DEVELOPMENT OF MACHINE LEARNING MODELS ON THE ANTI-ICING PERFORMANCE OF NADES FOR APPLICATION IN ANTI-ICING COATINGS

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INTRODUCTION

Ice formation is a prevalent issue that poses security risks across various sectors. Unwanted ice accumulation can lead to significant economic challenges and, in some instances, result in fatalities.

Figure 1. Ice formation

Natural deep eutectic solvents (NADES) represent a low-toxicity and efficient method for addressing this issue. Under cold conditions, NADES create a robust hydrogen bond network that lowers the melting point below freezing, effectively preventing ice growth. NADES are derived from plant metabolites, including sugars, amino acids, and organic acids.

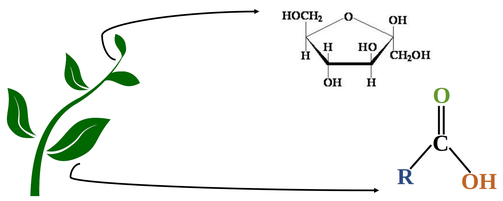

Figure 2. NADES derived from plant metabolites, including sugars, amino acids, and organic acids.

In this study, a machine learning (ML/QSAR) framework is developed to identify the key features influencing the performance of NADES as anti-icing agents. We developed three predictive models for Melting Temperature, Glass Transition Temperature, and Enthalpy of Melting Temperature, utilizing a combination of genetic algorithms (GA), multiple-linear regression (MLR) and non-linear methods.

ACKNOWLEDGMENTS

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METHODS

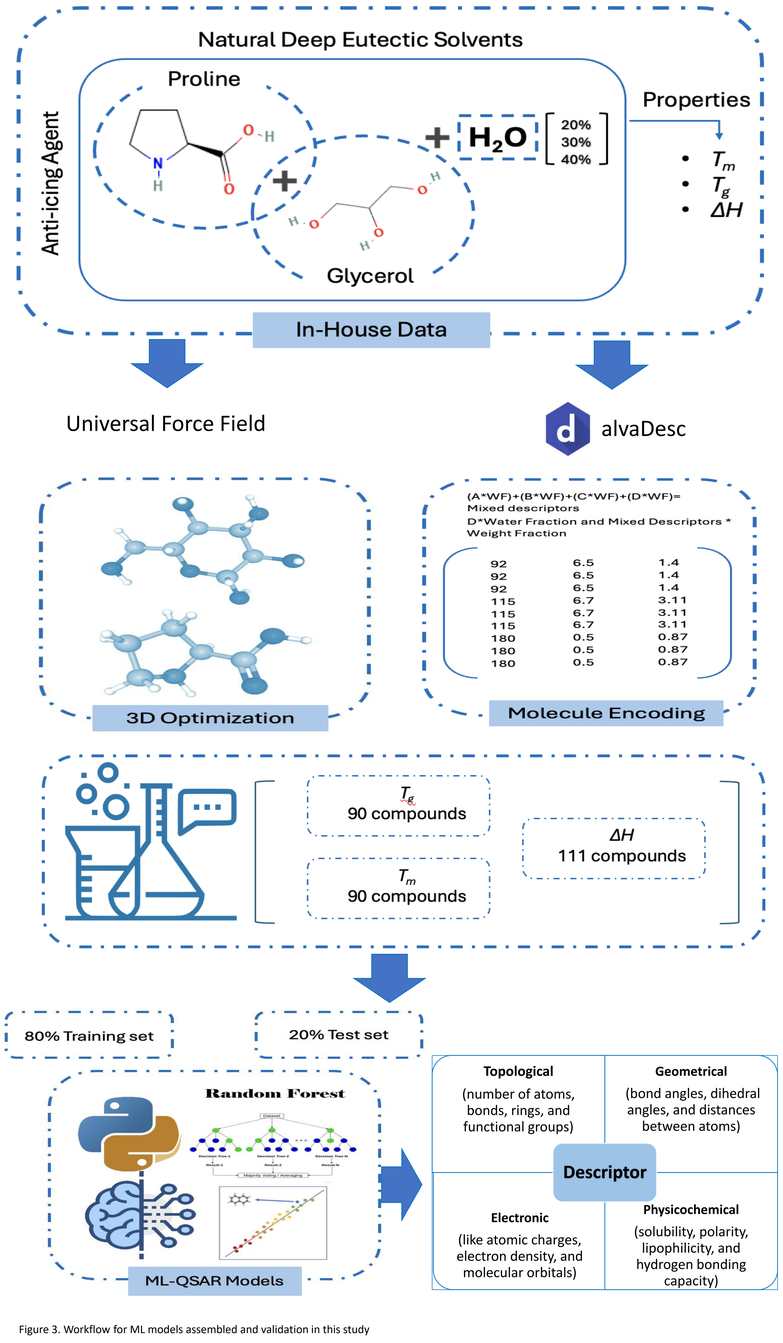
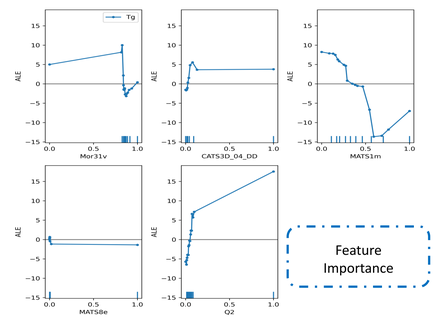


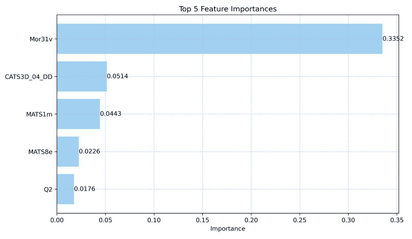
Figure 3. Workflow for ML models assembled and validation in this study

RESULTS & DISCUSSION

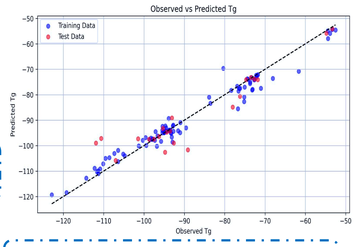
Machine learning (ML) techniques were employed to investigate the structure-property relationship of the NADES system, aiming to predict its Glass Transition Temperature, Melting Temperature, and Enthalpy. Random Forest (RF) and Multiple Linear Regression (MLR), were developed to develop the properties of NADES. Additionally, ML methods helped identify the most significant descriptors related to the system's properties and operations. This approach revealed essential chemical characteristics associated with enhanced anti-icing performance, providing valuable insights for designing anti-icing coatings.



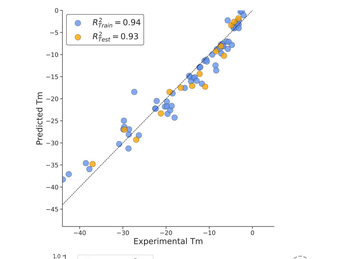
Feature Importance



Predictive Tg Model: R^2= 0.96 , R^2_{ext}= 0.8



Predictive T_m Model: R^2= 0.94 , R^2_{ext}= 0.93



Predictive ΔH Model: R^2= 0.9 , R^2_{ext}= 0.89