

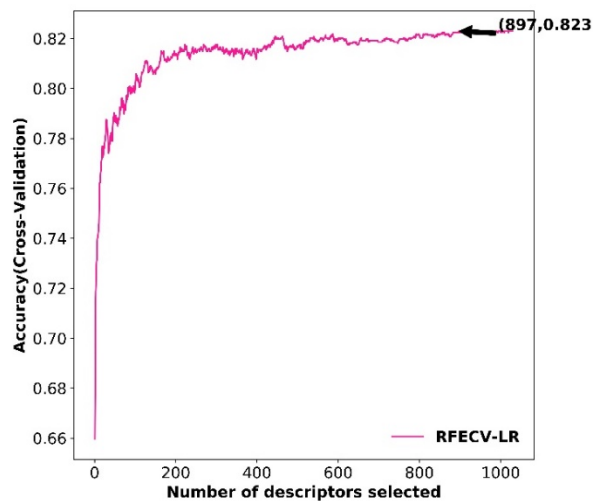
## Supplementary Information

# An Explainable Supervised Machine Learning Model for Predicting Respiratory Toxicity of Chemicals using Optimal Molecular Descriptors

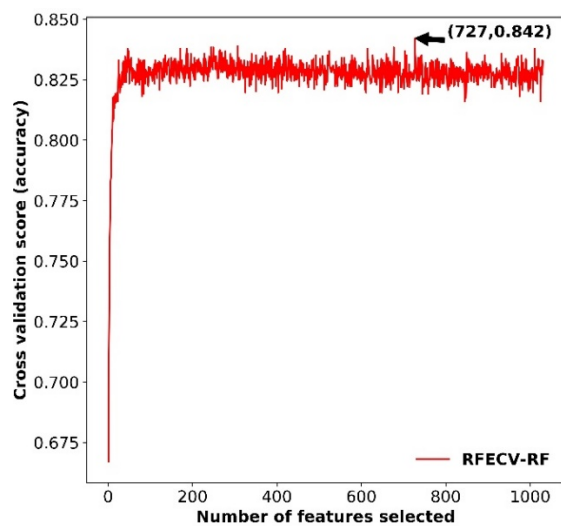
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### Content:

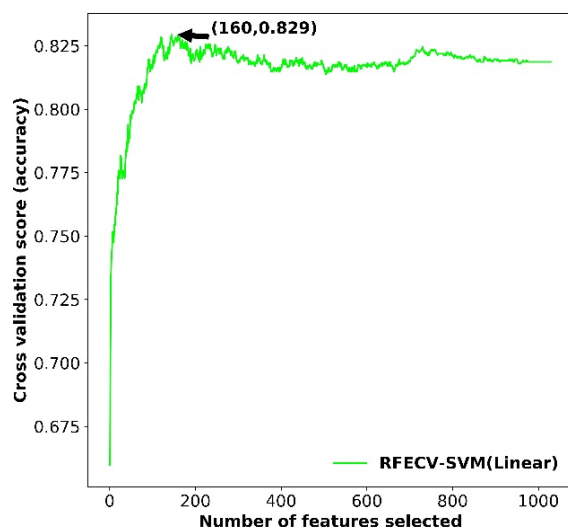
- **Table S1:** Training set compounds with molecular descriptors information.
- **Table S2:** Testing set compounds with molecular descriptors information.
- **Table S3:** External validation set compounds with molecular descriptors information.
- **Table S4:** The optimal parameter values of the machine learning models.
- **Table S5:** The performance of various single and hybrid feature selection methods.
- **Table S6:** The details of the selected optimal descriptors.
- **Table S7:** The performance of machine learning classifiers using the optimal descriptors.



**(a) Wrapper Method : RFECV-LR**

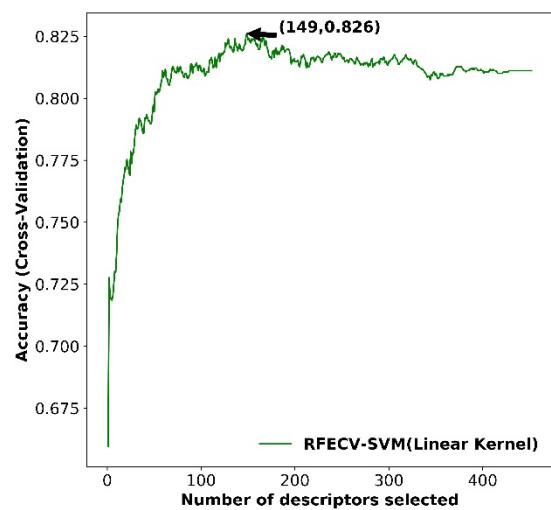


**(b) Wrapper Method : RFECV-RF**



**( c ) Wrappers Method: RFEC V-SVM**

**Supplementary Figure S1. Single Feature Selection Methods(a-c)**



**Supplementary Figure S2. Hybrid feature selection methods (Filter + Wrapper: Fs\_RFECV-SVM)**