

Evolution of analytical techniques towards a green laboratory in a water utility

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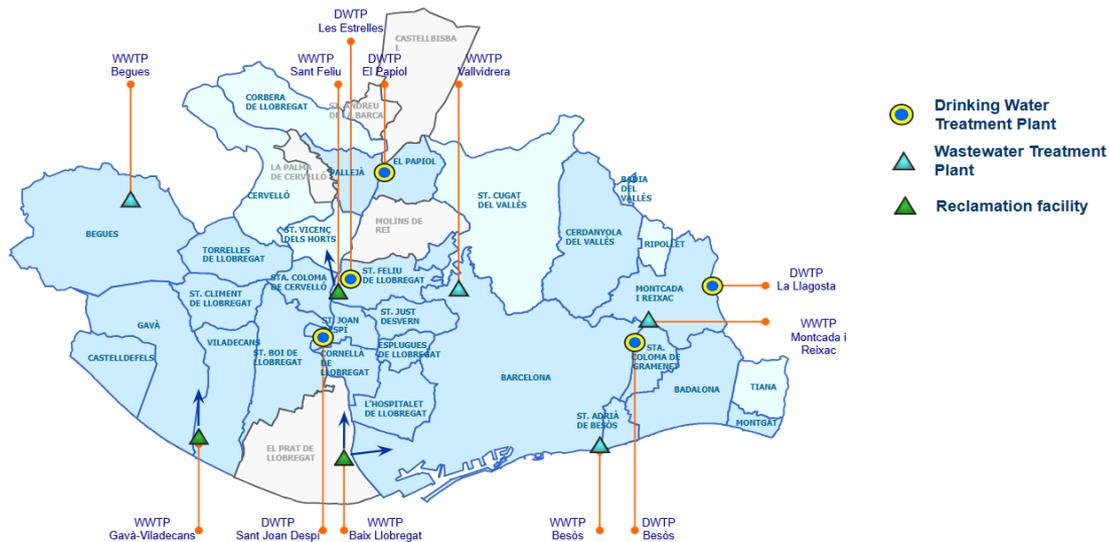
Founded in
1867



Serving
23
Municipalities



Supplying nearly
3 Million
Residents



- Drinking Water Treatment Plant
- Wastewater Treatment Plant
- Reclamation facility

Water Quality Department Activities:



Analytical activity (laboratories)



Management of the quality of water in its whole cycle



R&D + applied studies



Support activities



DRINKING WATER: AIGÜES DE BARCELONA management GROUP AGBAR management OTHER COMPANIES



Aigües de Barcelona

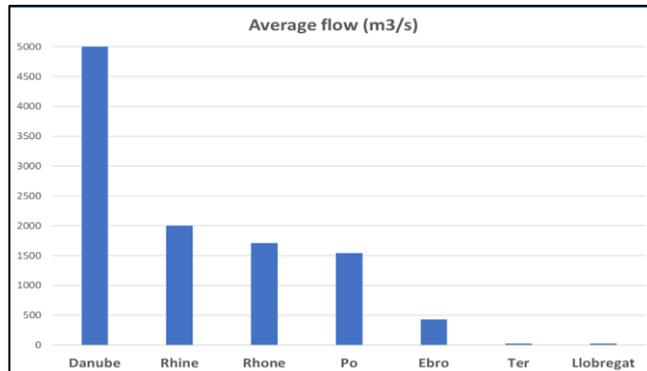
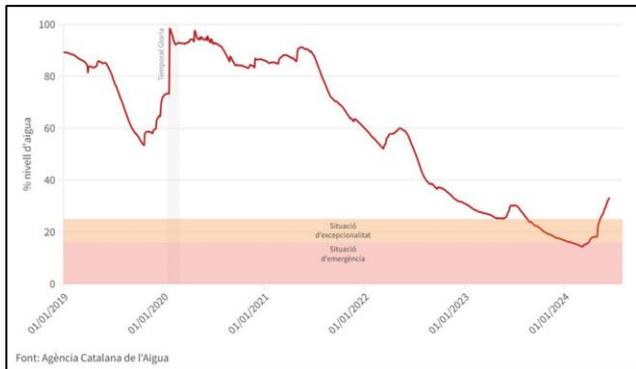
La gestió responsable

WATER RESOURCES

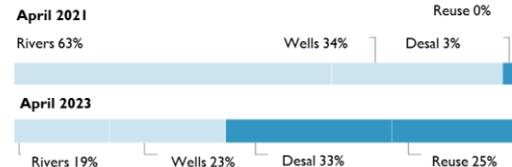


Water resources for Barcelona's metropolitan area water supply → Surface water from **Llobregat** and **Ter** rivers.

