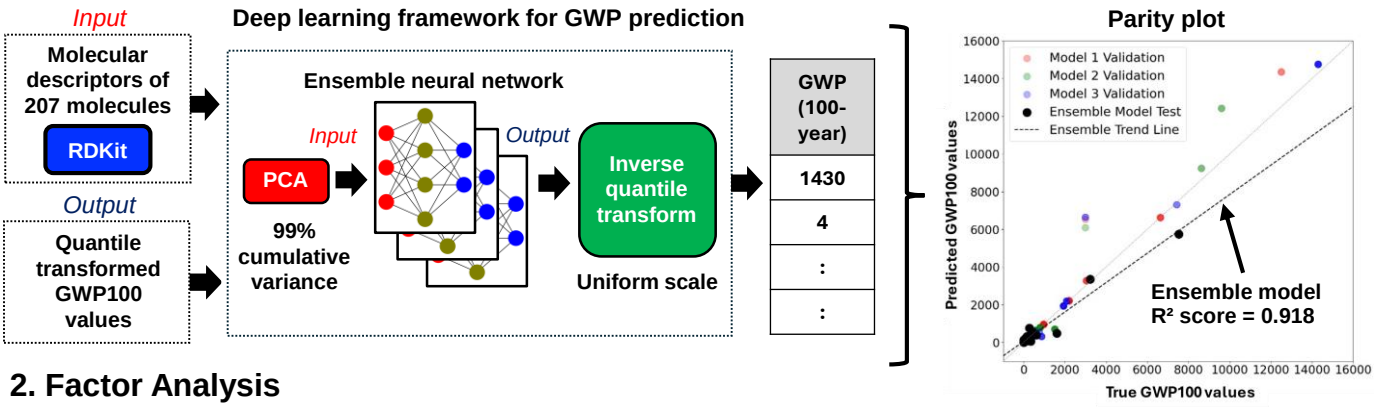
Global Warming Potential Prediction Using Multi-Sigma®

Refrigerants have global warming potentials (GWPs) thousands of times higher than CO_2, making them major climate contributors. As global policies like the Kigali Amendment push for low-GWP (<100) alternatives, this study presents an AI-based framework on the Multi-Sigma® platform to predict GWP100 values of 207 refrigerants, enabling fast and efficient screening for sustainable refrigerant design.

1. AI analysis

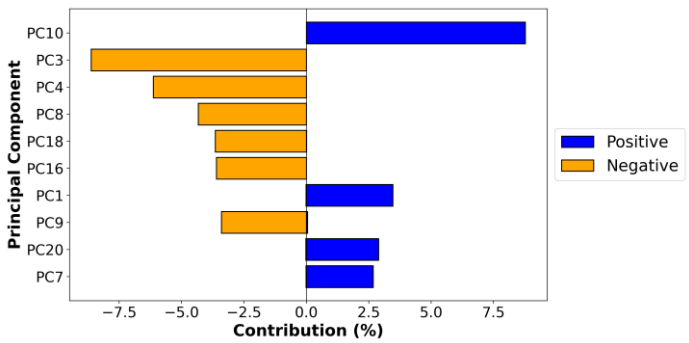
The AI model was built using RDKit descriptors to featurize refrigerants listed in the IPCC AR6 report. Principal Component Analysis (PCA) reduced the dimensionality of input features, and quantile transformation was applied to normalize the skewed GWP distribution. An ensemble of three neural network models, trained on the Multi-Sigma® platform, achieved the highest accuracy, reaching an R^2 score of 0.918 on the original GWP scale after inverse transformation.



2. Factor Analysis

Using Multi-Sigma®'s factor analysis (explainable AI module) identified the most influential principal components (PCs) in GWP prediction: PC10, PC3, and PC4. PC10, associated with molecular weight, lipophilicity, and allylic oxides, showed a strong positive correlation with GWP. In contrast, PC3, linked to aliphatic heterocycles and topological indices, and PC4, related to nitriles and volume-based descriptors, contributed negatively to GWP. These insights highlight key molecular features that can guide the design of low-GWP refrigerants.

Factor analysis in GWP prediction



Influencial molcular descriptors

Principle component	Descriptor
PC10	BCUT2D_MWLOW
PC10	SlogP_VSA6
PC10	fr_allylic_oxid
PC3	NumAliphaticHeterocycles
PC3	NumSaturatedHeterocycles
PC3	Chi2v
PC4	SMR_VSA10
PC4	SMR_VSA9
PC4	fr_nitrite

The developed GWP prediction model can be applied to screen chemical databases for refrigerant candidates that exhibit low GWP and align with key molecular features identified through factor analysis.

Note: The data used in this analysis was processed and edited based on the data published in the article below, under Creative Commons Zero 1.0 Universal (CC0 1.0) license.

Data Source: Rajapriya, Navin, and Kotaro Kawajiri. "Deep Learning for GWP Prediction: A Framework Using PCA, Quantile Transformation, and Ensemble Modeling." arXiv preprint arXiv:2411.19124 (2024).https://doi.org/10.48550/arXiv.2411.19124