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Національний фармацевтичний університет
Кафедра фармацевтичної хімії
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Predicting anticancer activity: machine learning analysis of 5,6-dihydro-tetrazolo[1,5-*c*]quinazolines against 74 cancer cell lines

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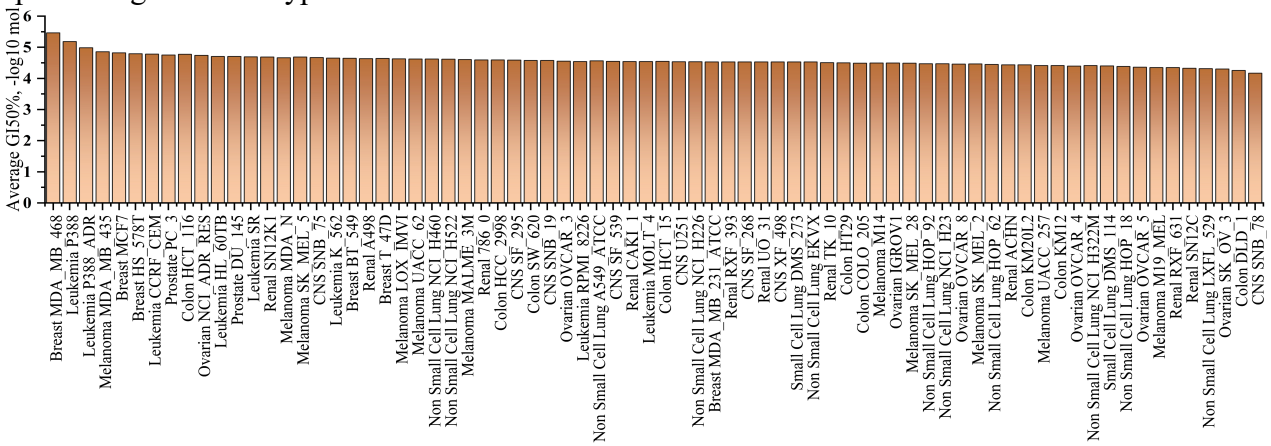
Introduction. The recent advances and considerations for machine learning (ML) models in cancer targeting are: a) Improved diagnosis and screening: They've shown particular promise in analyzing medical imaging with accuracy sometimes surpassing human experts; b) Personalized treatment planning: It helps oncologists tailor therapies to individual patients, potentially improving outcomes and reducing side effects; c) Drug discovery and development: ML accelerates the drug discovery process by predicting potential drug candidates, modeling drug-target interactions, and optimizing lead compounds; d) Predictive modeling: It helps in making more detailed decisions about treatment intensity and timing; e) Radiotherapy planning: The precision of therapy is improving by optimizing treatment plans and helping to more accurately target tumors while sparing healthy tissue; f) Challenges in data quality and quantity: Ensuring large, diverse, and high-quality datasets remains a challenge in the field; g) Interpretability concerns: As ML models become more complex, there's an ongoing challenge in making their decision-making processes transparent to clinicians; h) Integration with clinical workflows: Issues of user interface, training, and workflow disruption need to be addressed; i) Ethical and regulatory considerations: Its use raises important questions about data privacy, algorithmic bias, and the role of AI in medical decision-making; j) Multidisciplinary collaboration: The implementation of effective ML models require close collaboration between scientists, oncologists, radiologists, and other professionals.

Materials and methods. Prediction of anticancer properties among reported earlier series of 5,6-dihydro-tetrazolo[1,5-*c*]quinazolines was done *via* a pdCSM-cancer (using graph-based signatures to identify small molecules with anticancer properties) tool of Biosig Lab using SMILES of the compounds.

Results and discussion. Analysis revealed that the tested substances exhibited calculated average growth inhibition concentrations ($GI_{50\%}$, -log10 mol) ranging from 4.2 to 5.5 across 74 distinct cell lines representing 10 tumor types:



Conclusions. Continued advances in machine learning for oncology are expected to transform cancer treatment, enhancing efficacy while reducing both time requirements and reliance on animal testing. While studied substances did not demonstrate strong anticancer properties, their relatively mild effects on cell growth across diverse cancer cell lines suggest they may have low general cytotoxicity.

ЗМІСТ