Low flow with high flow peaks (Mediterranean climate)



Barcelona MA Water demand: ~7 m³/s



LABORATORY OVERVIEW & CAPABILITIES

KEY METRICS

- **LOCATION**
Barcelona (Spain)
- **WORKFORCE**
60 People (analysts, technicians, engineers, PhD)
- **VOLUME**
>100,000 sample/year
(Control, Management, Improvement)

EQUIPEMENT & TECHNOLOGY

ICP-OES, ICP-MS/MS, AFS, FIAS, Ion Chromatography, LC-MS/MS, GC_MS/MS, LC-HRMS, GC-HRMS, GC-MS & Olfactometry, GC-FID, Pyrolysis/MS, EEM, MALDI-TOF, Automated DNA Extraction, qPCR, Fluorescence, Microscopy, FilmArray, etc

ANALYSIS TYPE



ORGANIC

Pesticides, byproducts hydrocarbons, PAHs, PFAS, etc.



INORGANIC

Metals, anions, TOC, BOD₅, nutrients, solids, etc.



MICROBIOLOGICAL

Pathogens

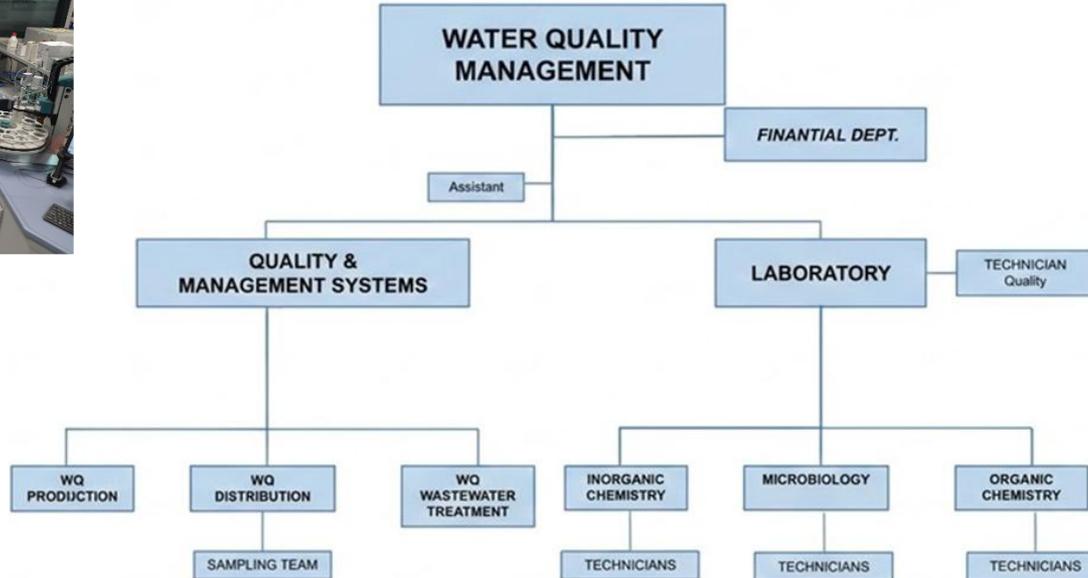
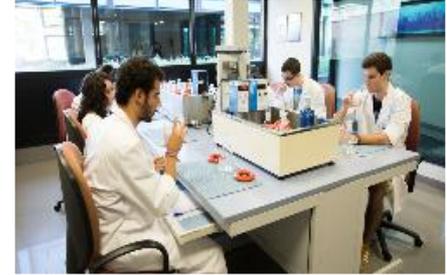
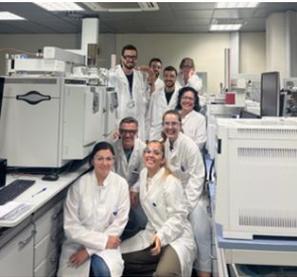
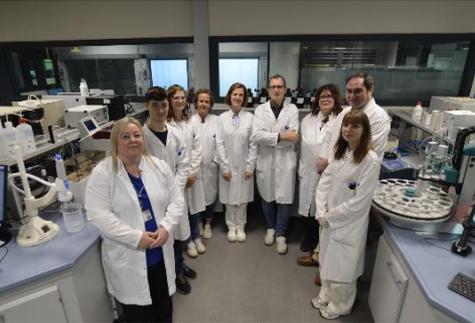
MATRICES

