J Dev Drugs 2018, Volume 7
DOI: 10.4172/2329-6631-C3-033

Molecular modelling, synthesis and biological evaluation of dihydropyrazole derivatives as potential as anticancer agents

Farah Nawaz and **Ozair Alam**
Jamia Hamdard University, India

A new series of dihydropyrazoles derivatives have been synthesized by Claisen Schmidt condensation reaction as potential epidermal growth factor receptor (EGFR) kinase inhibitors and their biological activities as potential antiproliferative agents have been evaluated against human tumour cell lines. Among these compounds, compound IVe exhibited most potent antiproliferative activity against cancer cell line variants (MCF-7), which showed the most potent EGFR inhibition activity (IC50=0.08 μM for EGFR). Molecular modelling simulation studies were performed to predict the desired interaction with the corresponding amino acids as compared to standard drug. Molecular docking into epidermal growth factor (EGFR) kinase active site (PDB code: 1M17) to get understanding the potency of the compounds and establish SAR. These results suggested that compound IVe may be a promising anticancer agent.

farahnwz5@gmail.com