A

Adaptive Management

Adaptive management, also known as adaptive environmental assessment and management, is a structured, iterative process of robust decision-making in the face of uncertainty with the aim of reducing uncertainty over time via system monitoring.

Adsorbable Organic Fluorine (AOF)

An organofluorine assay that first adsorbs these compounds from a sample onto polystyrene divinylbenzene–based activated carbon from which it is eluted and analyzed by combustion ion chromatography (CIC).

B

BP4NTA

Benchmarking and Publications for Non-Targeted Analysis is a working group formed to address challenges in nontargeted analysis studies using mass spectrometry (https://nontargetedanalysis.org/) (BP4NTA 2023).

C

Combustion Ion Chromatography (CIC)

A separation technique that first combusts organics at 900–1,000°C to inorganic ions that can be separated by ion (exchange) chromatography (IC).

Contaminant(s) of Emerging Concern (CEC)

Substances and microorganisms, including physical, chemical, biological, or radiological materials known or anticipated in the environment, that may pose newly identified risks to human health or the environment.

D

Dalton (Da)

A unit of mass that is equal to one-twelfth the mass of a free ^{12}Carbon atom at rest. The Dalton is also known as the unified atomic mass unit. One Dalton is approximately 1.66×10^{-27} kg.

Deconvolution

For gas chromatography–mass spectrometry (GC-MS) data, deconvolution is the process of computationally separating co-eluting components and creating a pure spectrum for each component. It is widely used to process complex data generated by high resolution mass spectrometry (HRMS).

Dynamic Light Scattering (DLS)

DLS is a noninvasive laser-based technique that is a useful tool for determining the hydrodynamic diameter and particle size distribution in suspension and for investigating colloidal properties of nanoparticles.

E

Effect-Directed Analysis

Effect-directed analysis is an emerging strategy for environmental profiling of complex samples that brings together

biological-effects testing using bioassays, sample preparation and fractionation, and chemical analysis to evaluate environmental toxicity and identify toxic pollutants.

Electrochemical Methods

These methods are based on the direct impact of individual nanoparticles in a suspension on the electrode surface. This leads to current spikes as a function of time that can correlate to various characteristics of an engineered nanoparticle's (ENP's) property.

Electron Impact (EI)

A strong gas-phase ionization technique applied widely in GC-MS that uses highly energetic electrons at 70 electron volts to produce ions from sample molecules. EI produces extensive but highly reproducible fragmentations of the parent molecule and yields mass spectra that can be easily compared across platforms.

Electrospray Ionization (ESI)

ESI is a technique used in mass spectrometry to produce ions using an electrospray in which a high voltage is applied to a liquid to create an aerosol. It is especially useful in producing ions from macromolecules because it overcomes the propensity of these molecules to fragment when ionized. ESI is typically used in high-performance liquid chromatography–mass spectrometry (HPLC-MS).

Engineered Nanoparticles (ENPs)

Specially designed chemical substances or materials with particle size between 1 and 100 nm in at least one dimension.

Exposure

Contact with a substance by swallowing, breathing, or touching the skin or eyes. Exposure may be short-term (acute exposure), intermediate duration, or long-term (chronic exposure) (ATSDR 1994).

Exposure Pathway

The physical course or path that a chemical or pollutant takes from the source via air, soil, water, and food to humans, animals, and the environment (USEPA 2003). Each exposure pathway includes a source or release from a source, an exposure point, and an exposure route.

Extractable Organic Fluorine (EOF)

An organofluorine assay that first extracts these compounds from a sample using ion-pairing sample preparation methods and then analyzes the extract by CIC. The EOF sample preparation method is highly customizable.

F

Features (Chemical)

Any ion detected in a mass spectrum that may be of importance. Features are defined by the mass-to-charge ratio (*m/z*), chromatographic retention time, and mass spectral peak intensity. After a feature is selected to be important, it can be designated as an unknown, and the analyst can then take further steps to identify it.

Flow cytometry

Flow cytometry is a technology that provides rapid multi-parametric analysis of single cells in solution. Flow cytometers use lasers as light sources to produce both scattered and fluorescent light signals that are read by detectors. These signals are converted into electronic signals that are analyzed by a computer and written to a data file. Cell populations can be analyzed and/or purified via flow cytometry based on their fluorescent or light-scattering characteristics.

