JF FOCANT

Title:

Extracting Disease-Specific Information from Complex Analytical Data Sets in Separation Science

Brief outline:

Today's Separation Science tools offer an unprecedented power. Very complex mixtures of molecules can be separated and identified when state-of-the-art chromatographic and spectrometric techniques are coupled. This, however, often resulst in the creation of very large matrices of data that become delicate to manipulate. Moreover, a large part of such matrices often contains significant amounts of data of low relevance in regards to the particular analytical question asked. Data reduction is thus needed prior to proper data exploitation using (un)-supeervised statistical tools such as PCA, HCA, etc... This will be illustrated in the case of GCxGC-(HR)TOFMS data produced from analyses of the VOC fraction of biological samples collected in the context of human disease research, including breathprint patterning of lung cancer and metabolomics of inflammatory bowel disease.

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