|  |
| --- |
| **Insilico Discovery of Novel Benzothiazole-Thiadiazole hybrid analogues as Src Kinase inhibitors** |
|  |
| |  |  | | --- | --- | | Author: | Ashish Shah, C N Patel | | Abstract: | Identification of specific target is very important for safe and effective cancer chemotherapy. Protein tyrosine kinase is considered as one of the important target for cancer. Src is prototypical member of tyrosine kinase family who plays critical role in various cellular process like signal transduction, proliferation, survival, differentiation etc. Mutation in Src leads to development of different types of cancer. Therefore Src consider as important target for cancer therapy. We designed benzothiazole-thiadiazole analogues targeting Src kinase using Insilico approach. Structure based virtual screening was performed to find out the novel compounds. Validations of ligands were done using ADME filtration and bioactivity prediction. All the designed compounds have passed Lipinski rule of five. Compounds 8a, 4a, 9a, 2a, 4sa, 3a and 3sa had higher binding affinity (low docking score) as compared to standard drug. Bioactivity prediction reveals that screened compounds may act through kinase inhibition or enzyme inhibition. The promising insilico results of compounds 8a, 4a, 9a, 2a, 4sa, 3a and 3sa opens newer directions to be explored as Src inhibitors. | | Keyword: | Src kinase, Virtual screening, benzothiazole, thiadiazole, Cancer | | DOI: | <https://doi.org/10.31838/ijpr/2020.12.02.277> | |

FULL TEXT : <http://www.ijpronline.com/ViewArticleDetail.aspx?ID=17165>