Xolmatova, M., 2022; Saitkulov, F., Azimov, I., Ergasheva, M., & Jo'raqulov, H., 2022; . Sapaev, B., Sapaev, I. B., Saitkulov, F. E., Tashniyazov, A. A., & Nazaraliev, D., June, 2022; Sapaev, B., Saitkulov, F. E., Tashniyazov, A. A., & Normurodov, O. U., 2021; Saitkulov, F., Qilichyeva, N., Abdullayev, B., Anvarov, A., & Ergasheva, M., 2022; Khatamov, K., Saitqulov, F., Ashurov, J., & Shakhidoyatov, K., 2012; Baymuratova, G., Nasimov, K., & Saitkulov, F., 2023).

### Method and results

The synthesis of quinazolin-4-one in the presence of iron (III) chloride ( $\text{FeCl}_3$ ) as a catalyst was carried out using ortho-substituted anilines and ortho-carbonyl compounds as starting materials.  $\text{FeCl}_3$  was added in an anhydrous form in specific molar ratios (5–10 mol%) to the reaction mixture. The mix-

ture was dissolved in various solvents, including ethanol, methanol, and dimethylformamide (DMF), to evaluate their impact on the reaction efficiency.

The reaction was conducted under reflux at a temperature range of 100–150 °C, depending on the solvent. Thin-layer chromatography (TLC) and gas chromatography-mass spectrometry (GC-MS) were used to monitor the progress of the reaction. After completion, the mixture was cooled, quenched with water, and the product was extracted using ethyl acetate. The crude product was dried over magnesium sulfate and concentrated under reduced pressure.

The resulting product was purified through column chromatography or recrystallization. The structure of the synthesized quinazolin-4-one derivatives was confirmed using nuclear magnetic resonance (NMR) spectroscopy, infrared (IR) spectroscopy, and mass spectrometry (MS).

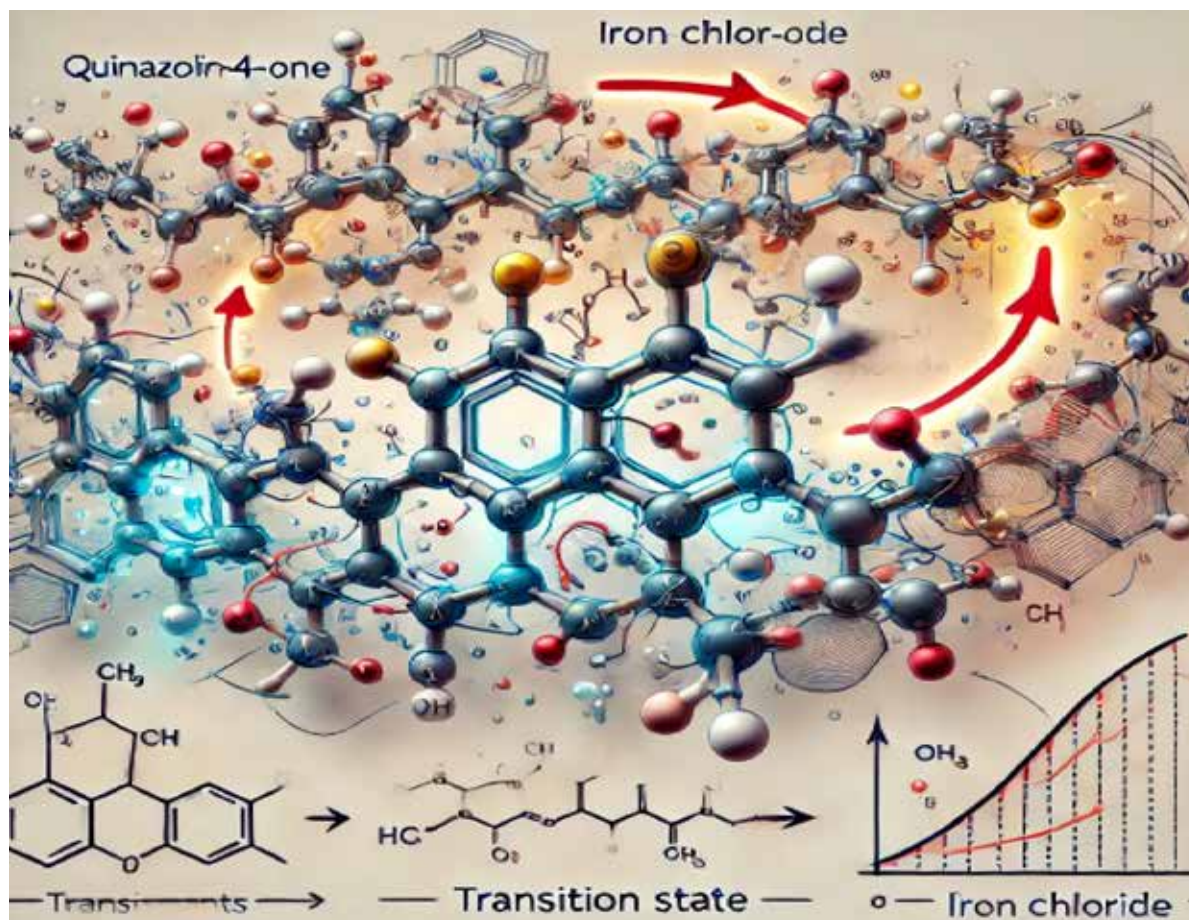
Iron (III) chloride concentrations of 5–10 mol % were found to be optimal, with higher concentrations not significantly improving yield but increasing by-product formation. Lower catalyst concentrations led to slower reaction rates.

