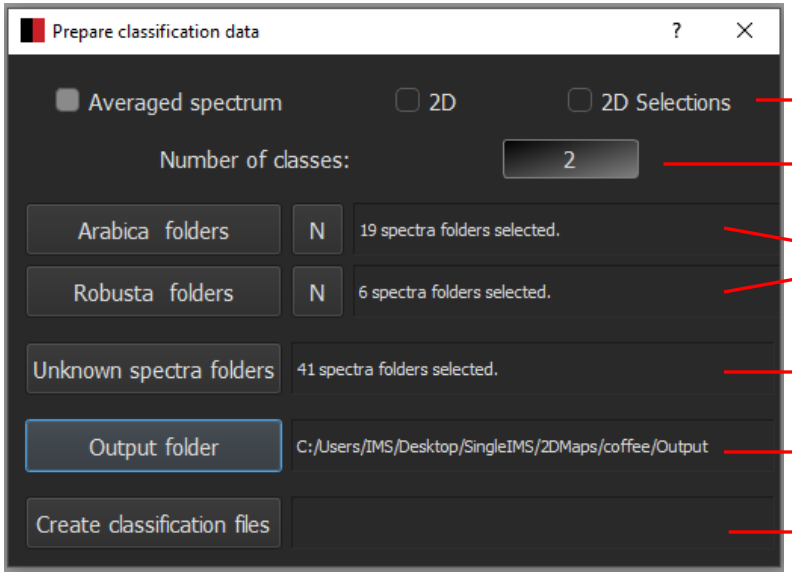
Machine learning classification of IMS spectra by MaSaTECH Chemometrics

Step1: Prepare classification data



Choose if you want to classify : Averaged spectrum along retention time, Complete 2 Dimensional Map or Selected areas from 2D Map

Select number of classes you want to use in your model

Choose recorded spectra of each class. This will create **Training Data**

Choose recorded spectra you **want to classify** (unknown class)

Choose Output folder where to save **prepared data**

Create classification files

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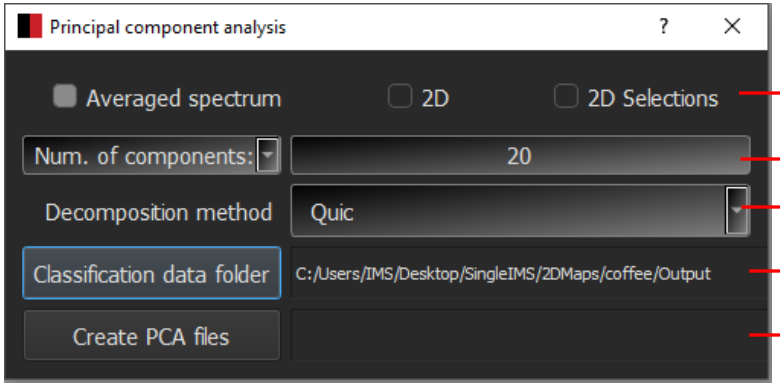
Step2: Principal Component Analysis



Choose if you want to use **PCA** for : Averaged spectrum along retention time, Complete 2D Map or Selected areas from 2D Map

Write number of **Principal Components** you want to use for classification

Choose decomposition method for PC generation

Choose folder where you saved your prepared data

Press to create PCA files

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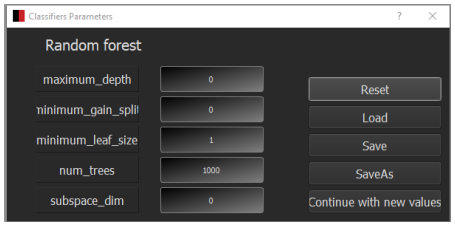
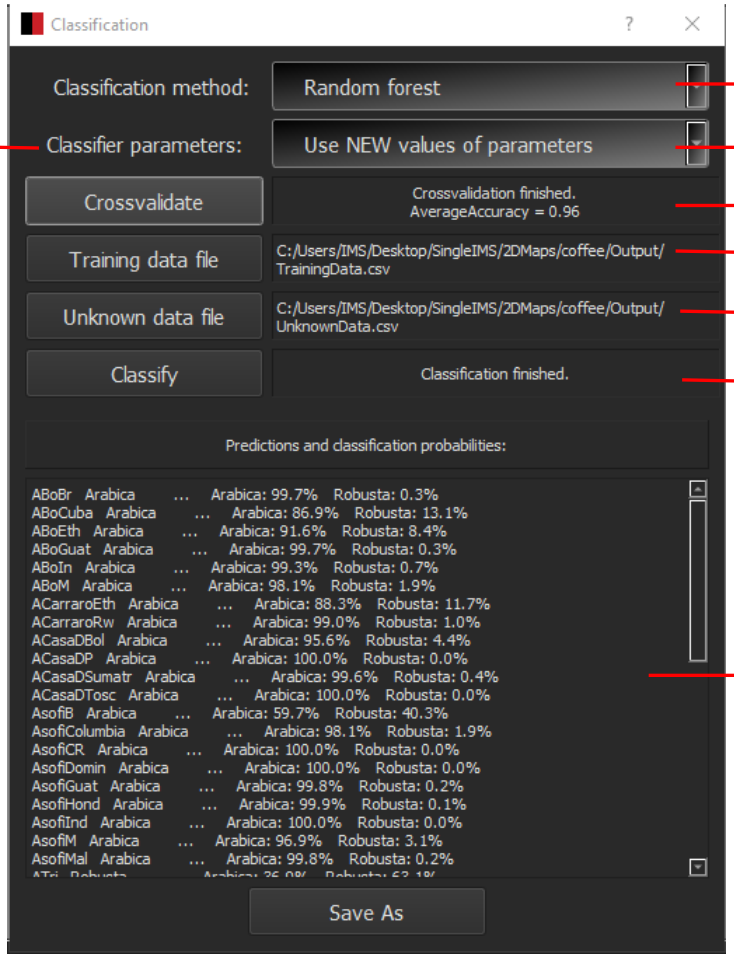
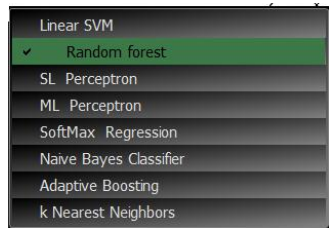
Step3: Classification







Choose **classification method**

User have possibility to **modify parameters** of classifier

Calculate **average accuracy** of your model

Select **Training data file** created in step 1

Select **Unknown data file** created in step 1

Press for **classification**

Results gives class information and percentage affiliation to each group.