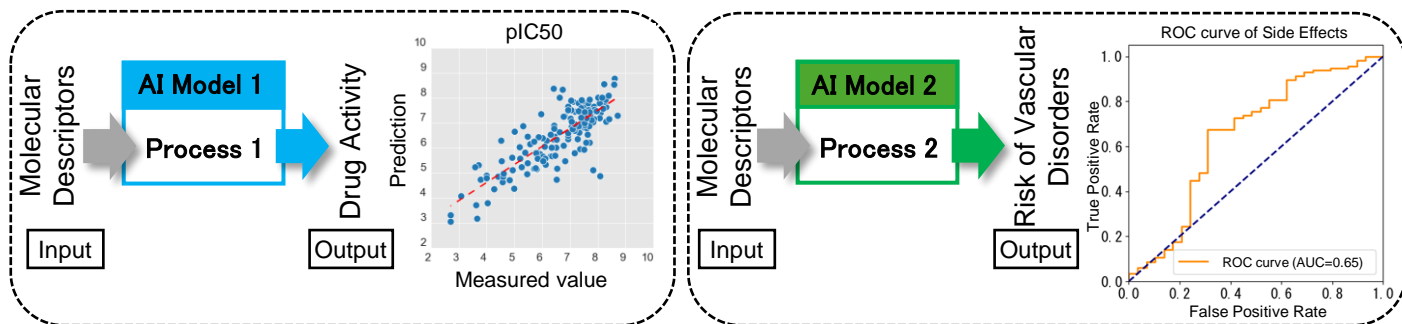


# Prediction Model Integration and Multi-Objective Optimization in Pharmaceutical Development Using Multi-Sigma™

This case study showcases Aizoth's Multi-Sigma, leveraging its AI chain analysis and multi-objective optimization to balance drug activity (pIC50) and side effects for BACE inhibitors, potential Alzheimer's treatments

## 1. Prediction of Drug Activity and Side Effects (Risk of Vascular Disorders)

Multi-Sigma's prediction functionality enables training of AI models using molecular descriptors and biological properties to capture their interrelationship.



## 2. Factor Analysis of Key Influences on Drug Activity and Side Effects (Risk of Vascular Disorders)

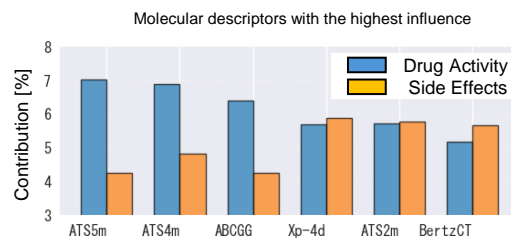
Multi-Sigma's factor analysis allows the identification of molecular descriptors that contribute to drug activity and the risk of vascular disorders, respectively.

Molecular Descriptors with Significant Impact on Drug Activity

1. ATS5m: +7.02%
2. ATS4m: +6.89%

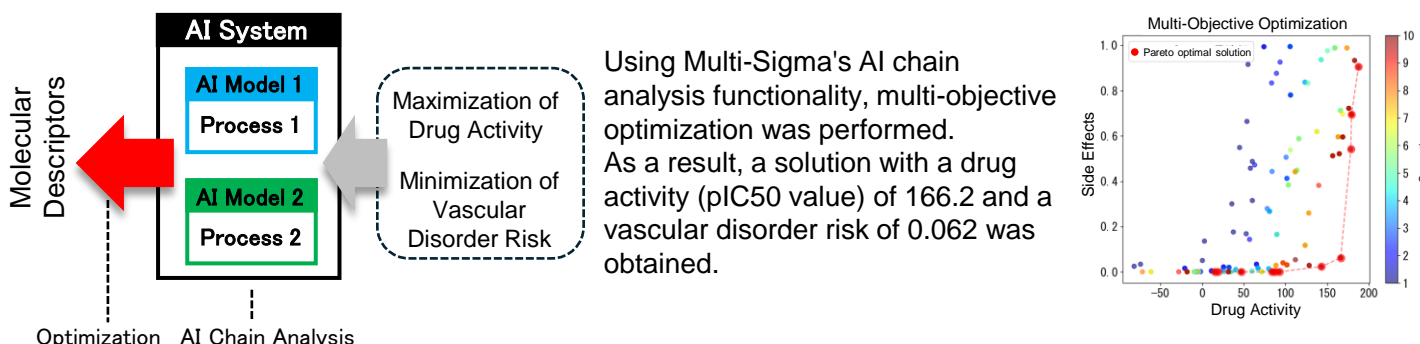
Molecular Descriptors with Significant Impact on the Risk of Vascular Disorders

1. Xp-4d: +5.88%
2. ATS2m: +5.77%



## 3. Optimization of Drug Activity and Side Effects (Risk of Vascular Disorders)

By combining Multi-Sigma's AI chain analysis and optimization functionalities, it's possible to propose combinations of molecular descriptors that maximize drug activity while minimizing the risk of vascular disorders.



(Note) Dataset: Molecular data obtained from the NCI database and MoleculeNet. Molecular descriptors calculated using the Mordred module. Also, data sourced from Kaggle (<https://www.kaggle.com/datasets/mmelahi/cheminformatics>).

AIZOTH inc. provides a range of AI services, including Multi-Sigma™, AI consulting, experimental condition optimization support, and contract research and development. Multi-Sigma™ is a cloud-based AI software designed for research and development, significantly reducing experimental workload and enabling researchers to discover innovative solutions to real-world challenges with minimal experimental datasets.

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