# *Analysis of FTIR imaging by using chemometric imaging methods*

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The management of high dimensional spectroscopic data has multidisciplinary challenges. Within the recent years, infrared imaging spectroscopy became a new and powerful tool for the rapid characterization of biological and in-organic samples. Using a typical IR-array detector, 4096 spectra can be recorded within a few minutes. Such large data sets allow the approach to a wealth of information. On the other hand, new strategies for data evaluation are required in order to point out the information of interest.

In this presentation we used FTIR-imaging spectroscopy to distinguish human brain tumors from normal brain tissue. A new, two-step chemometric imaging method was applied to derive classifiers in order to distinguish between normal tissue, astrocytoma grade II, astrocytoma grade III and glioblastoma. The first algorithm employed was a genetic optimal region selection routine. This program takes as input both the spectra of the tissue section and the histopathological designation of the sample. The histopathological designation is always used as 'gold standard'. With this information, the algorithm identifies a set of spectral subregions, which are subsequently used to classify spectra. The classification algorithm employs linear discriminant analysis to optimally partition the compressed spectra into groups. As result a training set for classification of 'unknown' tissue sections is obtained. The spectral analysis is based on more than 15 patients and over 40 000 spectra of each tissue class. The results reveal features characteristic of tumors with increasing malignancy. We achieved a classification success rate for prediction set samples greater than 87%. The impact of several data pre-processing steps such as derivation, base line correction, normalization and removal of outlier spectra are discussed and pre-processing routines that complicate classification are pointed out.