**Materials & methods**

Dataset: The experimental data of the OH radical degradation rate constants of 460 heterogeneous organic compounds were obtained from literature [1].

Descriptors: Zero, mono-, and bi-dimensional descriptors available in DRAGON 5.5 [2] (2D descriptors available at CADASTER web[3]) and ETA descriptors [4].

Quantum-chemical descriptors (HOMO, LUMO, ΔHOMO-LUMO) calculated by HYPERChem (AM1 method) were always added.

Method: Genetic Algorithm-Variable Subset Selection (GA-SSS), Multiple linear regression (MLR) and Ordinary Least Squares regression (OLS)

Data splitting: Random by response, K-ANN and K-means clustering

Statistical parameters: Internal (R², Q², RMSE, Q²(pred)) external (Q²-F[1], Q²-F[2], Q²-F[3]), ICC [8] and concordance correlation coefficient [9].

**Materials & methods**

Dataset: The experimental data of the OH radical degradation rate constants of 460 heterogeneous organic compounds were obtained from literature [1].

Descriptors: Zero, mono-, and bi-dimensional descriptors available in DRAGON 5.5 [2] (2D descriptors available at CADASTER web[3]) and ETA descriptors [4].

Quantum-chemical descriptors (HOMO, LUMO, ΔHOMO-LUMO) calculated by HYPERChem (AM1 method) were always added.

Method: Genetic Algorithm-Variable Subset Selection (GA-SSS), Multiple linear regression (MLR) and Ordinary Least Squares regression (OLS)

Data splitting: Random by response, K-ANN and K-means clustering

Statistical parameters: Internal (R², Q², RMSE, Q²(pred)) external (Q²-F[1], Q²-F[2], Q²-F[3]), ICC [8] and concordance correlation coefficient [9].

**Results and Discussion**

- **Unambiguous Algorithm**

The application of any QSAR models to chemicals without experimental data largely depends on model reproducibility.

Regular up-gradation of software almost abolishes the reproducibility

- **Validation**

Validation is the process by which the reliability and relevance of a procedure are established for a specific purpose.

- **Unambiguous Algorithm**

The application of any QSAR models to chemicals without experimental data largely depends on model reproducibility.

Regular up-gradation of software almost abolishes the reproducibility

- **Validation**

Validation is the process by which the reliability and relevance of a procedure are established for a specific purpose.

- **Unambiguous Algorithm**

The application of any QSAR models to chemicals without experimental data largely depends on model reproducibility.

Regular up-gradation of software almost abolishes the reproducibility

- **Validation**

Validation is the process by which the reliability and relevance of a procedure are established for a specific purpose.

- **Unambiguous Algorithm**

The application of any QSAR models to chemicals without experimental data largely depends on model reproducibility.

Regular up-gradation of software almost abolishes the reproducibility

- **Validation**

Validation is the process by which the reliability and relevance of a procedure are established for a specific purpose.

- **Unambiguous Algorithm**

The application of any QSAR models to chemicals without experimental data largely depends on model reproducibility.

Regular up-gradation of software almost abolishes the reproducibility

- **Validation**

Validation is the process by which the reliability and relevance of a procedure are established for a specific purpose.