[BIOINFO 2023]

Integration of multiple AI frameworks and data representations for enhancing the performance of predicting blood-brain barrier permeability

Erkhembayar Jadamba[1], Hyeonsu Lee, Sang-Heon Lee[1] and Hyunjin Shin[1]*

[1]*MOGAM Institute for Biomedical Research, Seoul 06730, Republic of Korea*

**Corresponding author: hyunjin.shin@mogam.re.kr*

Computationally predicting the permeability of the blood-brain barrier (BBB) is one of the most important challenges in developing neuroactive therapeutic agents.

While most existing approaches mainly utilize one or some of the structural (fingerprint), physicochemical (descriptors), 1D textual (SMILES), or 2D structural (graph) features in separate individual modeling frameworks. Therefore, the integration of all these feature representations within a single predictive model remains largely unexplored.

We propose a systematic AI platform that can merge LLMs, graph learning, and ensemble learning to exploit the collective power of the different feature representations. Our platform uses informative features and combines them with the textual and graphical knowledge derived from LLMs and graph learning in the frame of ensemble learning.

We also ran comparative study to thoroughly evaluate our approach over other state of the art method in terms of BBB permeability prediction power. Specifically, our platform achieved an AUROC score exceeding 0.95, while other methods performed below 0.90.

Finally, our platform not only enhancing predictive power BBB permeability but also introduces a potential time and cost-efficient way by accelerating the drug development process in the analytical stages, thereby reducing the resources expended on experimental procedures.