**CASE STUDY REPORT**

Toxicity prediction on Daily medication using Multi-Task Learning Approach.

Patent No: US20220383992 A1

Title No: Machine Learning Based Models of Analysing Drug like

Molecules.

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ABSTRACT:

There is a Provided method for Machine Learning based method analysing of drug like molecules by representing molecular quantum states of each drug like molecule as a quantum graph and feeding the quantum graph as an input to a Machine learning System.

METHODOLOGY:

1.Gather Drug Like Molecules with SMILES or InChI representations.

2.Convert Molecular representations into Quantum graphs where each nodes represent Quantum descriptors and edges represent Quantum Interactions.

3.Use Quantum Graph Neural Networks (QGNN) to process the data.

4.Feed Quantum graphs into Multi-Parameter Optimization (MPO) model to evaluate the performance based on the parameters.

ETHICAL CONSIDERATIONS:

1.Molecular Datasets should be accessed legally and transparently.

2.MPO can inherit biases from training data which can lead to in-inaccurate predictions.

3.Misuse of Predictive models should be avoided to prevent unethical Drug Synthesis.

CASE STUDY:

FDA MODERNIZATION ACT 2.0

Overview:

The FDA Modernization Act 2.0 allows the FDA to consider information other than that from animal studies, shining a spotlight on significant advancements in biology and technology that have occurred in the past several decades.

The study suggests that impaired cross talk between endothelial cells and cardiomyocytes can contribute to the pathogenesis of LMNA-related dilated cardiomyopathy and statin may be an effective therapy for vascular dysfunction in patients with cardio laminopathy.

Integrating iPSCs, AI, and computational biology into the process pipeline is transforming drug discovery and development from what used to be a slow and iterative process to an expedited, yet precise one.

Conclusion:

Advances in “clinical trials in a dish” that combine computational biology and human iPSCs may revolutionize drug development and reduce human risks by providing more relevant human-specific toxicity data.

The US Congress has recognized it and FDA regulators are keen to adopt many of these new alternative approaches for drug development.