

## Machine Learning Framework to Predict Glass Transition Temperature in Natural Deep Eutectic Solvents: A Step toward Green Functional Materials

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Table S1. List of the ML models developed.

| Model                            | R <sup>2</sup> Training | R <sup>2</sup> Test | Test MSE |
|----------------------------------|-------------------------|---------------------|----------|
| Random Forest                    | 0.96                    | 0.87                | 0.0001   |
| Gradient Boosting                | 0.99                    | 0.82                | 0.0002   |
| XGBoost                          | 0.99                    | 0.75                | 0.0003   |
| LightGBM                         | 0.99                    | 0.79                | 0.0003   |
| CatBoost                         | 0.99                    | 0.84                | 0.0002   |
| Lasso Regression                 | 0.1                     | 0.1                 | 0.0012   |
| Support Vector Regression (SVR)  | Failed                  | Failed              | -        |
| k-Nearest Neighbors (kNN)        | 0.73                    | 0.84                | 0.0002   |
| Gaussian Process                 | 1                       | Failed              | 2.2376   |
| Artificial Neural Networks (ANN) | 0.57                    | 0.68                | 0.0004   |