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PHYSICON 2025

The XXXVI Annual Conference of The Physiologycal Society of India

"Innovation in Physiology: From Cell to Systems"

Pre-Conference workshop
20th November,2025

Conference :
21st – 23rd November, 2025

Organized by :
Department of Physiology, AIIMS Bhubaneswar

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XXXVI (36th) Annual Conference of the Physiological Society of India
"Innovations in Physiology: From Cell to Systems"
21st – 23rd November 2025|Bhubaneshwar

A Multi-Phase Approach Using Supervised Algorithms And Clinical Models To Generate High- Accuracy Signatures For Pancreatic Cancer

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Keywords: methylation-driven differentially expressed genes, Machine learning in Pancreatic Cancer, Single Cell RNA seq, DNA methylation, Multi-Omics in Oncology, Molecular docking and dynamics, Drug target.

Abstract

Background: The in silico analyses provide evidence supporting the potential of methylation-driven differentially expressed genes as therapeutic targets across cancer types. This leads us to identify novel targets and their associated drug compounds for further progress towards pancreatic cancer treatment.

Objective: To identify targeted drugs based on methylation driven genes identified using bulk multi-omics data and single-cell level data to pinpoint important disease markers.

Methods: The workflow involves screening using the TCGA and ICGC databases, followed by validation with GEO datasets. The study employs supervised learning algorithms like kNN and random forests, and constructs a prediction model using adaptive LASSO-Cox regression. The process also includes pathway analysis, evaluation of survival status, and immune profile deconvolution, as well as multistage

evaluation of the methylation driven genes. We conducted drug targeting and molecular dynamic simulations, taking into account genes of interest.

Lastly, molecular docking and dynamics simulations were used to find out if the key MEDEGs could be utilized as drug targets.

Results: *CD36, UGT1A1, TFF1, S100P, MUC13, CALHM3* and *ANKRD44* were found to be top 7 methylation driven genes. The mutational profile was also documented

along with pathway analysis, which showed concordance with our observation based on their significant enriched terms namely "Maintenance of Gastrointestinal Epithelium", and "Digestive System Homeostasis". *CD36* had prognostic capabilities

and was seen to significant in terms of survival and also showed significant immune dysregulation. Our novel findings suggest *TFF1, S100P,* and *MUC13* were found to be associated with cell type specific expression as seen in single cell data and *UGT1A1* was found to be suitable for probable drug targeting. *CD36, UGT1A1, TFF1, S100P,* and *MUC13* showed concordance when observed at proteomics level and across other datasets. Apigenin-7-O-glucuronide emerged as the top binder for UDP-glucuronosyltransferase 1A1 (also known as

UDP 1A1), forming stable complexes with favourable interactions. Catechin and epicatechin were identified as the best ligands for *TFF1* and *S100P*, while rutin showed high-affinity binding to *MUC13*.

Conclusion: The study successfully identified and validated a panel of biomarkers specific to pancreatic cancer, with potential applications in early diagnosis and treatment. The findings highlight the importance of multi-omics data integration in cancer research and the potential of personalized medicine in improving patient outcomes. The *in-silico* drug targeting analysis provides a foundation for the development of novel drugs for PanCa treatment. Hence *TFF1, S100P, MUC13*, and *UGT1A1* showcased themselves as most promising biomarkers and novel drug targets.