論 文 内 容 の 要 旨

博士論文題目　Development of a cardiotoxicity prediction scheme using Sub-Graphed Transformer Neural Network
(サブグラフドトランスフォーマーニューラルネットワークを使用した心毒性予測ス キームの開発)

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（論文内容の要旨）

This study introduces a Sub-graphs-based Transformer Neural Network (GSTN) model, leveraging heterogeneous graphs to predict cardiotoxicity in pharmaceutical compounds. By defining distinct sub graphs and employing meta-paths, the model effectively aggregates and propagates intricate molecular structural information, crucial for identifying cardiotoxicity. We integrated the domain knowledge of cardiotoxicity, and addressed the challenges of non-uniform labeling standards by evaluating the impact of various thresholds on model performance, ultimately selecting a dual threshold strategy. These methodologies employed in GSTN markedly outperform traditional GCN models, achieving an impressive Accuracy of 90.5%, a Precision of 90.4%, a Recall of 90.4%, an AUC of 90.4%, and an F1 score of 90.0%. Additionally, we validated 56 FDA-approved drugs, assessing their potential cardiotoxicity to ensure safety in medical applications. Furthermore, to counter the "black-box" nature of deep learning models, we incorporated a visualization technique that assigns different weights to each atom, thus illuminating molecular regions contributing to toxicity. This advancement not only improves interpretability but also guides researchers in avoiding toxic molecular structures. In summary, this study contributes to the field of drug safety analysis by developing a robust, interpretable, and efficient GSTN model.

氏　名	WANG HUIJIA

（論文審査結果の要旨）

令和６年１月 12 日に開催した公聴会の結果を参考に，令和６年２月５日に本博士論文の審査を実施した．本博士論文は，本学位申請者が，独立した研究者として研究開発活動を続けていくために必要な素養を備えていることを示すものである．本論文は，博士（工学）の学位論文としての価値があるものと認める．