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***In silico* analysis of biological activity of 9'-methoxy substituted 6'H-spiro[cycloalkyl-1,5'-tetrazolo[1,5-c]quinazolines]**

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Introduction. The search for novel biologically active compounds remains a key direction in modern medicinal chemistry. Quinazoline derivatives are of particular interest due to their diverse pharmacological properties, including anticancer, antimicrobial, and anti-inflammatory activities. The introduction of methoxy substituents into the molecular structure can significantly influence their physicochemical and biological characteristics. *In silico* methods, such as molecular docking and ADMET prediction, provide an effective tool for the preliminary evaluation of potential biological activity and pharmacokinetic properties of these compounds, accelerating the process of drug discovery.

Materials and methods. The study employed SwissTargetPrediction to identify potential biological targets of the proposed compounds. Molecular docking was conducted to evaluate binding affinities to the predicted targets. ADME analysis was performed to assess pharmacokinetic parameters and drug-likeness profiles of the investigated molecules¹.

Results and discussion. ADME and target prediction analyses were carried out for a range of 9'-methoxy-6'H-spiro[cycloalkyl-1,5'-tetrazolo[1,5-c]quinazolines]. According to SwissTargetPrediction results, the investigated compounds demonstrated a high probability of interaction with several biologically relevant proteins, including nicotinamide phosphoribosyltransferase (NAMPT), cytochromes P450 (CYP11B1, CYP11B2), glycogen synthase kinase-3 beta (GSK3B), TRPM8 ion channel, and melatonin receptors MTNR1A/MTNR1B. Among these, GSK3B showed predicted to be the most promising therapeutic target for further docking studies².

The predicted toxicity class for all compounds was LD₅₀ ≈ 2500 mg/kg, indicating low acute toxicity³. ADME analysis revealed that all molecules comply with Lipinski's rule of five and have optimal physicochemical characteristics molecular weight 229–327, TPSA ≈ 65 Å², log P 2.2–3.2, supporting their potential as drug-like compounds. Solubility assessment (log S ≈ –2.5 to –4.7) indicated moderate to good aqueous solubility, suggesting both oral and parenteral usability.

Pharmacokinetic profiling predicted satisfactory permeability and acceptable interaction with CYP isoenzymes, confirming favorable biopharmaceutical parameters. Overall, the studied molecules, exhibit promising pharmacological potential as GSK3B inhibitors, which may be relevant for the treatment of neurodegenerative and metabolic disorders.

Conclusions. The conducted *in silico* study revealed that 9'-methoxy substituted 6'H-spiro[cycloalkyl-1,5'-tetrazolo[1,5-c]quinazolines] possess favorable ADME properties and low predicted toxicity. SwissTargetPrediction and docking results indicate potential GSK3B inhibitory activity, highlighting these compounds as promising candidates for further biological evaluation.

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Determination of total phenolics, flavonoids, and B-group vitamins in dried and fresh-frozen bee pollen.....	62
Stragauskyte Gabija, Liaudanskas Mindaugas, Sutkeviciene Neringa, Vaidotas Zvikas, Trumbeckaite Sonata	
Molecular docking and ADME evaluation of potential nootropics containing the pyrrolidin-2-one scaffold.....	63
Rustam Suleiman, Nataliia Kobzar, Angelica Solovyova, Lina Perekhoda	
Standardization and quality evaluation of dried propolis powder for pharmaceutical use	64
Michael Tarapata, Kukhtenko Oleksandr, Manskiy Oleksandr	
Chemical modulation of neuroinflammation: curcumin analogues as selective cyclooxygenase-2 inhibitors.....	65
Halina Tkaczenko, Natalia Kurhaluk	
Development dynamics of phenolic profiles and antioxidant capacity of walnut (<i>Juglans regia</i> L.) leaves during the vegetation period in Lithuania.....	66
Dalia Urbonaviciene, Ona Ragazinskiene, Saulius Mickevicius, Marina Sidorenko, Yelyzaveta Lohvinenko	
Synthesis and antimicrobial activity of 3-(4-oxo-3,4-dihydrothieno[3,2-d]pyrimidin-2-yl)propanamides.....	67
Sergiy Vlasov, Yuliia Nahorna, Victoriya Georgiyants	
The importance of using artificial intelligence in getting a higher education in pharmacy	68
Yaremenko V.D., Rakhimova M.V., Perekhoda L.O.	
Analysis of the quantitative and qualitative content of saponins in <i>Siraitia grosvenorii</i>	69
Valeriia Yavorska, Anne-Claire Mitaine-Offer, Victoriya Georgiyants, Olha Mykhailenko	
Individual phenolic compounds comparison of rapeseed honey and floral source	70
Ernesta Zaksaitė, Mindaugas Liaudanskas, Vaidotas Žvikas, Sonata Trumbeckaitė	
<i>In silico</i> analysis of biological activity of 9'-methoxy substituted 6'H-spiro[cycloalkyl-1,5'-tetrazolo[1,5-c]quinazolines].....	71
Angelina Zhmudenko, Oleksii Antypenko	
Порівняльна характеристика точності та відтворюваності титриметричного і спектрофотометричного методів визначення аскорбінової кислоти у фармацевтичному аналізі.....	72
Інна Абрамова, Ірина Івануса, Марія Михалків	
Чутливість резистентних і полірезистентних клінічних штамів мікроорганізмів щодо нових динамічних похідних стрептоміцину	73
Ірина Андрєєва, Тетяна Осолодченко, Ірина Рябова. Олена Батрак	
Чутливість резистентних і полірезистентних клінічних штамів мікроорганізмів щодо нових динамічних похідних амікацину	74
Ірина Андрєєва, Тетяна Осолодченко, Артур Мартинов, Надія Завада, Михайло Мануйлов	
Дослідження стану молекул води в складі косметичних засобів	75
Надія Антрапцева, Галина Біла, Мар'яна Матвійчук	
Оптимізація умов вилучення кислот з продуктів термообробки кристалогідратів для потреб сучасної косметології.....	76
Надія Антрапцева, Галина Біла, Вікторія Цюра	