

# 4<sup>th</sup> INTERNATIONAL WEBINAR ON **AI ML, DATA SCIENCE AND ROBOTICS** DECEMBER 16-17, 2023 | WEBINAR



## **Mr. Kadam Xess**

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**Identification of promising Drug Candidate for WNT and IL33 signaling pathways from Pterocarpus marsupium extracts for T2DM: insights from a transcriptomic study on beta and muscle cell dysfunction, molecular docking and ADMET profile.**

Molecular docking is a process through which small molecules are docked into the macromolecule structures to score their complementary values at the binding sites. Utilizing RNA-seq datasets representing pancreatic betacell dysfunction and muscle cell mitochondrial dysfunction, we identified 19 common differentially expressed genes (DEGs) and protein-protein interaction revealed 9 proteins, wnt2, and il33, which play a crucial role in regulating type 2 diabetes and cancer and promising protein target for computational drug development. We screened 100 portable compounds from Pterocarpus marsupium (Pia Sal) which have anti-diabetic and anticancer properties. Our study is conducted to identify compounds targeting our protein targets of inhibition to stop disease progression. Compounds like Amentoflavone, Stigmasterol, and myricetin have shown good binding affinity with our target proteins. In the current study, we focused on two proteins with high degree, "WNT2(PDB:2ygn) and IL33(PDB:4kc3)" that play an important role in anti-diabetic and anti-cancer properties. The top 15 Compounds like Amentoflavone, Stigmasterol, and myricetin were selected upon a binding affinity for our target protein and analysis of their ADMET properties. The outcomes of the virtual screening docking studies have identified few stable and effective compounds that exhibit the properties to inhibit these cancer and diabetic-inducing proteins.

**Keywords:** Type 2 diabetes, Cancer, Pterocarpus Marsupium, Beta-cell dysfunction, Muscle cell dysfunction, Drug discovery

### **Biography**

**Mr. Kadam Xess** is a student of genomic science from Central University of Kerala. He received his degree in genomic science from the Central University of Kerala. His research interest includes transcriptomic study in type 2 diabetes and drug discovery, and he is currently completing a transcription and drug discovery for type 2 diabetes using the Pterocarpus marsupium plant and Development of biomarkers for type 2 diabetes drug response: Identify and validate biomarkers that can predict which patients are most likely to respond to specific drugs for type 2 diabetes, and which patients may be at risk of adverse effects.