Wastewater, natural water, drinking water, recycled water

ACCREDITATION

ISO 9001, ISO 17025, ISO 22000, ISO 45001, ISO 14001

WATER QUALITY MANAGEMENT: ORGANIZATION



ISO 17025 ACCREDITATION

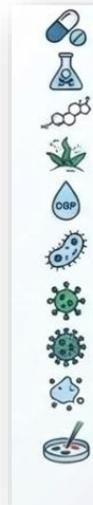
For a broad scope of parameters, including all regulated ones



LIMS automatically linked to analytical instruments, national reporting system, internal reporting system, SCADA, SAP, web page, etc.

ANALYTICAL CAPABILITIES NON-REGULATED CONTAMINANTS & PATHOGENS

- Pharmaceuticals
- Drugs of abuse
 - EDCs
 - Algae toxins
- Non-regulated DBPs
- *Salmonella, Campylobacter, etc.*
 - Bacteriophages
 - SARS-CoV-2
 - ARGs
 - Microplastics
- Identification of bacterial strains by MALDI-TOF
 - Metallic nanoparticles (Ti, Ag)



GREEN CHEMISTRY AT AIGÜES DE BARCELONA

Our analytical laboratory applies principles of the Green Chemistry by:

- **Minimizing solvent use** through direct injection instead of extraction, and using kits and FIAs
- **Eliminating hazardous reagents** by cleaning and reusing glassware responsibly, and optimizing specific analysis
- Generating nitrogen on-site and compressing air to **reduce our carbon footprint**, and using low-consumption electric vacuum pumps for filtration
- Improving **energy and waste efficiency** through modern instrumentation
- Using LIMS for **paperless laboratory management**



Inorganic Chemistry Laboratory



Inorganic Laboratory

Impact of switching from manual to COD kits (60 test/month)

- **Environment**
Mercury minimized
Hazardous waste reduced
- **Economic**
Hazardous waste disposal savings
- **Safety**
Reduction of mercury exposure risk
60-70% less concentrated acid handling
- **Operational**
70% faster analysis
Simplified regulatory compliance
Lower CO₂ footprint: 200-400 Kg/year

Impact of using FIAs for Phosphorous, Cyanide, Ammonia & Total Nitrogen

- **Environment**
Reduction 70-90% reagent consumption
80-85% reduction on chemical waste
60-75% less water usage
- **Economic**
Hazardous waste disposal savings
Reagent saving
- **Safety**
Minimal operator exposure to toxic reagents
- **Operational**
Faster analysis

Nitrogen Measurement Methods

Direct Kjeldahl vs. Indirect Calculation (TN- Inorganic N)

Direct Kjeldahl

- **Environment**
Waste generation
High energy consumption
- **Safety**
Hazardous reagents and toxic fumes (NH₃, SO_x)

Indirect calculation

- **Environment**
Prevention (less waste)
- **Safety**
Improved safety by reducing exposure
- **Operational**
Efficient



Indirect method offers lower environmental impact and improved safety, despite increased analytical complexity. Accredited method

