Machine learning methods for drug discovery and toxicology: How to develop a QSAR model using Python

ProtoQSAR

MOLDRUG AI Systems

Module 1: Introduction to chemoinformatics

1.1 Overview of computational methods
1.2 Practice Python for chemoinformatics

Module 2: QSAR classification model (step by step)

2.1 QSAR introduction and workflow
2.2 Data retrieval and curation for classification models
2.3 Descriptors calculation
2.4 Train/test splitting and scaling
2.5 Descriptor selection
2.6 Model development and optimization
2.7 Prediction and applicability domain for classification models

Module 3: QSAR regression model

3.1 Introduction to regression QSAR models
3.2 Data retrieval and curation for regression models
3.3 From descriptors calculation to model development and optimization
3.4 Prediction and applicability domain for regression models

Module 4: Develop a QSAR model (final project)

4.1 Final project: develop a full model by yourself