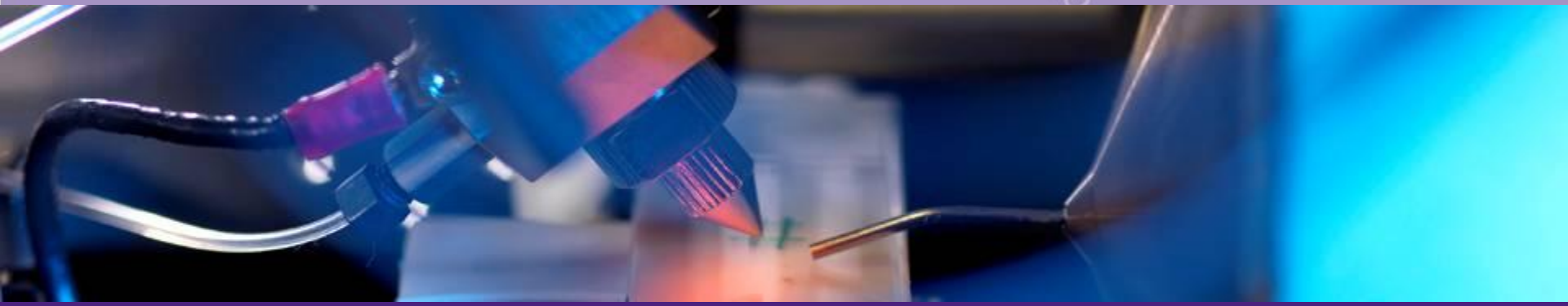
Setting standards
in analytical science



Science and Technology

Analysis for REACH Compliance

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Today's Talk

Setting standards in analytical science

- What is REACH
- What is the role of Analysis in REACH
- REACH Registration and Analytical Requirements
- Analytical Technologies for Substance Characterisation in support of REACH
- Issues with REACH

REACH

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- **It is a European Union regulation concerning the Registration, Evaluation, Authorisation and restriction of Chemicals. It came into force on 1st June 2007 and replaced a number of European Directives and Regulations with a single system**

REACH

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- **Aim is to provide a high level of protection of human health and the environment from the use of chemicals.**
- **To make the people who place chemicals on the market (manufacturers and importers responsible for understanding and managing the risks associated with their use.)**
- **REACH applies to substances manufactured or imported into the EU in quantities of 1 tonne or more per year. Generally, it applies to all individual chemical substances on their own, in preparations or in articles**

REACH

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- **Substance : a chemical element and its compounds in the natural state or obtained by any manufacturing process- toluene, chromium**
- **Preparation: is a mixture or solution composed of two or more substances- paint, detergent**
- **Article: is an object which during production is given specific shape, surface or design which determines its function to a greater degree than does its chemical composition- furniture, electronic equipment**

REACH

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- **A major part of REACH is the requirement for manufacturers or importers of substances to register them with a central European Chemicals Agency (ECHA). A registration package will be supported by a standard set of data on that substance.**
- **It applies to manufacturers, distributor, importers and downstream users in the supply chain**
- **No data No market**

The role of analysis in REACH

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- First and foremost, establishing substance identity (SID) for the purposes of a REACH registration/submission .
- Helps establish main categories of substance :
  - Well Defined Composition- Quantitative/Qualitative
  - UVCBs – Unknown or Variable composition, Complex reaction products or Biological materials
- Helps establish substances grouping:
  - Mono constituent – one main component at least 80%w/w
  - Multi component –one main component in a concentration >10% and <80%.
  - Defined by more than the chemical composition

The role of analysis in REACH

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- **Deciding which materials qualify as polymers**
- **Deciding whether a product is chemically identical to a substance found in nature**
- **Process and pre-release quality control to check that substances, mixtures and articles comply with restrictions, limits on SVHC[1]**