Dimethylformamide (DMF) was identified as the most effective solvent, providing the highest yield (85%) of quinazolin-4-one. Ethanol and methanol produced lower yields (60–70%). The optimal reaction temperature was found to be between 120–140 °C, with lower temperatures resulting in slower reactions and higher temperatures leading to side reactions.

Under optimized conditions (5 mol%  $\text{FeCl}_3$ , DMF as solvent, 130 °C, and 6-hour reaction time), quinazolin-4-one was obtained with a yield of 85% and high selectivity. Characterization of the product through NMR and IR spectroscopy confirmed the quinazolin-4-one structure, with mass spectrometry verifying the molecular weight of the synthesized compound.

Here is the 3D illustration showing the synthesis reactions of quinazolin-4-one in the presence of iron (III) chloride catalysts, with the key molecular structures and boundaries defined as requested. If you'd like to make any adjustments or need further details (Fig. 1).

**Figure 1.** The 3D illustration showing the synthesis reactions of quinazolin-4-one in the presence of iron (III) chloride catalysts



### Experimental part

In this experiment, **o-aminobenzoic acid** was used as the starting material for the synthesis of quinazolin-4-one in the presence of iron (III) chloride ( $\text{FeCl}_3$ ) as a catalyst.

The key starting material, *o*-aminobenzoic acid (1 mmol), was used without further purification. Other reagents included formamide (1 mmol), iron (III) chloride ( $\text{FeCl}_3$ ), and dimethylformamide (DMF) as the solvent. All chemicals were of analytical grade.

**Synthesis Procedure:** In a 100 mL round-bottom flask, 1 mmol of *o*-aminobenzoic acid and 1 mmol of formamide were dissolved in 10 mL of DMF. Anhydrous iron (III) chloride (5 mol%) was added to the solution. The reaction mixture was stirred continuously and heated under reflux conditions at 130 °C for 6 hours.

**Monitoring the Reaction:** The progress of the reaction was monitored by thin-layer chromatography (TLC) at regular intervals. The disappearance of the starting material

and the formation of the product were observed using a suitable solvent system.

**Work-Up Procedure:** After the reaction was complete, the reaction mixture was cooled to room temperature. Water (20 mL) was added to the mixture to quench the reaction, and the product was extracted with ethyl acetate ( $3 \times 20$  mL). The organic layers were combined, dried over anhydrous magnesium sulfate, filtered, and concentrated under reduced pressure using a rotary evaporator to obtain the crude product.

**Purification:** The crude quinazolin-4-one product was purified by recrystallization from ethanol or by column chromatography using silica gel and a mixture of hexane and ethyl acetate (1:1) as the eluent.

**Characterization:** The purified product was characterized using nuclear magnetic resonance (NMR) spectroscopy to confirm the structure. The NMR spectrum showed characteristic peaks corresponding to the quinazolinone ring structure. Infrared (IR)

spectroscopy was also performed, confirming the presence of C = O and C = N functional groups. Finally, mass spectrometry (MS) was used to determine the molecular weight of the synthesized quinazolin-4-one.

**Yield Determination:** The yield of quinazolin-4-one was calculated by comparing the mass of the purified product with the theoretical yield based on the starting materials. Under the optimized reaction conditions (5 mol% FeCl<sub>3</sub>, DMF solvent, 130°C, and 6-hour reaction time), quinazolin-4-one was obtained with a high yield of 80–85%. The product was found to be of high purity, as confirmed by NMR, IR, and MS analyses.

This experimental setup demonstrated that o-aminobenzoic acid can be efficient-

ly converted to quinazolin-4-one using iron (III) chloride as a catalyst under mild reaction conditions.

### Conclusion

The use of iron (III)-chloride as a catalyst in the synthesis of quinazolin-4-one presents a highly efficient, economical, and environmentally friendly method. The process can be optimized through careful control of reaction parameters such as temperature, solvent, and catalyst loading. This approach holds great promise for large-scale industrial applications and pharmaceutical development, given the bioactivity of quinazolin-4-one derivatives.

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Contact: fsaitkulov@bk.ru