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SYNTHESIS OF A THIOMOCHEVINA FRAGMENT BASED ON THE REACTION OF 6-AMINOQUINAZOLIN-4-ONE WITH ISOTHIOCYANATE

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Abstract

Today, it is important to purposefully create new biologically active compounds, successfully applying them in agriculture and medicine against various harmful insects and diseases. Of particular importance in this regard is the creation of inexpensive, highly effective and environmentally friendly topical preparations, the study of their physicochemical, biological and pharmacological properties. A study of condensed heterocyclic synthesis and biological activity found the production of mixtures, new drugs, including quinazoline-4-one derivatives and the determination of their bioactive derivatives the development of new drugs based on them is relevant.

Keywords: *o*-Aminobenzoic acid, formamide, quinazoline-4-on, nitration, reduction, tin (II)-chloride dihydrate ($SnCl_2 \cdot 2H_2O$), layered chromatography, IQ, and YaMR spectroscopy

Introduction

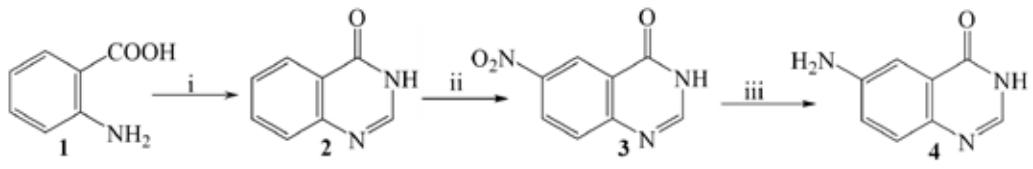
In recent years, various periparations based on many representatives of derivatives formed on the basis of heterocyclic compounds containing quinazoline have been introduced into agricultural and medical practice (Arun K. Ghosh., Margherita Bindisi. 2015). Currently, it is conducting scientific and practical research aimed at determining the specific aspects of optimal synthesis,

structure and reactivity of quinazolones and their new derivatives, as well as creating biologically active substances with new pharmacophore fragments in their composition (Asma Kh., Rabah A., Antonio I. M., Laiche A., Abdelmalek B., 2018). In medical veterinary practice and agriculture, medicinal products created on the basis of heterocyclic compounds – quinazolones and sulfonamides, formed from condensation with benzene Ringas, are widely used.n medical veterinary practice and agriculture, medicinal products created on the basis of heterocyclic compounds – quinazolones and sulfonamides, formed from condensation with benzene Ringas, are widely used. In particular, preparations created on the basis of compounds of this class are used as herbicides, fungicides (2–3-dimethlquinazolones), bactericides, antigelmints (quinazoline dressing), hypotensive (quinazoline bricmacs) preparations (Asma Kh., Rabah A., Antonio I. M., Laiche A., Abdelmalek B., 2018). Quinazoline is widely used as an inhibitor of harmful substances involved in a large number of biochemical processes in the body. Therefore, scientific research is carried out to carry out the targeted synthesis and modification of new derivatives of these heterocyclic compounds, to determine their structure on the basis of modern methods, to check the various biological properties of the compounds obtained, to create new drugs based on selected biologically active substances (Alagarsamy V., Murugesan S., Dhanabal K., 2007).

Derivatives based on quinazoline have been introduced into various periparatlarr agricultural and medical practices, created on the basis of a very large number of Representatives. Briquettes based on quinzoline have been widely used against viruses, microbes, fungi, colds and cancer (Arun K. Ghosh., Margherita Bindisi. 2015), as well as stimulants for plants (Asma Kh., Rabah A., Antonio I. M., Laiche A., Abdelmalek B., 2018). Substances created on the basis of quinazoline are part of various preparations agricultural and medical practices, created on the basis of a very large number of representatives. Based on quinzoline have been widely used against viruses, microbes, fungicide, colds and cancer (Raffaella S., Daphne W., Daniel A., Jeffrey S., 2004), as well as stimulants for plants (Asma Kh., Rabah A., Antonio I. M., Laiche A., Abdelmalek B., 2018). In recent years, drugs such as imatinib, erlotinib, afatinib, which are used against tuberculosis and cancer patients, can be cited as examples. To this end, the synthesis, modification of various representatives of the biologically active – quinazoline ring in State 6, as well as the determination of their structure, gained relevance. Today, a lot of scientific work is being done on the synthesis and effective use of this type of substance (Imtiaz K., Aliya I., Waqas A., Aamer S.).