Fourier Transform Infrared (FTIR) Microscopy

FTIR microscopy is a combination of conventional light microscopy and clear chemical identification using FTIR spectroscopy. FTIR microscopy can yield chemical area maps or single point scans in an optical field.

Fourier Transform Infrared (FTIR) Spectroscopy

FTIR is a vibrational spectroscopy technique that uses an infrared light source to induce vibrations. It is conducted in the frequency domain to rapidly produce infrared absorption spectra to identify organic, inorganic, and polymeric materials in a sample.

Full-Scan Mode

Full-scan mode is used in quantitative mass spectrometry to detect parent ions in a sample. A mass analyzer set to scan from the lowest to highest *m/z* ratio in a user-defined range.

G

Gas Chromatography–Mass Spectrometry (GC-MS)

A common hybrid analytical method that combines gas-phase chromatographic separation with a single mass spectrometer acting as a mass filter and detector. Once separated via GC, compounds can be identified by their full-scan EI ionization mass spectrum by a spectral match from a spectral library. A total ion chromatogram can be generated to document compound elution with time. Alternatively, more sensitive quantitation can be performed in selective ion monitoring (SIM) mode. GC-MS is typically used for the analysis of volatile and semi-volatile thermally stable compounds.

H

Hazard

A condition or physical situation with a potential for an undesirable consequence, such as harm to life or limb (ITRC 2020).

High Resolution Mass Spectrometry (HRMS)

HRMS is an analytical tool that measures the *m/z* ratio of ions to an accuracy of 0.001 Da or lower. These instruments can be used to distinguish between compounds with a similar nominal mass, determine elemental compositions, and identify unknowns. A type of HRMS widely used today is the quadrupole time-of-flight (QTOF) mass spectrometer.

Homologous Series

In organic chemistry, a homologous series is a group of compounds that contain the same functional group or structure and differ by a repeating unit (e.g., CH_2 or CF_2). Compounds in a homologous series tend to have similar chemical and physical properties.

I

Instrumental Neutron Activation Analysis (INAA)

A nuclear technique used to determine the concentration of trace and major elements in a variety of matrices. A sample is subjected to a neutron flux resulting in the production of radioactive nuclides, which upon radioactive decay, emit gamma rays whose energies are characteristic for each nuclide. Comparison of the intensity of these gamma rays with those emitted by a standard permit a quantitative measure of the concentrations of the various nuclides.

Ion Chromatography (IC)

IC is a separation technique that measures the concentration of ionic species using an ion exchange resin.

L

Laser Direct Infrared Microscopy

An infrared spectrometer using a quantum cascade laser coupled to a rapidly scanning imaging system.

Liquid Chromatography (LC)

LC is an analytical technique that separates compounds from their mixtures through a column or stationary phase using solvents or mobile phase. In the analytical chemistry realm, LC is typically performed at high pressure to shorten elution times and is more commonly known as high-performance liquid chromatography (HPLC).

M

Mass Spectrometry (MS)

Mass spectrometry is an analytical tool that measures the *m/z* ratio of ions.

Matrix-Assisted Laser Desorption or Ionization (MALDI)

An ionization technique for mass spectrometry that uses a laser-energy–absorbing matrix to create ions from large molecules with minimal fragmentation.

Metabolomics

Metabolomics is an emerging field and is broadly defined as the comprehensive measurement of all metabolites and low-molecular-weight molecules in a biological specimen using primarily mass spectrometry.

Metagenomics

Analysis of the genome of multiple organisms in bulk/environmental samples using next-generation sequencing (NGS) methods. Metagenomics is often used to study a specific community of microorganisms, such as those residing on human skin, in the soil, or in a water sample.

Metatranscriptomics

Metatranscriptomics is the science that studies gene expression of microbes within natural environments. It allows one to obtain whole gene expression profiling of complex microbial communities.

Microarray

A microarray is a laboratory tool used to detect the expression of thousands of genes at the same time. Deoxyribonucleic acid (DNA) microarrays are microscope slides that are printed with thousands of tiny spots in defined positions, with each spot containing a known DNA sequence or gene.

Microplastics (MPs)

Particles that are greater than 1 nanometer (nm) and less than 5 millimeters (mm) in their longest dimensions and are composed of solid polymeric materials to which chemical additives or other substances may have been added.

