

Cheminformatics Analysis of RNA-Binding Ligands

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This project focuses on the analysis and classification of RNA-binding molecules through cheminformatics and machine learning techniques. It involves an extensive examination of various chemical databases containing RNA ligand structures to identify distinctive properties or structural features that set these compounds apart from protein ligands. Additionally, the project leverages advanced machine learning approaches, notably ensemble methods and graph neural networks, to facilitate the identification and classification of RNA ligands. The primary goal of this work is to deepen our understanding of the interactions between small molecules and RNA. This insight is pivotal for the development of novel therapeutic strategies aimed at treating RNA-related diseases. This project illustrates the value of combining cheminformatics and machine learning to decipher the complexities of RNA-ligand interactions, contributing significantly to the progress in medical science and drug discovery.

Bibliography :

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