DOI: https://doi.org/10.36094/sc.v92.2026.Computatioal_Prediction_of_Molecular_Toxicity.Pathak.270

ARTICLE

Sci. and Cult. 92 (3–4) : 270-272 (2026)

COMPUTATIONAL PREDICTION OF MOLECULAR TOXICITY USING MULTI-ENDPOINT RANDOM FORESTS AND GRAPH NEURAL NETWORKS

AMIT KUMAR PATHAK[1,2], SUBRATA SINHA[3] AND SUBRATA GHOSH*[1,2]

Accurate prediction of molecular toxicity is critical for early-stage drug discovery and chemical risk assessment. In this study, three artificial intelligence–based models were developed using the Tox21 dataset: (i) a descriptor-based Random Forest for global toxicity screening, (ii) a multi-endpoint Random Forest for pathway-specific prediction, and (iii) a graph neural network that learns toxicity directly from molecular structure. The baseline model achieved a ROC-AUC of 0.75, while endpoint-specific learning improved performance to a mean ROC-AUC of 0.819. The graph-based model achieved a competitive ROC-AUC of 0.789 without relying on handcrafted descriptors. These results demonstrate that endpoint-aware ensemble learning and structure-based deep learning provide robust and scalable solutions for predictive toxicology.