[1] Substances of Very High Concern http://guidance.echa.europa.eu/index_en.htm,

The role of analysis in REACH

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- **Shows whether different industrial products are the same REACH substance, and establishing a single joint specification**
- **Providing evidence of structural similarity between substances, to support the read-across of valuable data on physicochemical, toxicological and ecotoxicological properties**
- **Filling gaps in supply chain data, such as for imported materials - for example, establishing whether they are multi-constituent substances or deliberate mixtures.**
- **Enforcement, such as testing whether a substance is really what it is claimed to be, checking the nature and concentrations of substances in mixtures and articles, and policing restrictions.**

REACH Registration and Analytical Requirements

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- **Registrations must include:**
- **Tests for elemental composition and purity**
- **For Organic materials the minimum spectral package should include UV/VIS, IR and NMR**
- **Plus HPLC or GC data and method or other appropriate test methods**
- **Any other technologies which can provide complementary data to confirm structure or define the whole substance**
- **Interpretation and verification by a technically qualified individual**

What need to be measured?

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- All constituents and impurities which are known to make up 1% or more of a substance should be identified and quantified.
- At least 99% and ideally 100% of the substance should be accounted for and any unknown impurities listed
- Looking to produce a dossier to include purity based on concentration of the main components plus impurities
- For substances /articles SVHV levels <1% need to be measured

Analytical Technologies For REACH support

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Techniques for Confirmation of Structure

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Analytical Tool Box	Main Substance Organic (80%)	Main substance Inorganic (80%)	Substance <10%	Substance < 0.1%	UVCB
IR*	✓	✓	✓		✓
NMR*	✓		✓		✓
UV/VIS*	✓				
MS	✓				
Raman	✓	✓	✓		✓
XRD		✓	✓		✓
XRF		✓	✓		✓
AA		✓	✓	✓	✓
ICP/MS		✓	✓	✓	✓
ICP/OES		✓	✓	✓	✓

Instrumental Techniques for Purity/Impurity Profiles

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Analytical Tool Box	Main component Organic (80%)	Main component Inorganic (80%)	Substance <10%	Substance <0.1%
XRF		✓	✓	
AA		✓	✓	✓
ICP/MS		✓	✓	✓
ICP/OES		✓	✓	✓
GC	✓		✓	✓
HPLC	✓	✓	✓	✓
Thermal Analysis	✓		✓	

Impurity Investigative Techniques

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Analytical Tool Box	Main Substance Organic (80%)	Main substance Inorganic (80%)	Substance <10%	Substance < 0.1%	UVCB
GC/MS	✓		✓	✓	✓
GC/GC/MS	✓		✓	✓	✓
HPLC/MS	✓		✓	✓	✓
HPLC/MS/MS	✓		✓	✓	✓
HPLC/ ICP/MS	✓	✓	✓	✓	✓

Probe Techniques

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Analytical Tool Box	Isomers	Branching	Chiral	Crystallinity	Salts	Molecular weight D	Speciation
IR	✓	✓			✓		
NMR	✓	✓					
Raman					✓		
XRD				✓	✓		
XRF					✓		
AA					✓		
ICP/MS					✓		
ICP/OES					✓		
GC	✓						
HPLC	✓						
GPC							
GC/MS	✓	✓	✓				
GC/GC/MS	✓	✓					
HPLC/MS	✓		✓				
HPLC/MS/MS	✓	✓					
GPC						✓	
HPLC/ICP//MS							✓

Additional Technologies

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- **Karl Fischer – water content**
- **Materials Analysis- Particle Size, Surface Area, Shape, Hardness, Density, Refractive Index.**
- **Biological property measurements – Catalytic activity for enzymes and amino acid sequencing**

Issues with REACH

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- Guidance documents are not comprehensive
- Difficult if there are no reference standards or spectral databases
- To effectively compare substances the same analytical method has to be used
- May have to explore batch to batch variation and sample homogeneity

Health Warnings

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- Compounds can appear the same or different depending on what analytical technique is used.
- Easier to detect difference than sameness
- The harder you look more you find
- Ultimate aim is to produce relevant, reliable ,adequate and defensible data

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Questions?