



A STRUCTURE BASED DRUG DESIGN STUDY ON VEGFR-2 INHIBITORS

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Condition: New. Publisher/Verlag: LAP Lambert Academic Publishing | Exploiting Molecular Docking and In-Silico Validation | VEGF (Vascular Endothelial Growth Factor) is a potent angiogenic signal implicated with a key role in several pathological processes, including tumour vascularization, angiogenesis, and endothelial cell growth. The members of VEGF family bind to tyrosine kinase receptors on the cell surface to initiate a signalling cascade. VEGFR-2 is one such Receptor Tyrosine Kinase (RTK) that is found to mediate a majority of the cellular responses to VEGF. A structure based drug design study was performed on VEGFR-2 inhibitors based on the article Hetaryl imidazoles: A novel dual inhibitors of VEGF receptors 1 and 2. The target protein was retrieved from the Protein Data Bank (I.D. 2OH4), based on the Ramachandran plot. The structures of reported inhibitors were obtained in 3-D format using standard software packages. These 3-D analogues were docked to the protein of choice using Molegro Virtual Docker. Based on a correlation between experimentally obtained log IC50 values and the results of the docking study, direct drug design was carried out. Novel inhibitors with significantly higher moldock scores were obtained with simple modifications to the original structure. | Format: Paperback | Language/Sprache: english |...



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