Molecular Ion Peak

In a mass spectrum, the peak representing the molecular ion is called the molecular ion peak. Excluding any peaks due to the presence of heavier isotopes, the molecular ion peak is the peak with the highest *m/z* ratio.

Monoisotopic Molecular Ion

Ion composed of only the most abundant stable isotopes of its constituent elements.

N

Nanoparticle Tracking (NT)

NT passes a laser beam into the particle suspension. When the particles in suspension appear in the scattered light path, they can be clearly visualized and recorded frame by frame using a high-sensitivity camera or charged coupled device (CCD) detector. The motion trail of the particles is obtained and analyzed through the recorded frames by means of a microscope. Further calculation of hydrodynamic sizes is completed with the average distance between each particle, temperature, and solution viscosity through the Stokes-Einstein equation.

Nanoplastics

Plastic/polymeric particles less than 1,000 nm in their longest dimension.

Next-Generation Sequencing (NGS)

NGS is a massively parallel sequencing technology that offers ultra-high throughput, scalability, and speed. The technology is used to determine the order of nucleotides in entire genomes or targeted regions of DNA or ribonucleic acid (RNA).

Nominal Mass

Mass of a molecular ion or molecule calculated using the isotope mass of the most abundant constituent element stable isotope of each element rounded to the nearest integer value and multiplied by the number of atoms of each element.

Non-target Analysis or Screening (NTA or NTS)

NTA aims to detect "unknown-unknown" compounds without any *a priori* criteria to identify potential new molecules or molecular fragments. Because no structural information is available in advance, a full nontargeted identification starting from the exact mass, isotope, adduct, and fragmentation information needs to be performed using HRMS. NTA can result in acquiring structural information and compound identity but does not yield quantitative information with respect to concentration.

NORMAN Network (Network of Reference Laboratories, Research Centers and Related Organizations for Monitoring of Emerging Environmental Substance)

NORMAN is a network that facilitates the exchange of information and data collection of CEC, promotes method validation and harmonization, and shares knowledge of CEC across networks (https://www.norman-network.net/?q=NORMAN%20Network) (NORMAN 2023).

Nuclear Magnetic Resonance (NMR)

An NMR instrument allows the molecular structure of a material to be analyzed by observing and measuring the interaction of nuclear spins when placed in a powerful magnetic field.

P

Particle-Induced Gamma Ray Emission (PIGE)

PIGE spectroscopy is a surface analysis technique for quantification of elemental fluorine in which an accelerated beam of protons strikes the surface of the sample of interest, exciting ^{19}F nuclei. Gamma rays emitted upon de-excitation provide a unique signature proportional to the number of fluorine atoms on the surface.

Polymerase Chain Reaction (PCR)

PCR is a method widely used to rapidly make millions to billions of copies of a specific DNA sample, allowing scientists to take a very small sample of DNA and amplify it to a large enough amount to study in detail.

Proteomics

Proteomics is the systematic, large-scale analysis of proteins using techniques such as mass spectrometry. It is based on the concept of the proteome as a complete set of proteins produced by a given cell or organism under a defined set of conditions.

Public

A people as a whole; a populace having common interests (ITRC 2020).

Pyrolysis GC-MS

A GC-MS (see GC-MS) where samples are introduced via a pyrolizer, which provides a heated and inert environment where complex molecules are broken down into fragments/pyrolyzates.

Q

Quantitative Polymerase Chain Reaction (qPCR)

A laboratory analytical technique for quantification of a target gene. In qPCR, the accumulation of amplification nucleic acid product is measured as the reaction progresses, in real time, with product quantification after each cycle.

R

Raman Spectroscopy

Raman spectroscopy is a spectroscopic technique typically used to determine vibrational modes of molecules, although rotational and other low-frequency modes of systems may also be observed. Raman spectroscopy is commonly used in chemistry to provide a structural fingerprint by which molecules can be identified. Raman spectroscopy relies upon inelastic scattering of photons, known as Raman scattering.

Resolution (in mass spectrometry)

In mass spectrometry, resolution is defined as the ability of the mass spectrometer to separate ions of similar *m/z* ratio.

Reverse Transcription qPCR (RT-qPCR)

Reverse transcription qPCR (RT-qPCR) is used when the starting material is RNA. In this method, RNA is first transcribed into complementary DNA (cDNA) by reverse transcriptase enzyme from total RNA or messenger RNA (mRNA). The cDNA is then used as the template for the qPCR reaction.

