Abstract

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Kurt Varmuza, Peter Filzmoser, Irene Hoffmann, Jan Walach, Hervé Cottin, Nicolas Fray, Christelle Briois, Paola Modica, Anaïs Bardyn, Johan Silén, Sandra Siljeström, Oliver Stenzel, Jochen Kissel, Martin Hilchenbach:

Significance of variables for discrimination: Applied to the search of organic ions in mass spectra measured on cometary particles.

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The instrument Cometary Secondary Ion Mass Analyzer (COSIMA) on board of the European Space Agency mission Rosetta to the comet 67P/Churyumov-Gerasimenko is a secondary ion mass spectrometer with a time-of-flight mass analyzer. It collected near the comet several thousand particles, imaged them, and analyzed the elemental and chemical compositions of their surfaces.

In this study, variables have been generated from the spectral data covering the mass ranges of potential C-, H-, N-, and O-containing ions. The variable importance in binary discriminations between spectra measured on cometary particles and those measured on the target background has been estimated by the univariate *t* test and the multivariate methods discriminant partial least squares, random forest, and a robust method based on the log ratios of all variable pairs.

The results confirm the presence of organic substances in cometary matter—probably a complex macromolecular mixture.