Using **Ion Mobility Spectrometry** to Determine the Origin of Wine

*The ion mobility spectrometry (IMS) technique offers advantages like high sensitivity (ppb range), fast response (ms range), compact design, operation in atmospheric pressure and ability to separate the isomeric compounds. In combination with presseparation technique like GC or MCCGC is IMS suitable for analysis of complex matrix like coffee, oil, **wine**….*

The determination origin of the wine is important in order to protect producers and consumers. There exist huge amount of falsification of wine what making price pressure on local producers, tax avoidance as well like quality decrease for final consumer.

In this short report we will demonstrate potential of **IMS** supported by **machine learning classification** for determination origin of the **Wine**. Despite the small amount of samples we reach excellent results that demonstrate the ability of IMS supported by Machine learning for determination origin of the wine.

Experiment

The MCC-GC AIMS – **Peak-Machine** from **MaSa**TECH was used in this experiment.

The operation parameters of **Peak-Machine** are listed in Table 1.

Working pressure	**600 mbar**
Working temperature	**80 °C**
Drift Gas	**Zero Air**
Drift gas flow	**800 mL/min**
MCC-GC temperature	**50 °C**
MCC-GC flow	**20 mL/min**
Polarity	**Positive**

*Table1. Working parameters of **Peak-Machine***

The 18 samples of wine was used in this study. The origin of the wines was determined according to standard OIV-MA-AS311-05 based on isotopes $^2H/^1H$ ratio. From the 18 samples there was 15 samples of Slovak Republic origin and 3 samples of foreign origin. The 1mL amount of the sample was injected to vial. The vials was in next step analyzed by **Peak-Machine,** head space injection was automated by HTA sampler.

Results and discussion

The **IMS** spectrum of one of such sample is shown on figure 1. The retention time was 15 min with IMS duty cycle 150ms. As we can see from the figure huge amount of volatiles was recorded from the sample.

The classification model was created from recorded spectra in **MaSaTECH Chemometric** software. Based on the small amount of samples **only 18** and non-equal distribution (**15** samples of Slovak origin and **3** samples of foreign origin), the **Random Forest** classification method was chosen as most appropriate one. The classificator used only 2 classes of origin *Slovak* and *Foreign*. After creation of the classification model the sample was analyzed once again. The classification model was used for assigned of recorded spectra. The output from the classificator is shown on figure 2.
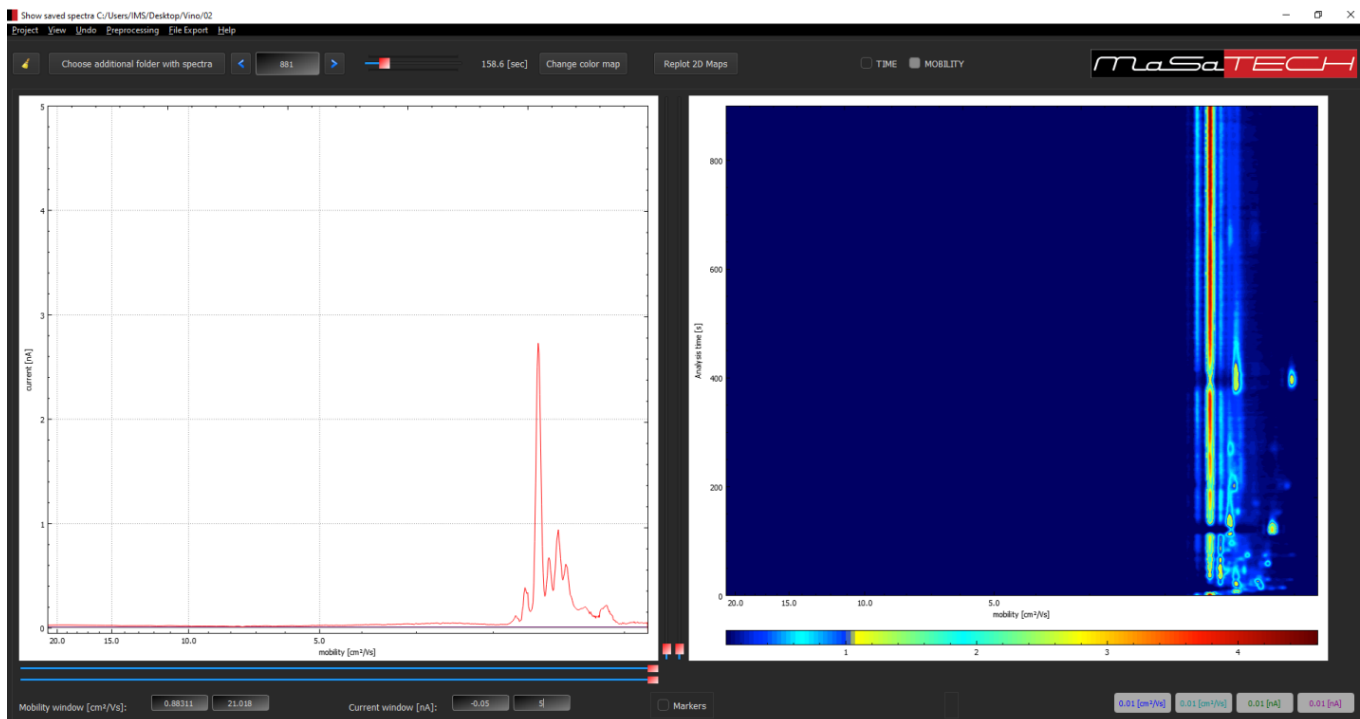

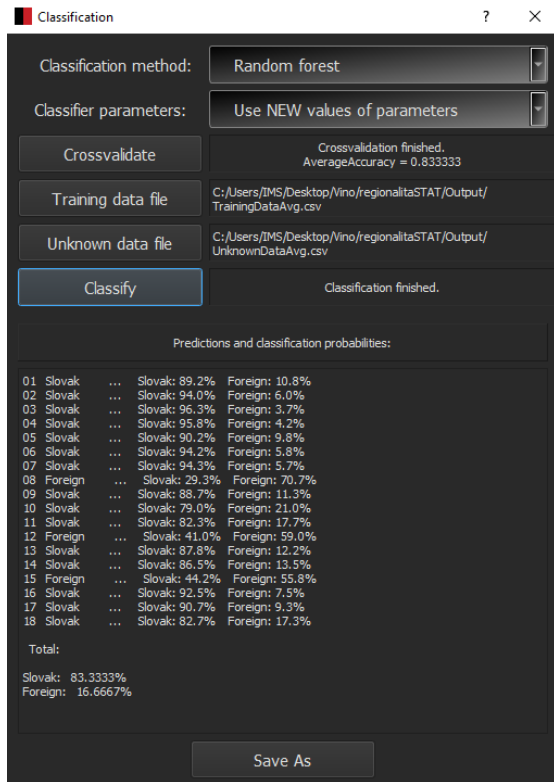*Figure 1. 2D spectrum of wine samplerecorded by* **Peak-Machine**

Figure 2. Results of **Random Forest** classification method

As we can see from this figure the accuracy of classification model was 83%, while the correct assigned to the region was **100%**.

Conclusion

In this short report we demonstrate the potential of MCC-GC **IMS** for classification the origin of wine. Despite the small amount of samples and them non-equal distribution (15 Slovak 3 Foreign) we reach the 83% classification accuracy and **100%** accuracy for the correct assignment. It has to be also note that samples was of various attributes like color (red, white, pink) and sugariness. The higher amount of samples with the same attributes will significantly improve the accuracy of classification model.