Microbiology Laboratory

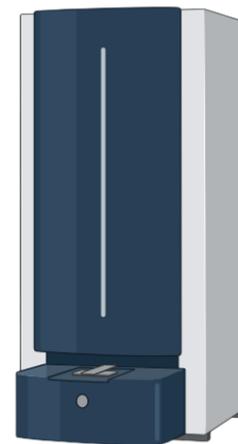


Microorganisms identification method

Replacement of single-use miniaturized strips → mass spectrometry



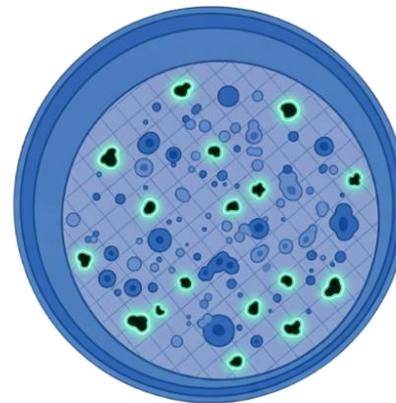
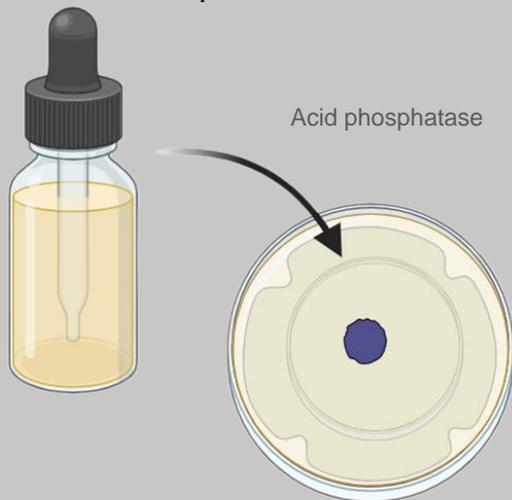
MALDI-TOF



- **Elimination of plastic waste and consumables per test**
- Reduction of hands-on time, costs and results per test

Clostridium perfringens detection method

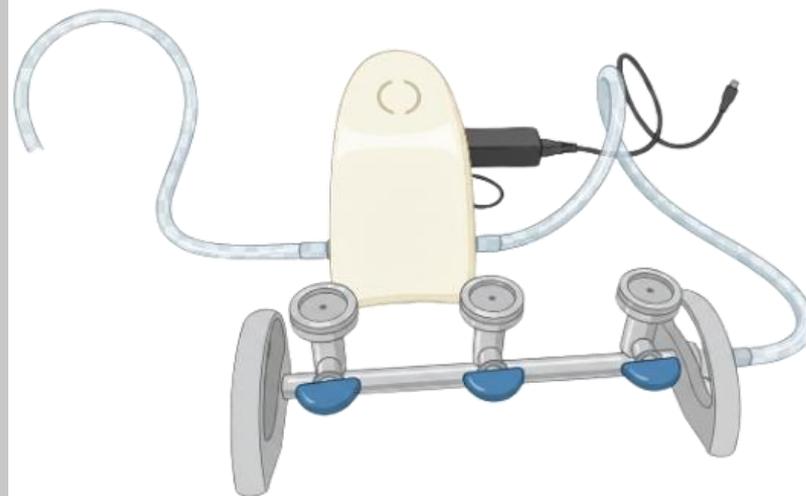
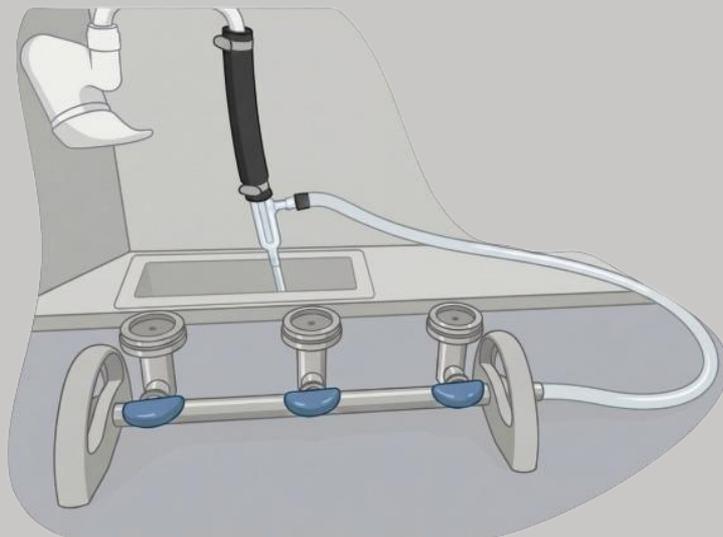
Replacement of carcinogenic reagent → fluorescent colonies detection



- **Elimination of carcinogenic reagent**
- Reduction of hands-on time and results per test
- Accepted method by RD3/23

