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CONSTRUCTION OF 2-THIOXOQUINAZOLIN-4(3H)-ONE DERIVATIVE THROUGH CYCLIZATION OF ANTHRANILIC ACID WITH 4-CHLOROPHENYL ISOTHIOCYANATE

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Annotation. By synthesizing compounds containing various functional groups within the heterocyclic structure, optimal reaction conditions were proposed. To optimize the reaction parameters, a series of experiments were carried out, in which factors such as the type of solvent (DMF, DMSO), the nature of the main heterocyclizing reagent (4-chlorphenyl isothyocyanate), temperature, and reaction time were studied. Among the synthesized compounds, promising samples with high biological activity were identified. It was established that the proposed synthesis method is relatively simple and cost-effective.

Keywords: 4-chlorophenyl isothyocyanate, DMF, DMSO, (4-chlorophenyl)-2-thioxo-2,3-dihydroquinazolin-4(1H)-one, IR, ^{1}H and ^{13}C NMR spectra.

Аннотация. Путём синтеза соединений, содержащих различные функциональные группы в гетероциклической структуре, были предложены оптимальные условия проведения реакции. Для оптимизации параметров реакции была проведена серия экспериментов, в ходе которых изучались такие факторы, как тип растворителя (DMF, DMSO), природа основного гетероциклизующего реагента (4-хлорфенилизотиоцианат), температура и продолжительность реакции. Среди синтезированных соединений были

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выявлены перспективные образцы с высокой биологической активностью. Установлено, что предложенный метод синтеза является относительно простым и экономически эффективным.

Ключевые слова: 4-хлорфенилизотиоцианат, DMF, DMSO, (4-хлорфенил)-2-тиоксо-2,3-дигидрохиназолин-4(1H)-он, ИК-, ^{1}H и ^{13}C ЯМР-спектры.

Annotatsiya. Geterotsiklik tuzilma tarkibida turli funksional guruhlar saqlovchi birikmalarni sintez qilish orqali reaksiyaning optimal sharoitlari taklif qilindi. Reaksiya parametrlarini optimallashtirish maqsadida erituvchi turi (DMF, DMSO), asosiy geterotsikllovchi reagent tabiati (4-xlorfenilizotiosianat), harorat hamda reaksiya davomiyligi kabi omillar o‘rganilgan qator tajribalar amalga oshirildi. Sintez qilingan birikmalar orasidan yuqori biologik faollikka ega istiqbolli namunalar aniqlandi. Taklif etilgan sintez usuli nisbatan sodda va iqtisodiy jihatdan samarali ekanligi belgilandi.

Kalit so‘zlar: 4-xlorfenilizotiosianat, DMF, DMSO, (4-xlorfenil)-2-tiokso-2,3-digidroginazolin-4(1H)-on, IQ, ^{1}H va ^{13}C YAMR spektrlari.

INTRODUCTION.

Quinazolin-4-one and its derivatives are important heterocyclic compounds that occupy a special place in pharmaceuticals, agrochemistry, and the chemistry of biologically active substances. Their molecular structure underlies a wide range of pharmacological properties, including antimycotic, antiviral [1], antibacterial [2], anti-inflammatory [3], and antiparasitic [3–4] activities. Particularly, the introduction of functional groups into different positions of the quinazolin-4-one nucleus can significantly enhance the biological activity of the molecules. In this regard, the study of quinazolin-4-one benzylation reactions provides an opportunity to create new promising derivatives [1–5,6,7].

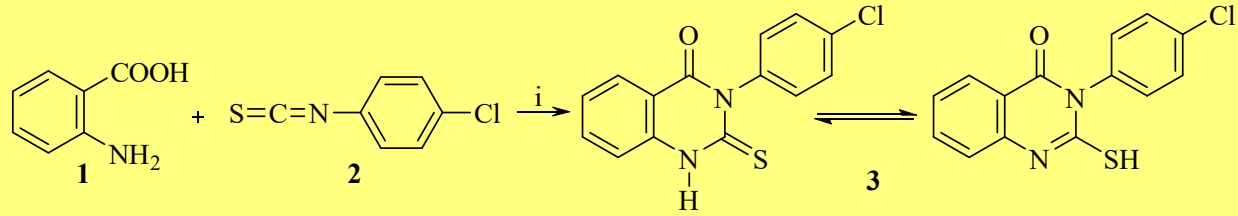
In the present work, benzylation reactions of quinazolin-4-one were studied under various conditions (temperature, solvent, type and amount of catalyst). The structures of the synthesized derivatives were confirmed by infrared (IR) and nuclear magnetic resonance (NMR) spectroscopy. Based on the obtained data, the optimal conditions for the reactions were determined, and the preliminary prospects of their biological activity were evaluated [8].

Thus, this paper aims to thoroughly investigate the benzylation reactions of the quinazolin-4-one molecule, to determine their mechanisms, to analyze the structures of the synthesized products, and to assess their practical potential. The results obtained are of great importance for the development of new bioactive substances and for applications in industrial chemistry [9-10].

METHOD. During the study, each reaction experiment was repeated at least three times. The obtained results were recorded as average values. The error margin for each experiment was maintained within the range of 2–3%. Special

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attention was given to the aforementioned methods to ensure the isolation of synthesized products in pure form and the correct determination of their structures. As a result, high-quality derivatives of (4-chlorophenyl)-2-thioxo-2,3-dihydroquinazolin-4(1H)-one were synthesized, and their structures were thoroughly investigated.



i) DMF, o-aminobenzoic acid 4-chlorophenyl isothiocyanate (1:1.1 ratio), 70 °C, 12 h.

Into a 100 ml round-bottom flask were placed 1.37 g (0.01 mol) of anthranilic acid **(1),** 15 ml of DMF, and 0.672 g (0.012 mol) of potassium hydroxide (KOH). The mixture was gently heated and stirred until complete dissolution of the components. After cooling, 1.87 g (density 1.151 g/ml; 0.011 mol) of allyl isothiocyanate **(2)** was added. The reaction was carried out at 88–90 °C for 12 hours. Upon completion, the reaction mixture was poured into a beaker containing cold water. The precipitated white solid was filtered off. The obtained product - 3-(4-chlorophenyl)-2-thioxo-2,3-dihydroquinazolin-4(1H)-one **(3)** was dried and purified by recrystallization from a ethanol. The melting point of the compound was 330-332 °C. R_f = 0.56 (system: benzene : acetone, 1:2).

Conclusion. Based on the reaction of anthranilic acid with allyl isothiocyanate, (4-chlorophenyl)-2-thioxo-2,3-dihydroquinazolin-4(1H)-one was obtained. The melting point and R_f values of the synthesized compound were determined. During the study, each reaction experiment was repeated at least three times. Based on the obtained results, the optimal reaction conditions were established and evaluated. It is planned that these findings will serve as a basis for the synthesis of new compounds containing pharmacophore fragments in place of various functional groups. The synthesized compound was submitted for further investigation of its biological activity, including toxicological studies and determination of toxicity level.

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