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Inhibition Of Pdk3 by Artemisinin, A Repurposed Antimalarial Drug in Cancer Therapy

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Cancer has emerged as a global concern, claiming one-sixth of lost total lives. Despite advancements in technologies and cancer therapy, there is still a need for easily available novel therapies. The development of new drug molecules is tedious, expensive, and laborious process that can take years to reach in clinical trials. In recent years, drug repurposing has gained popularity as it accelerates selecting new candidates for anticancer therapeutics. One such repurposed candidate is the antimalarial drug artemisinin (AMS), which has anticancer potential. AMS is known to work against the major hallmarks of cancer. The compound halts some of the major signaling pathways involved in cancer, such as Wnt/ β -catenin and PI3K signaling pathways. Pyruvate Dehydrogenase Kinase 3 (PDK3) is overexpressed in many cancer types and thus being considered as an attractive drug target for cancer therapy. In the current study, we investigated the binding and PDK3 inhibitory potential AMS using combined computational and spectroscopic methods. We observed a significant binding affinity of AMS for PDK3. In addition, the kinase activity of PDK3 is significantly inhibited by AMS. We further complemented our findings with molecular docking and MD simulation studies. After getting the required clinical validation, artemisinin may be explored as anticancer therapeutics. enters to become trauma- informed that would help this recognition.

Recent Publications

1. Anwar, S., DasGupta D., Azum N., Alfaifi S., Asiri A., Alhumaydhi A, Suliman A., SharafA., Sharaf., Shahwan M., & Hassan, M. I. Inhibition of PDK3 by artemisinin, a repurposed antimalarial drug in cancer therapy. *Journal of Molecular Liquids* 355, 118928, 2022.
2. Anwar, S., DasGupta, D., Shafie, A., Alhumaydhi, F.A., Alsagaby, S.A., Shahwan, M., Anjum, F., Al Abdulmonem, W., Sharaf, S.E. and Hassan, M.I. Implications of Tempol in Pyruvate Dehydrogenase Kinase 3 Targeted Anticancer therapeutics: Computational, Spectroscopic and Calorimetric Studies." *Journal of Molecular Liquids* *Journal of Molecular Liquids*.350, 118581, 2022.
3. Anwar, S., Khan, S., Anjum, F., Shamsi, A., Khan, P., Fatima, H., Shafie, A., Islam, A. and Hassan, M.I Myricetin inhibits breast and lung cancer cells proliferation via inhibiting MARK4. *Journal of Cellular Biochemistry* 123(2) 359-374, 2022.

Biography

Saleha Anwar is an academic researcher from Jamia Millia Islamia. She has her expertise in cancer therapeutics and has published more than 20 publications in International Journals.

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