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«100 РОКІВ УСПІХУ ТА ЯКОСТІ»,

присвячений 100-річчю кафедри
фармацевтичної хімії
Національного фармацевтичного
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MINISTRY OF HEALTH OF UKRAINE
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PHARMACEUTICAL CHEMISTRY DEPARTMENT

МІНІСТЕРСТВО ОХОРОНИ ЗДОРОВ'Я УКРАЇНИ
НАЦІОНАЛЬНИЙ ФАРМАЦЕВТИЧНИЙ УНІВЕРСИТЕТ
КАФЕДРА ФАРМАЦЕВТИЧНОЇ ХІМІЇ

100 РОКІВ УСПІХУ ТА ЯКОСТІ

Матеріали міжнародного науково-практичного симпозиуму,
присвяченого 100-річчю кафедри фармацевтичної хімії
Національного фармацевтичного університету

100 YEARS OF SUCCESS AND QUALITY

Materials of the international scientific and practical symposium,
dedicated to the 100th anniversary of pharmaceutical chemistry
department of National University of Pharmacy

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С 81 **100 років успіху та якості**: матеріали міжнар. наук.-практ. симпозиуму, присвяченого 100-річчю кафедри фармацевтичної хімії Національного фармацевтичного університету (18 жовтня 2021 р., м. Харків) = 100 years of success and quality: materials of the international scientific and practical symposium, dedicated to the 100th anniversary of pharmaceutical chemistry department of National University of Pharmacy (October, 18, 2021, Kharkiv). – Електрон. дані. – Х.: НФаУ, 2021. – 89 с.

Збірка містить матеріали Міжнародного науково-практичного симпозиуму «100 років успіху та якості», присвяченого 100-річчю кафедри фармацевтичної хімії Національного фармацевтичного університету, які згруповано за напрямками, представленими науковцями в ході роботи симпозиуму. Розглянуто теоретичні та практичні аспекти цілеспрямованого конструювання та синтезу біологічно активних сполук; створення на лікарських субстанцій; стандартизації ліків, фармацевтичного аналізу субстанцій, фітопрепаратів та екстемпоральної рецептури.

Для широкого кола наукових і практичних працівників фармації та медицини.

The collection contains materials of the International Scientific and Practical Symposium «100 years of success and quality», dedicated to the 100th anniversary of Pharmaceutical Chemistry Department of National University of Pharmacy, which are grouped by the topics of the scientific reports presented during the symposium. It contains the theoretical and practical aspects of targeted design and synthesis of biologically active compounds, development on medicinal substances, standardization of drugs, pharmaceutical analysis of substances as well as plant drugs and individually prepared formulations.

The book is published for a wide number of scientific and practical workers in pharmacy and medicine.

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Search for anti-inflammatory agents among the products of (1*H*-tetrazolo-5-yl)aniline's [5+1]-cyclocondensation

Oleksii Antypenko^{1*}, Sergiy Kovalenko¹

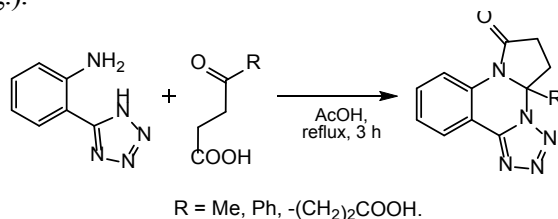
¹Zaporizhzhia State Medical University, Organic and Bioorganic Chemistry Department, Zaporizhzhia, Ukraine

*Corresponding author e-mail: antypenkoan@gmail.com

Introduction. Its known that, unfortunately, the pandemic of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is still spreading all over the world. A timely anti-inflammation treatment, including glucocorticoids, inflammatory cytokines antagonist (IL-6) Tocilizumab, janus kinase inhibitors (Baricitinib or Jakotinib), and chloroquine/hydrochloroquinolone is of pivotal importance and should be tailored in individual patient to achieve the most favorable effects¹. Lately it was reported that substituted pyrrolo[1,2-*a*][1,2,4]triazolo-([1,2,4]triazino)-[*c*]quinazoline-4*a*(5*a*)-propanoic acids had promising anti-inflammatory properties². So, products of (1*H*-tetrazolo-5-yl)anilines cyclocondensation are of interest to be investigated for above-mentioned activity.

Materials and methods. Studies of the inhibitory activity of 15-LOX were performed using the Lipoxygenase Inhibitor Screening Assay Kit. Nordihydroguaiaretic acid was used as a reference compound. Molecular docking to the active site was performed to reveal the ability to bind to 15-LOX (PDB ID - 4NRE).

Results and discussion. Thus, the aim of the study was to search for 15-LOX inhibitors among dihydropyrrolo[1,2-*a*]tetrazolo[1,5-*c*]quinazolines, to discuss the relationship between structure and activity, and to select promising compounds for further biological studies. New condensed dihydropyrrolo[1,2-*a*]tetrazolo[1,5-*c*]quinazolines were obtained by condensing of (1*H*-tetrazolo-5-yl)aniline with ketocarboxylic acids according to a previously tested method³ (Fig.).



The affinity according to the docking was in the range of -7.5--10.3 kcal/mol. The best value was observed for compound with a phenyl residue. Thus, it can be stated about the high affinity towards 15-LOX. This fact was confirmed according to the studies of 15-LOX inhibition. Thus, the compound with a phenyl residue inhibited 15-LOX by 9.64%. The best activity showed a compound with a methyl residue, the level of inhibition – 64.87%.

Conclusions. Dihydropyrrolo[1,2-*a*]tetrazolo[1,5-*c*]quinazolines showed a high level of 15-LOX inhibition indicating potential anti-inflammatory activity. Studies of the synthesized compounds will be carried out in the future.

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