Linking Mass Spectrometry with Toxicology for Emerging Water Contaminants

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Introduction

Mass spectrometry is the cornerstone of environmental chemistry, allowing trace levels (pg-ng/L) of contaminants to be detected in rivers, lakes, soils, and air. Further, advances in mass spectrometry instrumentation has allowed the discovery of toxicologically important ("emerging") contaminants that go beyond the "legacy" contaminants commonly associated with environmental contamination (e.g., PCBs, PAHs, dioxin). In much of the new discovery work, research groups are increasingly combining toxicology with mass spectrometry, such that mass spectrometry methods and measurements are focused on those contaminants that might pose the greatest risk in the environment.

Methods

Mass spectrometry tools include liquid chromatography (LC)/electrospray ionization (ESI)-mass spectrometry (MS)/MS, with triple quadrupoles serving as the "gold standard" for quantification, and time-of-flight (TOF) and quadrupole/TOF instruments commonly used to provide exact mass information that is key to identifying unknown contaminants or their environmental degradation products. Ultra performance (UP)LC is also increasingly used in environmental research to improve separations of highly complex environmental samples, which can contain hundreds of contaminants. LC or UPLC/MS/MS is ideal for many emerging contaminants, such as pharmaceuticals and perfluorinated compounds. Gas chromatography (GC)/MS is still preferred for other contaminants, including drinking water disinfection by-products (DBPs).

Preliminary Results

This overview presentation will discuss the benefits of combining mass spectrometry with toxicology. These benefits will be described for 3 main areas: (1) Toxicity assays used to test new environmental contaminants previously identified using mass spectrometry, such that further quantitative MS methods development is focused on those contaminants that pose the greatest toxicological risk; (2) Toxicity used in conjunction with mass spectrometry, such that fractions (size or polarity) are collected and tested for toxicity, and toxicity results are used to focus MS identification efforts on the most toxic fractions; and (3) Toxicity assays used to test environmental degradation products or treatment products of specific contaminants identified using mass spectrometry, such that the risk of the degradation/reaction products can be determined. Examples will be given for drinking water DBPs (regarding fractionation and toxicity testing helping to focus further measurement and formation research) and for other emerging contaminants, such as pharmaceuticals (for determining whether an environmental degradation product or a reaction product formed by ozone in drinking water treatment retains the toxicity of the parent compound). Integrated toxicology-mass spectrometry research is expected to provide meaningful results for addressing public health and regulatory issues.