Characterizing an ESI-MS Interface Based on the Ion Utilization Efficiency

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Overview

• Study of the electric current transmitted through different electrospray ionization mass spectrometry (ESI-MS) interfaces.
• Evaluation of the ionization efficiency and the ion transmission efficiency for the different ESI source and MS interface configurations.
• Establishment of a general metric, based on the ion utilization efficiency, to evaluate the overall efficiency of any ESI-MS interface designs.

Introduction

Achievable sensitivity of ESI-MS is largely determined by 1) ionization efficiency in the ESI source, and 2) ion transmission efficiency through the ESI-MS interface. These characteristics are difficult to evaluate and compare among different ESI source and ESI-MS interface designs. We present a universal method based on the ion utilization efficiency, to evaluate performance of ESI-MS interfaces. ESI-MS interface ion utilization efficiency is defined as the percentage of analyte molecules in a sample solution being converted into gas phase ions and transmitted through the interface. It is determined by measuring the total gas phase ion current transmitted through the interface and the ion abundance in the corresponding mass spectrum.

Methods

Instrument configurations

The theoretical maximum ion current, $I_J$, for a mixture of N compounds under the complete ionization condition:

$$I_J = \sum_{i=1}^{N} (\sum_{j} \frac{z_i J_i}{z_i J_i})$$

The ion utilization efficiency, $\epsilon_J$, for analyte J and mixture of analytes in the sample mixture:

$$\epsilon_J = \frac{\sum_{i} i(J)}{\sum_{i} \frac{z_i J_i}{z_i J_i}}$$

Where $\Delta_i$ is the ion utilization efficiency for a single emitter single inlet ESI-MS interface and $\epsilon_J$ for all the analytes in the sample mixture:

$$\epsilon_J = \frac{\Delta_i}{\sum_{i} \frac{z_i J_i}{z_i J_i}}$$

Results

Electric current transmitted through the high pressure ion funnel RF voltages and $\epsilon_J$ for 3+ neurotensin (m/z = 558.3) at different high-pressure ion funnel RF voltages and with different interface configurations.

$\Delta_i$ and analyte peak intensity for a) single emitter/single inlet ESI-MS interface and b) single emitter/SPIN interface at different flow rates.

Conclusions

• The ion cloud transmitted through ESI-MS interface contains both fully desolvated gas phase ions and ‘residue’ not fully desolvated charged analyte/solvent clusters/particles.
• The portion of fully desolvated gas phase ions correlates well with the final intensity of the ion current detected by MS.
• Over an order of magnitude increase in transmitted analyte ion current was observed by using 10 emitters/SPIN-MS interface compared to using a standard single-emitter/single-heated capillary inlet ESI-MS interface.
• Of the interfaces evaluated in this study, an emitter array/SPIN-MS interface demonstrated the greatest ion current, highest MS-signal intensity, and consequently the best ion utilization efficiency at a given total ESI flow rate.

Acknowledgments

Portions of this work were funded by the NIH National Cancer Institute (1R01CA135229), General Motors Science (GM0484955-1D), the Laboratory Directed Research and Development Program at Pacific Northwest National Laboratory (PNNL), and the Department of Energy Office of Biological and Environmental Research (BER) Genomes Sciences Program under the Panomics project. The experimental work was performed in the Environmental Molecular Sciences Laboratory, a DOE-BER national scientific user facility on the PNNL campus. PNNL is a multiprogram national laboratory operated by Battelle for the DOE under contract DE-AC05-76RL01830.

References