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Drugs for epimutation obtained from natural products *In silico* drug design

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Prognostication of cancer can be advanced by certain epimutational events. Gene silencing caused by the ectopic methylation in tumour suppressor genes is one such event. The concatenation of DNA methylation is a series of demethylation, de novo methylation and maintenance of methylation. One of the promising treatments of cancer is to inhibit the enzyme responsible for DNA maintenance. This enzyme is DNA methyltransferase 1 (DNMT1). The interminable activity of this enzyme is required to maintain the framework of epimutation. In this study, the crystal structure of the enzyme has been used to develop non-nucleoside DNMT1 inhibitors using virtual screening (VS), absorption, distribution, metabolism, elimination/toxicology analysis and molecular docking studies. To create a subset of lead-like natural products, VS was done on 48,531 natural products. Out of all, three of them were found to interact with the catalytic site of DNMT1 (Cys 1226) through the formation of hydrogen bonds. Thus, from this study some potential lead compounds have been identified for the treatment of epimutation.

Biography

Lekshmi Mohan is in her 4th year of BTech in Biotechnology at VIT Vellore, Tamil Nadu, India. She has been working in the area of cancer biology from the past three years and is working on the foresaid project since the last six months.

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