Methods and results

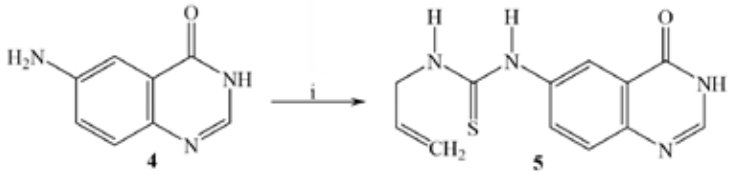
Result and discussion. In the course of our research, an effective and convenient method of synthesizing quinazolin-4-one **(2)** in the presence of o-aminobenzoic acid **(1)** and formamide was implemented and obtained with a quantitative yield (98%). The resulting substance was nitrated under the action of a nitrating agent to synthesize 6-nitroquinazolin-4-one **(3)** in 95% yield. The resulting 6-nitroquinazolin-4-one was reacted with tin (II) chloride dihydrate ($SnCl_2 \cdot 2H_2O$) and HCl to synthesize the corresponding 6-aminoquinazolin-4-one **(4)** in 67% yield.



i) *o*-aminobenzoic acid : formamide (1:2 ratio), 140-145 °C, 2 h.
ii) HNO_3+H_2SO_4 0-2 °C, 1 h; 20-24 °C, 1 h; 60-65 °C, 2 h.
iii) $SnCl_2 \cdot 2H_2O$, HCl/EtOH. 20-24 °C, 2 h; 65-70 °C, 2 h.

The resulting substance **(4)** was thoroughly dissolved by placing 1 mmole in a 20 ml flask, connected to a magnetic mixer at 5 ml DMF, and 1.1 mmole allyl isothiocyanate was added on top. Connected to the refrigerator, the reaction was carried out and mixed

