derivatives

October 2023

DOI: 10.52711/0974-360X.2023.00782

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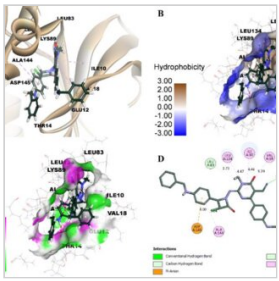
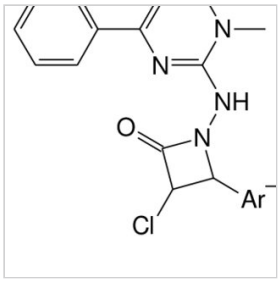
Abstract

A molecular docking study is advance technique of structure based drug discovery and help to develop more heterocyle with promising pharmacological activity. In the present study molecular docking analysis was carried out for the various pyrimidine fused heterocycle derivatives (6a-y and 7a-r)which are planned, using the C-Docker protocol. Roscovitine-complexed X-ray crystallographic enzyme (CDK2) substrate.The result of molecular docking studies showed that 6r, 6l and 6p compounds showed higher docking scores compared to those in the series. Compound 6rexhibited one H-bonding interaction between the nitrogen of Cyanide group of pyrimidine at 5th position with LYS89 (1.80 Å) and four Pi-Alkyl bond with LEU134, ILE10, VAL18 and ALA144 (4.47, 4.46, 5.29, 5.04 Å respectively) one carbon-hydrogen bond with LEU83 (2.73 Å), one Pi-Donor Hydrogen Bond interaction with GLU12 (3.18 Å) and one Pi-Anion interaction with Asp145 (4.00 Å).All synthesized derivatives (6a-y and 7a-r) will be confirmed by the TLC, IR, NMR and MASS spectroscopy. Molecular docking studies give idea regarding the interaction of synthesized compound with protein of interest. The series of 6a-y and 7a-r will be synthesized, confirmed and tested for the in-vitro anticancer activity using human cancer cell line using MTT assay.

Molecular docking, synthesis and study of substituted 1-Methyl-6-Oxo-2-[(2z)-2-(3-Oxo-4-Phenylazetidin-2-Ylidene)Hydrazinyl]-4-Phenyl-1,6-dihydropyrimidine-5-carbonitrile derivatives

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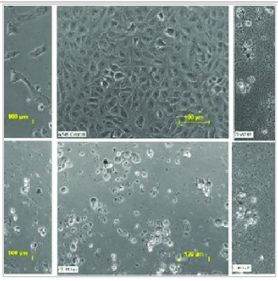

MW	R	R1
449.48	H	OCH3
532.79	OH	Br
446.52	H	H
448.45	H	NO2
528.37	H	OCH3
419.45	OH	H
561.24	H	Br
488.56	H	H
445.49	H	H
536.60	H	H

oncentration µL/mL

		HT-29
40	80	Compound
-54.7	-49.2	7c
33.7	-59.1	7e
-12.4	-31.3	7f
71.3	39.5	7g
-31.2	-50.6	7l
-29.5	-59.1	7m
32.1	10.1	7n
-29.0	-49.4	7o
-35.6	-56.8	7p
78.6	61.4	7r
48.5	42.4	ADR

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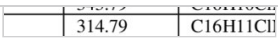

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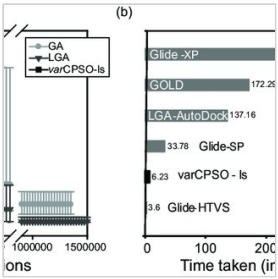

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