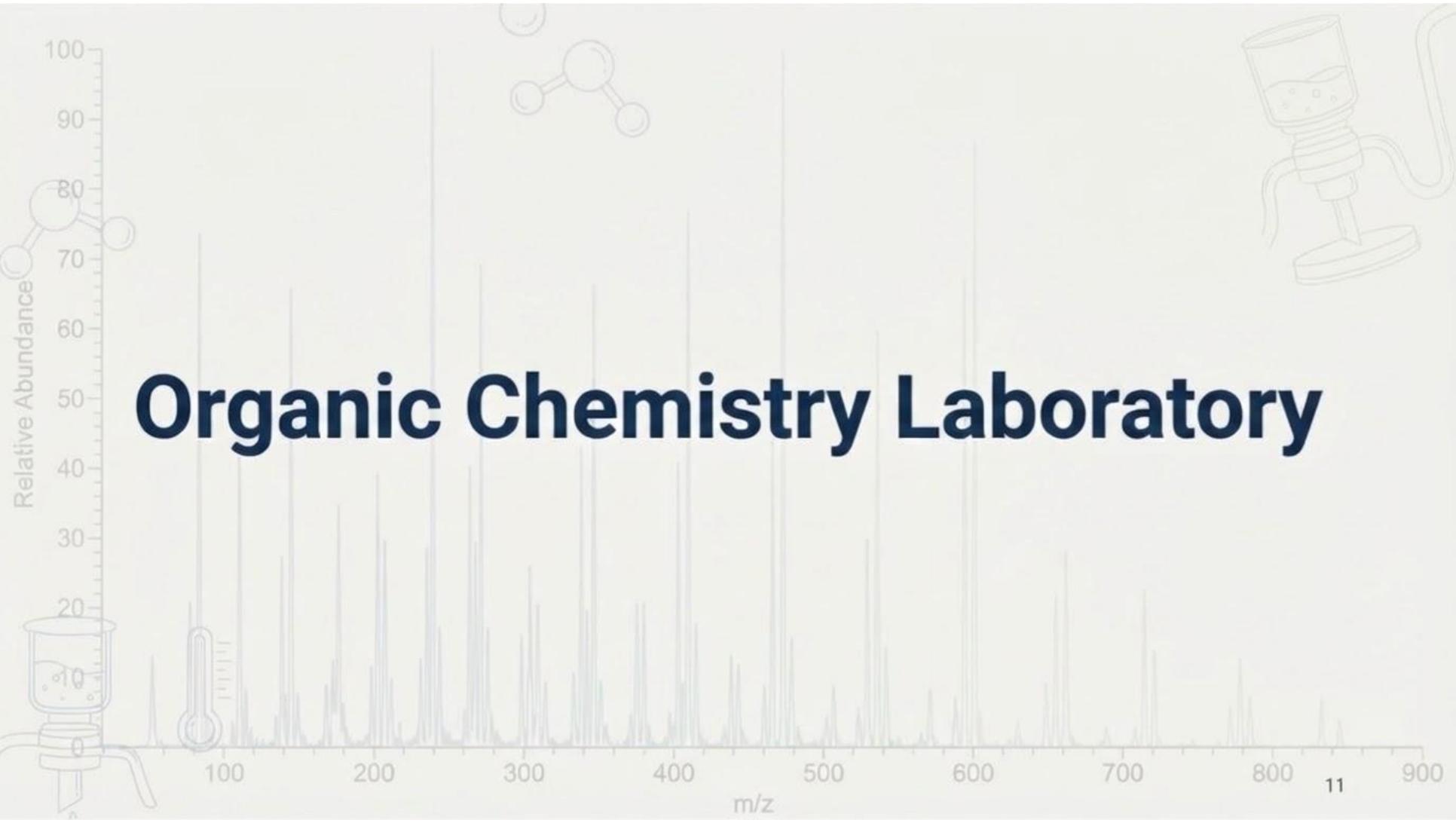
Sample filtration

Replacement of vacuum pumps → low consumption electric peristaltic pumps



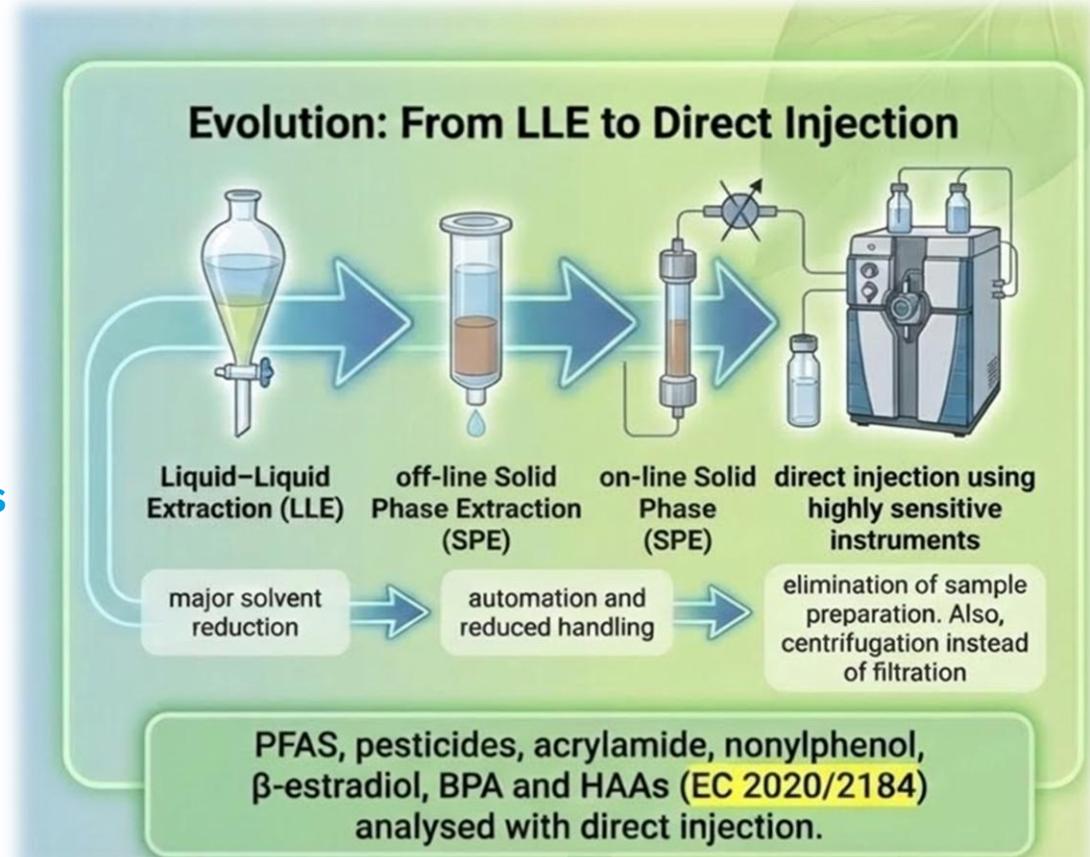
→ Reduction of water consumption

Organic Chemistry Laboratory



Sample Preparation

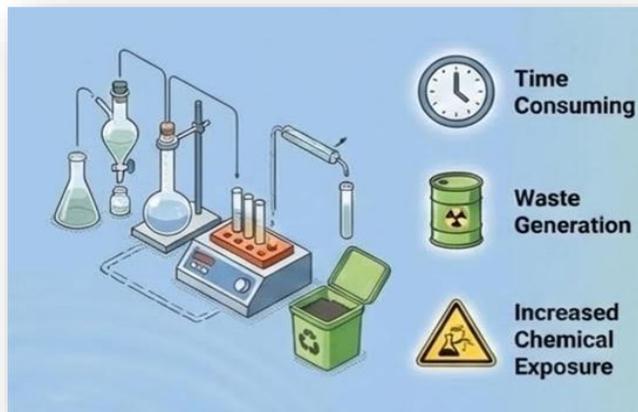
- Strategies to **reduce solvent consumption and toxicity** (SPME, Twister, direct injection, etc.)
- **Minimization** of organic solvent volumes
- Selection of **les toxic solvents** (ethanol, ethyl acetate...)
- Optimization of extraction **times and energy consumption**



Example: Haloacetic acids (HAAs)

Conventional method (GC-MS)

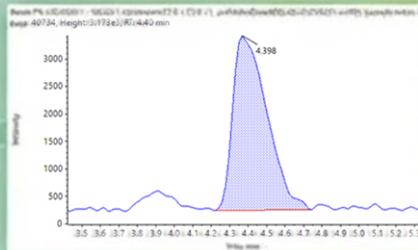
- Derivatization with acidic methanol (EPA). Requires significant sample preparation.



Aigües de Barcelona Method (LC-MS/MS)*



Direct analysis of 9 HAA in water (**LOQ = 4 µg/L**) using LC-MS/MS (Qtrap). No derivatization, direct injection.