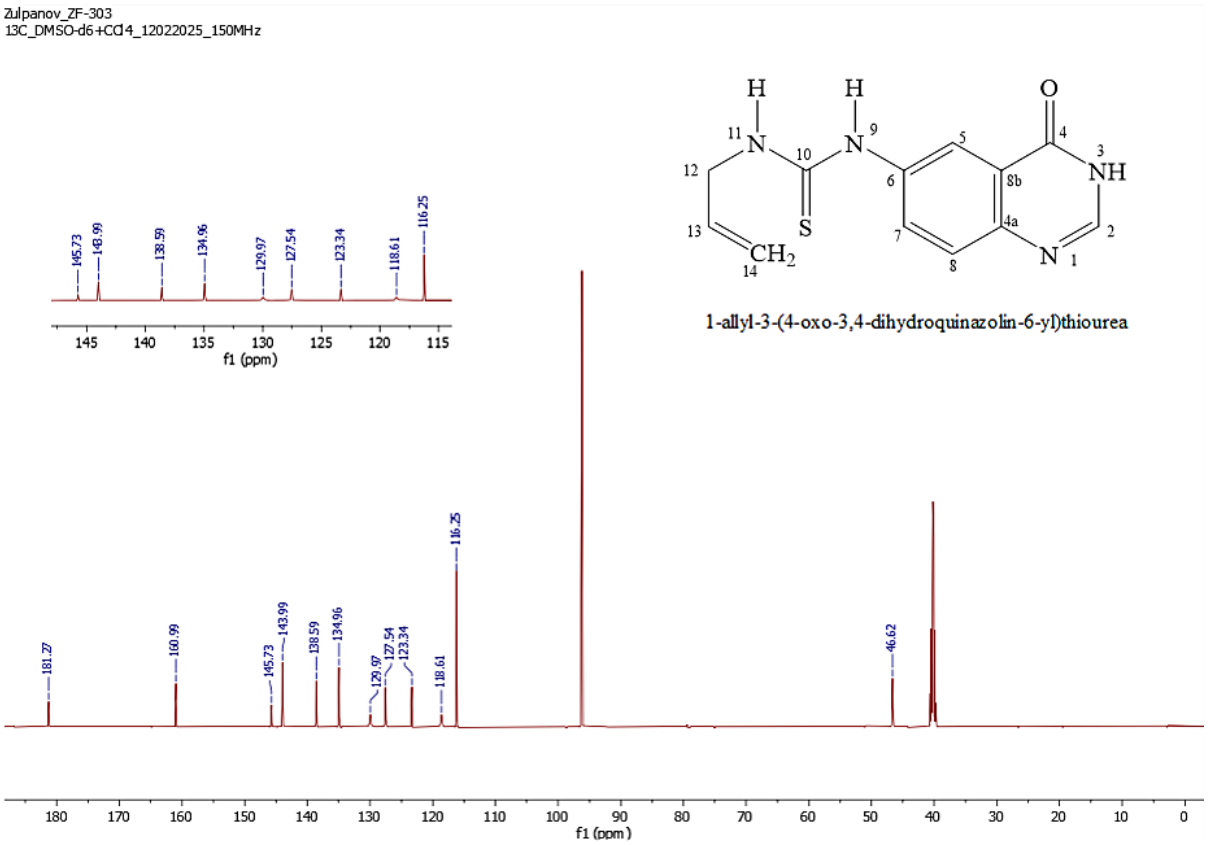
in a magnet at 58–60 °C for 24 hours. The reaction was examined every 2 hours using thin-layer chromotography. Rsulting substance **(4)** was thoroughly dissolved by placing 1 mmole in a 20 ml flask, connected to a magnetic mixer at 5 ml DMF, and 1.1 mmole allyl isothiocyanate was added on top. Connected to the refrigerator, the reaction was carried out and mixed in a magnet at 58–60°C for 24 hours. The reaction was examined every 2 hours using thin-layer chromotography. When the starter substance was completely finished, it was rolled into the ice-cold water in the glass. The precipitate was filtrated and dried on 1-allyl-3-(4-oxo-3,4-dihydroquinazolin-6-yl)thiourea **(5)** at filter paper. DMF: recrystallized in the water system (taken in a ratio of 1 to 1) and dried thoroughly. 1-allyl-3-(4-oxo-3,4-dihydroquinazolin-6-yl) thiourea was obtained with 86% **(5).**



i) Allyl isocyanate, DMF, 63-65 °C, 24 h.

The liquefaction temperature of the resulting substance was determined by the values of 202–204 °C and Rf = 0.61 (sistema; benzene acetone, 1:3 ratio), the structure of which was determined using the spectrum of modern physical research methods^{1}H NMR and^{13}C NMR (**Fig. 1**, **Fig. 2).**

