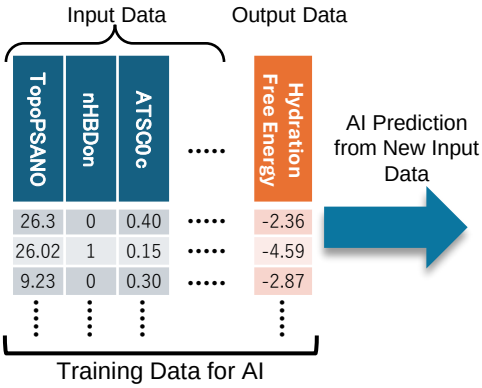
Hydration Free Energy Prediction in Molecular Design Using Multi-Sigma®

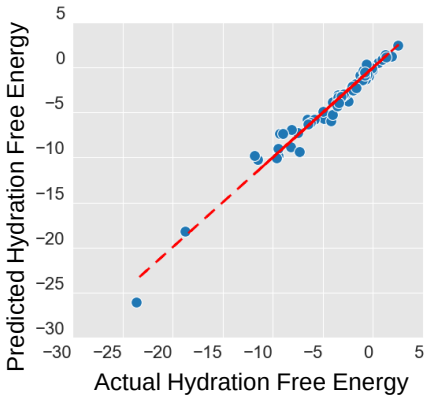
This case study introduces the use of AIZOTH's AI analytics platform, Multi-Sigma®, to predict, analyze key factors influencing, and optimize hydration free energy, a critical property in the drug discovery process.

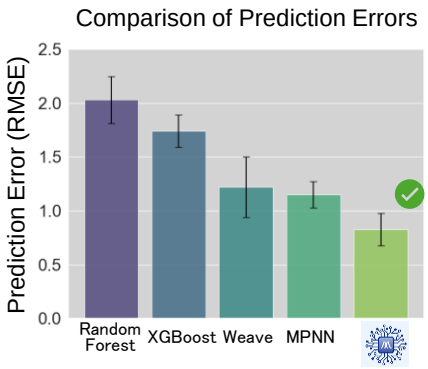
1. Prediction of Hydration Free Energy

The AI prediction capabilities of Multi-Sigma® enable the construction of AI models that capture the relationship between input data and output data through model training. Using this AI model, it is possible to accurately predict hydration free energy values from new molecular descriptors.



AI Prediction from New Input Data





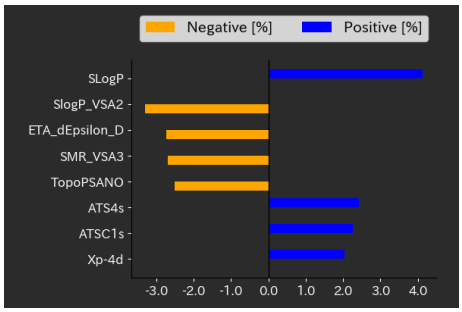
Wu, Zhenqin, et al. "MoleculeNet: a benchmark for molecular machine learning." Chemical science 9.2 (2018): 513-530.

2. Factor Analysis on Hydration Free Energy

The factor analysis functionality of Multi-Sigma® allows the identification of molecular descriptors that positively (and negatively) contribute to hydration free energy.

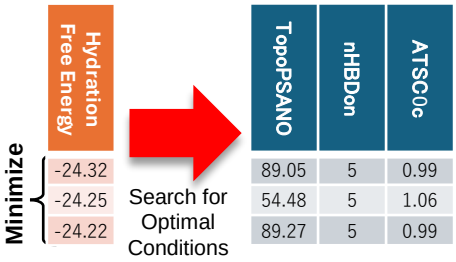
Strong Positive Influence
1. SLogP: +4.12%
2. ATS4s: +2.42%
3. ATSC1s: +2.25%
4. Xp-4d: +2.04%

Strong Positive Influence
1. SlogP_VSA2: -3.29%
2. ETA_dEpsilon_D: -2.72%
3. SMR_VSA3: -2.68%
4. TopoPSANO: -2.50%



3. Optimization to Minimize Hydration Free Energy

The optimization functionality of Multi-Sigma® can propose combinations of molecular descriptors that minimize hydration free energy.



Expected Outcomes:

1. Significant Streamlining of the Drug Discovery Process
2. Reduction in Experimental Costs
3. Realization of Innovative Molecular Design
4. Shortening of Development Time

Advantages of Optimization with Multi-Sigma®:

For instance, optimization can be conducted under the condition that nHBDon takes only integer values. Moreover, optimization can also be carried out by constraining the range of input values.

(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).