Risk

The potential for realization of unwanted, adverse consequences to human life, health, property, or the environment. Estimation of risk is usually based on the expected value of the conditional probability of the event occurring multiplied by the consequence of the event, given that it has occurred (ITRC 2020).

Risk Communication

Actions, words, and other messages, responsive to the concerns and values of the information recipients, intended to help people make more informed decisions about threats to their health and safety.

Risk communication is the formal and informal process of communication among and between regulatory agencies and organizations responsible for site assessment and management, and the various parties who are potentially at risk from or are otherwise interested in the site.

S

Schymanski Confidence Levels or Scale

Schymanski Confidence Levels are used to communicate confidence in structural identification of compounds using HRMS. It is named after the first author of the paper (dx.doi.org/10.1021/es5002105) that first presented the scale (Schymanski et al. 2014).

Selective Ion Monitoring (SIM)

SIM is a mass spectrometry scanning mode in which only a limited *m/z* ratio range is transmitted/detected by the instrument, instead of the full spectrum range. This mode of operation typically results in significantly increased sensitivity.

Single Particle Inductively Coupled Plasma–Mass Spectrometry (ICP-MS)

SP ICP-MS is a type of mass spectrometry that uses an inductively coupled plasma to ionize the sample. It atomizes the sample and creates atomic and small polyatomic ions, which are then detected. It is known and used for its ability to detect metals and several nonmetals in liquid samples at very low concentrations. It can detect different isotopes of the same element, which makes it a versatile tool in isotopic labeling.

Solid-Phase Extraction (SPE)

SPE is a sample preparation technique used in analytical laboratories. It extracts and preconcentrates analytes from a complex liquid matrix prior to quantitative analysis.

Study Reporting Tool (SRT)

SRT is an open-source guide for reporting NTA data. It provides a framework for NTA design, data communication, and

reporting performance metrics to ensure high-quality data are gathered and interpreted.

Subpopulation

Groups of individuals who respond biologically at lower levels of exposure to a contaminant or who have more serious health consequences than the general population (USEPA, OW 2000).

Suspect Screening

Suspect Screening is a technique that uses HRMS to identify “suspect” compounds in a sample. Although reference standards may not be available for suspect screening, exact mass, mass fragmentation, and other experimental data can be used to increase the confidence of the identification.

T

Tandem Mass Spectrometry (MS/MS)

Mass spectrometry technique that breaks a precursor ion (parent ion) into fragments. These fragments are used to reveal the chemical structure of the precursor ion.

Target Screening or Target Analysis

Target analysis is a technique that uses tandem mass spectrometry to identify and quantify known compounds in a sample using available reference analytical standards and/or libraries.

Tentatively Identified Compound (TIC)

A compound detected in a sample, typically using a GC-MS method, that is not in the target analyte list for the method.

Thermal Desorption GC-MS

Uses heat and a flow of inert (carrier) gas to extract volatiles from a solid matrix (no solvent required), which is then analyzed via GC-MS. One such standardized method, USEPA Method 8275A, could be used to include the decomposition products of MPs.

Thermally Labile

Easily breaks down upon heating. The term also describes compounds not amenable to separation via gas chromatography because of the high temperature or thermal gradient applied to the GC. These compounds are usually separated using liquid chromatography.

Total Ion Chromatogram

A total ion chromatogram is the sum of the ion intensities versus time for a full chromatographic run.

Total Oxidizable Precursor (TOP)

The TOP assay is the most selective of perfluoroalkyl and polyfluoroalkyl substances (PFAS) surrogate analytical methods in that it selects only for compounds that can be oxidized to form targeted perfluoroalkyl acids (PFAAs). This method was developed to infer and indirectly quantify the total amount of chemical “precursors” to PFAAs in a sample by comparing the concentrations of specific PFAAs by HPLC-MS/MS both before and after oxidation of the sample by an excess of hydroxyl radicals.

Toxicological Reference Value or Toxicity Reference Value (TRV)

A concentration or dose that represents a threshold or defined level of toxic effects.

U

Ultra (High) Performance Liquid Chromatography (UPLC or UHPLC)

Liquid chromatography employing a shorter and more tightly packed analytical chromatography column (owing to smaller particle size of the stationary phase) that allows faster separation of analytes at a higher operating pressure than HPLC.