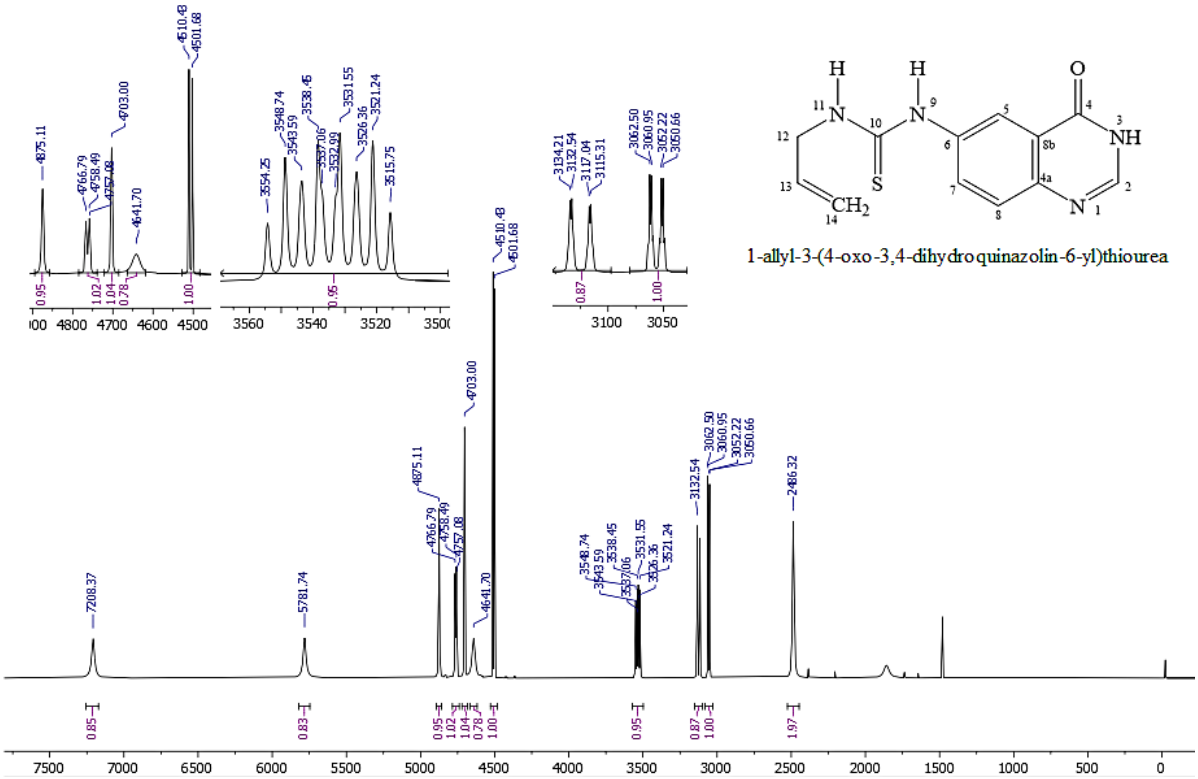
Figure 1.



1HNMRspectrumofquinazlin-4-one (400 *M*Hz, CD3OD, δ, ppm, *J*/Hz): 8.25 (1H, s, H-2), 8.16 (1H, dd, *J*=8.0, 1.6, H-5), 7.76 (1H, ddd, *J*=8.3, 7.2, 1.6, H-7), 7.62 (1H, dd, *J*=8.2, 1.1, H-8), 7.49 (1H, ddd, *J*=8.2, 7.1, 1.2, H-6).**13C NMR spectrum of quinazlin-4-one** (150 MHz, DMSO-d6+CCl4, δ, ppm): 149.13 (C-2), 162.59 (C-4), 122.90

(C-4a), 128.55 (C-5), 127.37 (C-6), 135.67 (C-7), 127.83 (C-8), 149.01 (C-8a).**1H NMR spectrum of 1-allyl-3-(4-oxo-3,4-dihydroquinazolin-6-yl)thiourea** (400 *M*Hz, CD3OD, δ, ppm, *J*/Hz): 8.32 (1*H*, s, H-2), 7.84 (1H, s, H5), 7.94 (1H, d, J=8.3, H7), 7.51 (1H, d, J=8.7, H8), 7.73 (1H, s, H3), 12.01 (1H, s, H9), 9.63 (1H, s, H11) 4.14 (2H, s, H12), 5.89 (1H, s, H13), 5.21 (1H, dd, J=17.2, 1.7, H14a), 5.09 (1H, dd, J=10.28, 1.55, H14b).**13C NMR spectrum of 1-allyl-3-(4-oxo-3,4-dihydroquinazolin-6-yl)thiourea** (150 MHz, DMSO-d6+CCl4, δ, ppm): 145.73 (C-2), 160.99 (C-4), 143.99 (C-4a), 134.96 (C-5), 129.97 (C-6), 123.34 (C-7), 127.54 (C-8), 118.61 (C-8a), 181.27(C-10), 46.62 (C-12), 138.59 (C-13), 116.25 (C14).

Figure 2.



Conclusion

Quinazoline-4-on **(2)**, which has a geretocyclic structure, was obtained in absolute units in the simplest and most convenient way. After nitrolizing the resulting substance **(3),** a recurrence reaction was carried out. As a result of the reaction of the resulting substance **(4)** with isothiocyanate, the **(5)** compounds stored in the thiomochevina fragment were synthesized in high flour.

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