MCAA standard injected at LOQ

Haloacetic acids (HAAs)

60 µg/L



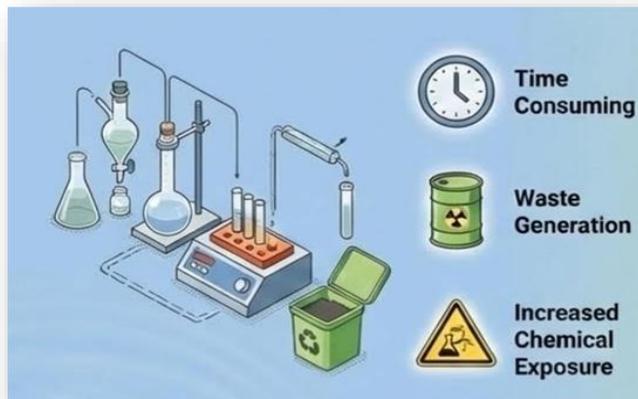
Complies with EC 2020/2184 (L 435/36)

*US EPA Method 557 (Determination of Haloacetic Acids, Bromate and Dalapon in Drinking Water by Ion Chromatography Electrospray Ionization Tandem Mass Spectrometry)

Example: AMPA & Glyphosate

Conventional method (GC-MS)

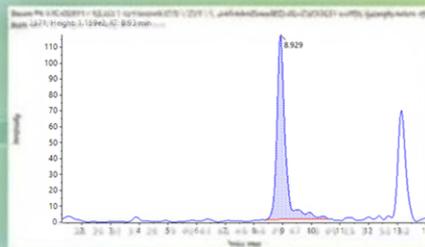
- Requires derivatization with perfluoroalcohols (GC-MS) and FMOC-C (LC-MS/MS).



Aigües de Barcelona Method (LC-MS/MS)*



Direct analysis of AMPA and Glyphosate in water (LOQ = 30 ng/L) using LC-MS/MS (Qtrap). No derivatization, direct injection.



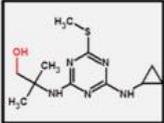
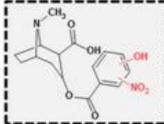
AMPA and Glyphosate

LOQ = 30 ng/L

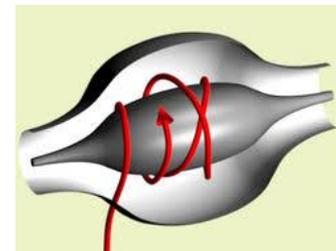


Complies with EC 2020/2184 (L 435/36)

Non-targeted Analysis

Example	Identification confidence	Minimum data requirements
	Level 1: Confirmed structure by reference standard	MS, MS ² , RT, Reference Std.
	Level 2: Probable structure a) by library spectrum match b) by diagnostic evidence	MS, MS ² , Library MS ² MS, MS ² , Exp. data
	Level 3: Tentative candidate(s) structure, substituent, class	MS, MS ² , Exp. data
$C_6H_5N_3O_4$	Level 4: Unequivocal molecular formula	MS isotope/adduct
192.0757	Level 5: Exact mass of interest	MS

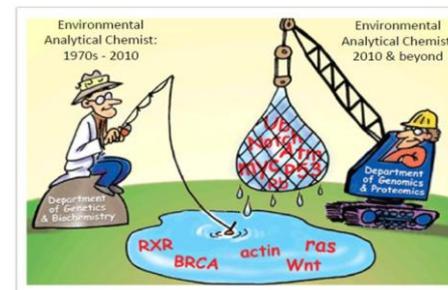
Schymanski. E., et al. *Environ. Sci. Technol.* 2014, 48, 4, 2097–2098



PubChem



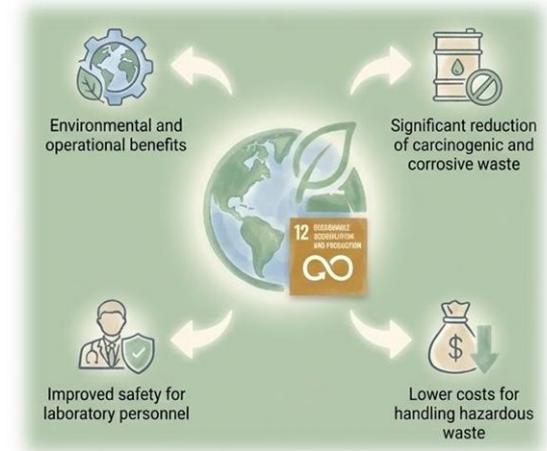
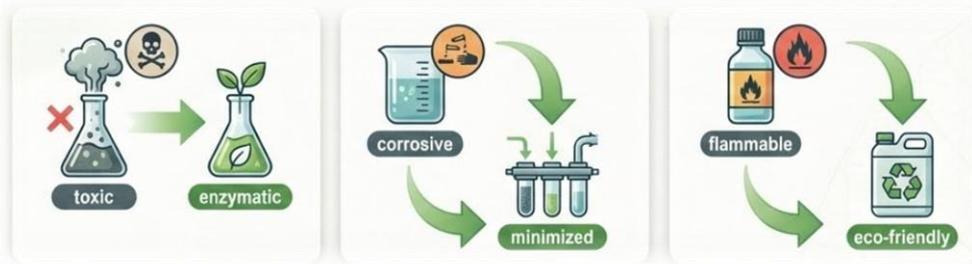
NIST



