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J Proteomics Bioinform 2018, Volume 11
DOI: 10.4172/0974-276X-C1-113

In silico study of repositioning of drugs against a candidate drug target implicated in type-2 diabetes

Prateek Kumar
Indian Institute of Technology Mandi, India

Diabetes is the 7th major cause of deaths throughout the world. In 2015, 415 million people were living with diabetes and Type-2 Diabetes (T2D) consists about 90% of cases. T2D is characterized by hyperglycemia and caused due to improper production of insulin. Few years back, the genetic architecture of T2D was not clear. After 2007, several high throughput studies such as Genome Wide Association (GWA) studies and Next Generation Sequencing (NGS) have been conducted on the different populations. These studies have confirmed the association of several genes with T2D. GWA studies have proved the association of gene *KCNJ11*, potassium inwardly rectifying channel subfamily J member 11, in T2D signaling pathway. *KCNJ11* regulates the insulin secretion in pancreatic beta cells by inhibiting ATP sensitive potassium channel. Several drugs are available for the treatment of T2D but either due to their improper binding or their stability in the target protein they cause side effects. The crystal structure of human *KCNJ11* has not been solved yet, so structure modeling of *KCNJ11* was performed using computational approaches. To identify the interaction of drugs targeting *KCNJ11*, *in silico* docking was performed and the binding effects of these drugs were analyzed by molecular dynamic simulation. This study may provide a valuable insight on further structure-based drug design approaches for *KCNJ11* for the treatment of type-2 diabetes.

kumar.prateek3@yahoo.com