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Human DHFR inhibitors: From *in silico* to novel leads

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Background & Aim: Human dihydrofolate reductase is the pivotal enzyme received much attention with its gold standard inhibitor methotrexate. With this inspiration, the research was aimed to design and synthesize dihydrofolate reductase inhibitors (DHFR) for anti-cancer activity.

Methods: *In silico* screening of some Quinazolines by Vlife MDS 4.2 software, their synthesis *in vitro* and *in vivo* pharmacological screening were performed to obtain quinazoline leads for hDHFR inhibition. Structure of the ligands were drawn by Marvinsketch to convert 2D molecules to Mol file followed by optimization of ligands by energy minimization and was carried by molecular mechanics force field (MMFF) on V-Life MDS 4.2 software. Lastly Docking was done and docking scores were compared with standard drug Methotrexate for prioritization of molecules. Further these prioritized molecules were synthesized. The reactions were monitored by TLC and synthesized molecules were characterized IR and NMR spectroscopy. At the end the molecules were evaluated for ***in vitro*** anticancer assay on ten different cell lines as per National Cancer Institute, Bethesda guidelines, followed by ***in vivo*** assay.

Results & Conclusion: Molecules showed comparable inhibition both in *in-silico* and *in-vitro* assays to that of Methothrexate taken as standard.

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Biological effects of dietary plant unsaturated fatty acids (UFAs)

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Dietary UFAs plays considerable roles in human body particularly in modulating plasma cholesterol concentrations and determining the risk for coronary heart disease (CHD). UFAs are characterized by the presence of one or more double bonds, and they are classified as omega-3 (n-3) and omega-6 (n-6) based on the location of the last double bond relative to the terminal methyl end of the molecule. The significance of unsaturated fatty acids (UFA) in normal mammalian physiology was first established by Burr and Burr in 1929, who showed that linoleic acid (LA, C18:2n-6) and α-linolenic acid (ALA, C18:3n-3), are required for normal health and development but are not produced by the human body. Because they must be supplied by the diet, they are called essential fatty acids. LA and ALA are the simplest members of the most biologically significant polyunsaturated fatty acid (PUFA) families, called n-6 and n-3 PUFA respectively that regulate a wide variety of biological functions, which range from blood pressure and blood clotting to the correct development and functioning of the brain and the nervous system. Epidemiological evidence has been shown for the inclusion of n-9 monounsaturated fatty acids (MUFA) with n-6 and n-3 PUFA for replacement of dietary saturated fatty acids to provide added health benefits. The focus of the present paper is to review the dietary requirements, sources, and the biological effects of dietary plant n-9 MUFA, and n-6 PUFA on the human body.

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