19th International Conference on
Medicinal Chemistry & Multi Targeted Drug Delivery
&
International Conference on Catalysis and Pyrolysis
November 05-06, 2018 | San Francisco, USA

Evaluation of an inverse molecular design algorithm in a model binding site for the *in silico* design of a *YEATS2* gene blockador for the depletion of *YEATS2* and its interactions between YEATS domain and acetylated histones for the reduction of the ATAC complex-dependent H3K9ac promoter levels targeting to the deactivation of the essential NSCLC genes

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The computational molecular design is a useful tool in modern drug discovery. Virtual screening is an approach that docks and then scores individual members of compound libraries. In contrast to this forward approach, inverse approaches construct compounds from fragments, such that the computed affinity, or a combination of relevant properties, is optimized. We have recently developed a new inverse approach to drug design based on the dead-end elimination and A* algorithms employing a physical potential function. It has recently been identified that the YEATS domain as a novel acetyllysine-binding module regulating the functional importance of YEATS domain-containing proteins in human non-small cell lung cancer (NSCLC) for cancer cell growth and survival. *YEATS2* binds to acetylated histone H3 via its YEATS domain. Here, we have discovered for the first time an *in silico* predicted and computer-aided molecular designed *YEATS2* gene blockador for the reduction of *YEATS2*-containing ATAC co-localized complex with H3K27 acetylation (H3K27ac) promoters of actively transcribed NSCLC genes as a histone H3K27ac inhibitor that regulates a transcriptional program essential for NSCLC tumorigenesis by utilizing the Microcrylaq™ cluster of algorithms for large-scale protein-ligand docking experiments.

Biography

Ioannis Grigoriadis has completed his PharmacistD at the age of 24 years from Aristotle University of Thessaloniki. He is the scientific director of Biogenea Pharmaceuticals Ltd., a premier biotechnology personalized cancer vaccination service organization. He has published more than 200 papers in reputed drug designing journals.

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