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Experiment No: 01

**Aim:**

A case study on Recent Innovations in the field of AI-based papers published in IEEE/ ACM/ Springer or any prominent journal.

**Theory:**

**Paper:** *Drug Discovery and Drug Identification using AI.*

**Video:**<https://youtu.be/QrcO2i0dEHE>

**Summary:**

They implemented a process using the Intel pen VINO toolkit for the identification of drugs. With this detection technique, we can identify the reactants which are added as drugs and automates the entire flow. They used intel OpenVINOtoolkit with a custom object detection technique to train the model using the faster Region-Based Convolutional Neural Network (R-CNN) method with labeled drugs (organic compounds) that act as Reactants. Using this approach, the entire drug discovery process of a clinical trial for the process can be reduced to a very small time of 3-4 months(which generally takes 10-12 years). Using this technique they can generate simulated drugs to see the behavior and implementation faster. The catch here is to find a virtual compound that helps to take a decision and reduce the time for unnecessary walkthroughs for the process. AI model reproduces natural chemical diversity for desired molecules. There were multiple phases of testing namely phase 1, phase 2, and phase 3 mostly testing failed at phases 2 and 3. Using robotics, data processing/control software, liquid handling devices, and sensitive detectors, high-throughput screening allows researchers can quickly conduct millions of chemical, genetic, or pharmacological tests. Through this process can rapidly identify active compounds, antibodies, or genes that modulate a particular bio-molecular pathway. The results of these experiments provide starting points for drug design and for understanding the non-interaction role of a particular location. Using the main approach which is known as Objective-Reinforced-GAN (ORGAN).

ORGAN3 allows to :

* Generate samples that are both diverse and interesting.
* To direct the generative process towards certain objectives as an approach to Reinforcement Learning.
* To work with discrete sequence data which is SMILES.

Chemical interaction plays a key role in predicting candidate drugs. SMILES are generally known as Simplified Molecular Input Line Entry Systems which is aString. As an example, the Canonical SMILES for the Benzene molecule is represented as C1=CC=CC=C1. They used generative and predictive molecules.

This model gives a good use case of deep learning and computer vision; introducing a computer vision recipe using the model optimizer and inference engine of the Intel® Distribution of OpenVINO™toolkit.

**CONCLUSION :**

While performing this experiment we learned various applications of AI in the real world whether it is in the field of Science, Industry, or Education. While researching, we learned that predictive and general models used AI applications in drug discovery. Using this model drug discovery decreased to months.