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CURRENT TRENDS IN DESIGN OF NEW 3-METHYLXANTHINE DERIVATIVES AS POTENT ANTICANCER AGENTS

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Introduction. The leading reason of death worldwide is cancer, which accounts for approximately 10 million deaths in 2021. Discovering new anticancer drugs remains a serious problem to overcome many tumor – and drug-related obstacles such as side effects, systemic dysentery, and drug resistance. Universal phenomenon in tumor formation is the stepwise exactness of genetic information variations. Several receptor tyrosine kinase (RTK) inhibitors have been accepted by the FDA for the treatment of a variety of malignancies. Also, many RTK inhibitors face the limitations of acquired resistance and durable efficiency due to many resistance pathways. For example, it has been reported that hyperactivation of PI3K/AKT/mTOR signaling is frequently related to resistance of EGFR-mediated endocrine chemotherapy and various other forms of targeted therapy. Activation of upstream tyrosine kinase growth factor receptors or oncogenes, inactivation of the tumor suppressor PTEN (a phosphatase and tensin homolog deleted on chromosome 10), mutation or amplification of PI3K itself is accountable for common PI3K pathway dysregulation in human cancer.

Materials and methods. A substantial portion of modern anticancer drug discovery yet concentrated on the lead finding and optimization of ligands by evaluating, among other properties, their affinity to the primary target, because such targets are proteins that are related to diseases. If a drug interacts with a target, that drug can possibly be used to treat the corresponding disease. An anticancer-drug target should be essential, have a unique function in the pathogen and show an activity that can be rearranged over by tiny molecules.

Results and discussion. To faster the process, a possible direction is to predict new interactions for novel drugs based on known drug-target interactions using in silico approaches before conducting laboratory experiments. Existing computational approaches, that are widespread, are docking simulation and machine learning.

Conclusion. At this time, the search for new drugs is aimed at reprocessing known structures and refining and adjusting them to design new substances. Research on 3-methylxanthine derivatives fits well with this trend, nevertheless, 3-methylxanthines are not currently the drug of choice for cancer treatment, they are promising and valuable group of substances in medical chemistry.