

<p><b>Title:</b> (Capitalize the first letter of each <u>key</u> word)</p>	<p>A Chemometric Optimization Study of Electrospray Ionization Parameters for the Determination of Organic Acids by CE-MS</p>
<p><b>Abstract:</b> (Your abstract <u>must</u> use Normal style and <u>must</u> fit in this space), Times New Roman Font, 12 point</p>	<p>Aerosol particles influence the radiation balance of the earth and have a crucial relevance for atmospheric chemistry. Apart from inorganic salts they consist of a wide variety of organic compounds, most of which are still unknown. Carboxylic acids are an important fraction of the organic particulate matter and are found in all parts of the world (Saxena and Hildemann, 1996).</p> <p>The aim of this study was to develop and optimize a method which allows the determination of aliphatic and aromatic organic acids in aqueous extracts of atmospheric particulate matter.</p> <p>A capillary electrophoresis (CE) System (Agilent), coupled via an electrospray ionization (ESI) to an ion trap mass spectrometer (esquire 3000+, Bruker) was used as instrumentation.</p> <p>Based on earlier work in our group (Inuma and Herrmann, 2003), a 20 mM Ammoniumacetate electrolyte with pH 9.1 was used for separation which exhibited a good resolution of different carboxylic acids in a standard solution. The optimization of different parameters influencing the efficiency of the electrospray (thereby the sensitivity of the system) was done by means of chemometric methods. The use of experimental design allows a systematic and efficient approach to optimization studies. Furthermore, interaction effects having a significant impact on the responses can be identified.</p> <p>A fractional factorial design was used for a first screening of seven parameters which might influence the spray performance (distance CE-capillary to sprayer tip, isopropanol fraction in sheath liquid, flow rate of sheath liquid, pressure of nebulizing gas, electrospray voltage, temperature of dry gas, flow rate of dry rate). Two significant effects were found for signal intensity: i) the fraction of isopropanol in the sheath liquid and ii) an interaction between the sheath liquid organic fraction and the nebulizing pressure. These effects were investigated in more detail by means of a central composite design. Additionally their influence on separation efficiency and background noise was evaluated. The optimal values were found as 100% isopropanol (sheath liquid) and 4 psi (nebulizing pressure). The figures of merit for the method were determined and it was applied to real samples.</p> <p>Inuma, Y., and H. Herrmann, <i>Journal of Chromatography A</i>, 1018 (1), 105-115, 2003.</p> <p>Saxena, P., and L.M. Hildemann, <i>Journal of Atmospheric Chemistry</i>, 24 (1), 57-109, 1996.</p>