Abstract

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Evaluation of mass spectra from organic compounds assumed to be present in cometary grains. Exploratory data analysis.

From about 60 organic compounds, mass spectra have been measured by ^{252}Cf ionization mass spectrometry (PDMS). The substances and the data are relevant for future experiments near a comet by the space research project COSIMA (a time-of-flight mass spectrometer for secondary ions) on board of the ESA mission ROSETTA.

The spectra have been transformed into a set of appropriate spectral features (*x*-variables); the corresponding chemical structures have been characterized by binary substructure descriptors (*y*-variables).

PLS-2 mappings exhibit good correlations between the *x*- and the *y*-components. PLS spectrum-substructure mappings supported the detection of structural classes that are well reflected by spectral data.

PCA with spectral data was less efficient for this purpose.

The found structural classes are candidates for the development of spectral classifiers for the COSIMA project. Interpretation of the loading plots indicated spectral properties which are characteristic for substance classes.