9th International Conference on Pharmaceutical Research and Drug Discovery
8th International Conference on Analytical Chemistry and Chromatographic Methods
July 27, 2022 | Webinar

Computational drug design and synthesis of pharmacophore based hybrid oncological molecules

Ankita Pathak* **and Md. Shahar Yar**
Anjuman-I-Islam's Kalsekar Technical Campus, India

We, herein report a well-established method used to design 13 novel compounds by studying the scaffold via Sitemap and then 3D-QSAR of marketed molecules to develop hypothesis. Obtained molecules were then subjected to validation via docking with VEGFR receptor PDB ID 4ASE by using glide (Schrodinger LLC) and synthesized aiming at developing a potent anti-neoplastic agent which could act on different scaffolds simultaneously to show anti-angiogenic effects with improved binding affinity available along with good pharmacokinetic profile to reduce cytotoxic effects as associated with the conventional anti-angiogenic drugs. Benzimidazole and oxindole are one of the most recent molecules tested for anticancer potential and also considered to be biologically active moieties. A series of new 2- oxindole substituted derivatives (5a-m) as anti-cancerous compounds was synthesized and identified of their spectral and elemental analysis via ultraviolet (UV)-visible, MS, Infrared (IR) spectroscopy and 1H NMR (nuclear magnetic resonance). The compounds 5d, 5b, 5f and 5h were active against seven different cancer cell lines. The compound 5b was found to follow p38/MAPK pathway while regulating MMP9 with therapeutic *in vivo* potential at 50mg/kg bw of the drug. This research work is executed keeping in mind patients, suffering from cancer having high angiogenic profile to avoid metastasis and resistance development. Next objective devised by us is to approach targeted drug delivery *in vivo* to check the concentration of drug at target site..

Speaker Biography

Ankita Pathak is a PhD scholar in Pharmaceutical Chemistry, School of Pharmaceutical Education and research, Jamia Hamdard. Her current research work is focused on duly oriented study with computational (Homology Model guided 3D-QSAR and MD using FEP+ algorithm, Schrodinger LC) and microbiological approach for anti-angiogenic inhibitors. She is a GOLD medalist from her university in Masters' and was awarded Best Poster for her group work on new derivatives of 2-aminobenzthiazole for diuretic activity. Her area of expertise is computer Aided Drug Design (on Shcrodinger LC and AutoDock) and microbiology of therapeutic targets. She has a good hands-on experience in the field of pharmaceutical chemistry and analytical laboratory techniques..

ankitapathak_sch@jamiahamdard.ac.in

Received Date: June 05, 2022; **Accepted Date:** June 08, 2022; **Published Date:** July 29, 2022