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Ashish Patel

Parul University, India

Design, synthesis and biological evaluation of novel mTOR inhibitors as anti-cancer agents

mTOR, a PI3K related kinase (PIKK) family member, is a component of the mTORC1 and mTORC2 serine/threonine kinase complexes, which play key roles in cell homeostasis and growth and are abnormally regulated in tumor cells. Aberrant activation of the PI3K signaling cascade stimulates cell growth, survival, proliferation and migration. More than 50% of all solid tumors have gene mutations, deletions, or amplifications that lead to unregulated PI3K/mTOR signaling. Therefore, blocking the mTOR signaling pathway by inhibiting mTOR serine/threonine kinase activity provides an innovative strategy for cancer therapy. Benzothiazole derivatives were docked against our target mTOR retrieved from our protein data bank (PDB Id: 3Qk0). Docking results revealed that, with respect to their free binding energy RB1, RB2, RB3, RB9, RB17 and RB19 compounds have highest binding energy by interaction with Try876, Asp964, ASN951, ILE831 amino acid residues. The designed molecules showed better binding affinity in terms of estimated docking scores with respect to the already reported system; hence suggesting that newly designed molecules may serve as potential lead compound for developing new mTOR inhibitors.

Biography

Ashish Patel has pursued his PhD from RK University, Gujarat. He is currently working as HOD in the Department of Pharmaceutical Chemistry in Parul Institute of Pharmacy, Parul University. He has published more than 16 papers in reputed journals and 3 patents on recent development of anti-TB molecules and anti-cancer molecules. He was awarded as Best Teacher for outstanding academic performance as well as Best Academician award from Parul University. He has published one book *The Pearson Guide to the* GPAT. He is working as an Associate Professor with aim to provide the better education and better platform to students.

patel_ashish2388@yahoo.com
aashishpatel2388@gmail.com

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