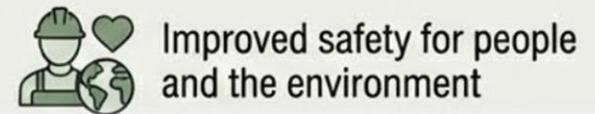
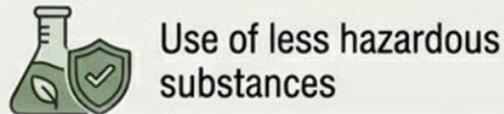
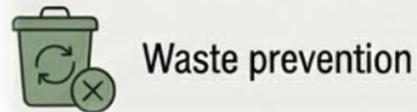
Other aspects - General

Material Cleaning

- ✓ Elimination of chromic mixture -> replaced with enzymatic detergents
- ✓ Minimization of the use of nitric acid
- ✓ Minimization of the use of methanol



Overall impact



Nitrogen Generator (and air compression)

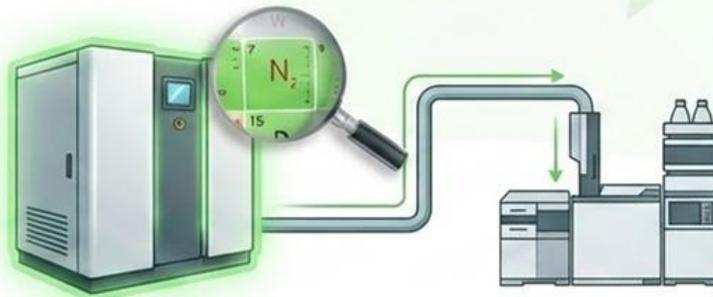
5 LC/MSMS → Laboratory consumption: 134 L/min → 20 cylinders /day

❌ Conventional Cylinders (Before)



Daily CO₂: 246–492 kg
Annual CO₂: 61,500–123,000 kg

✅ Nitrogen Generator (After)



Daily CO₂: <1 kg
Annual CO₂: <200 kg



No transportation of cylinders → Reduces road emissions



No cylinder manufacturing → Reduces steel demand & industrial energy use



Minimal risk of leaks or wasted gas



Continuous supply → Avoids overstocking or laboratory slow down



Economical savings (approx. 100.000 €/year)

Laboratory Information Management System (LIMS)

1. Paperless operations.

Digital records eliminate paper waste. Electronic signatures and reports.

2. Reduced Re-Analysis.

Quality controls prevent errors. Less waste from repeating testing.

3. Efficient Resource use (stock control).

Track stocks and instrument maintenance scheduling

4. Quality Control .

Follow quality control directly on LIMS (no excel)



5. Better sample management.

Prevent sample loss and expiration. Minimize re-sampling needs.

6. Sustainability Metrics.

General consumption reports. Support environmental certification (ISO14001)

Take home messages

We have made our lab greener by:

- ✓ **Minimizing solvent consumption:** Direct injection methods instead of extraction plus kits and FIAs Systems,
- ✓ **Eliminating hazardous reagents:** Responsible glassware cleaning and reuse, optimized methods for specific analyses (e.g., Clostridium perfringens, derivatization, etc)
- ✓ **Reducing carbon footprint:** On-site nitrogen generation, air compression, and low consumption electric vacuum pumps replacing water-aspirated pumps for filtration,
- ✓ **Improving efficiency:** Modern instrumentation for reduced energy consumption and waste generation,
- ✓ **Digital management:** LIMS implementation for paperless operations.

Thank you

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**Aigües de
Barcelona**

La gestió responsable

