

The Application of Pharmacoinformatics Approaches to Study Post COVID-19 Complications and Prioritize Drug Targets and Effective Therapeutics: A Focus on Metabolomic Disturbances and Post-COVID-19 Diabetes

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Abstract

COVID-19 pandemic continues to impact an increasing number of people, and many are experiencing long-term debilitating complications including on post-COVID-19 metabolomic disturbances that often lead to post-infection latent autoimmune disease in adults (LADA), which is autoimmune diabetes that progresses slowly. Herein, we applied pharmacoinformatics approaches to study disease mechanisms of LADA and prioritize therapeutic targets and disease-modifying drugs. Key findings herein, highlighted the "Histone deacetylases in Prostate Cancer"," Transcription_Epigenetic regulation of gene expression","COVID-19 immune dysregulation" and " Type 2 diabetes (general schema)" as to enrichment results. Our results uncovered an important link between histone deacetylases (HDACs) and post-COVID-19 metabolomic disturbances, indicating the involvement epigenetics in disease processes leading to LADA. HDACs (e.g., HDAC3 and HDAC4) and SIRTUINs (e.g., SIRTUIN3, SIRTUIN6) as top scoring target hypotheses to treat post COVID-19 LADA. This approach can be applied to prioritize drug discovery hypotheses for many other diseases and receptor systems.

Keywords: COVID-19, diabetes, HDAC, LADA, pharmacoinformatics.