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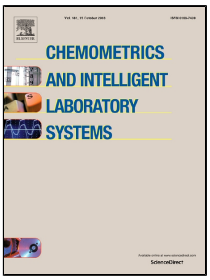

simsMVA: A tool for multivariate analysis of ToF-SIMS datasets

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simsMVA: A tool for multivariate analysis of ToF-SIMS datasets

Running title: simsMVA: A tool for multivariate analysis of ToF-SIMS datasets

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Abstract: Imaging mass spectrometry datasets are every year larger and more complex, with unsupervised multivariate analysis (MVA) becoming a routine procedure for most researchers. Moreover, the increasing interdisciplinarity of the field demands the development of software for rapid and accessible MVA for researchers of various backgrounds. This paper presents a MATLAB-based software for performing principal component analysis (PCA), non-negative matrix factorisation (NMF) and *k*-means clustering of large analytical chemistry datasets with a particular focus on of time-of-flight secondary ions mass spectrometry (ToF-SIMS). All five modes of operation (spectra, profiles, images, 3D and multi) are described with a few examples of typical applications at The Surface Analysis Laboratory of the University of Surrey: point spectra analysis of wood growth regions, depth profiling of a metallic multi-layered sample, imaging of an organic coating on a metal substrate and 3D characterisation of an automotive grade polypropylene.

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