Analytical strategies to highlight and identify organic compounds in groundwater

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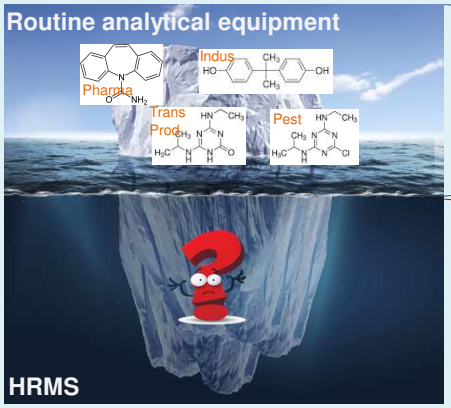
1. Nowadays it is increasingly important for public policy to know what compounds are present in groundwater and which of them must be monitored. This implies the need of specific analytical methodology to identify these micropollutants, emerging substances or transformation products present at low concentrations. The high resolution mass spectroscopy (HRMS) has gained increasingly in importance for monitoring these organic compounds. Its high resolving power, mass accuracy and the sensitive full spectrum acquisition are the key points.

2. Interest of High Resolution Mass Spectrometry (HRMS)



Search of information known

- Mainly quadrupole analyzer
- List of compounds known
- Limited number
- Regulated compounds
- Relevant compounds

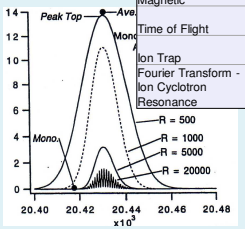
Search of information unknown

- Compounds unknown
- Unlimited number

a. High resolution

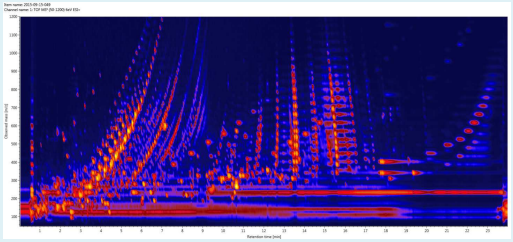
The resolution measures the ability to distinguish two peaks of slightly different mass-to-charge ratios *ΔM*, in a mass spectrum. The higher the resolution is the higher the accurate mass is.

Analyzer	Resolution
Quadrupole	2,000
Magnetic	20,000
Time of Flight	20,000 - 60,000
Ion Trap	5,000 - 20,000
Fourier Transform - Ion Cyclotron Resonance	1,000,000



b. What is the acquired information?

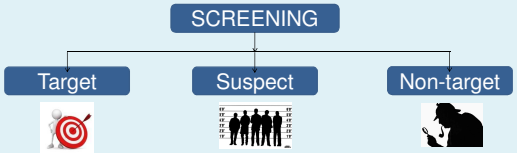
All accurate masses, retention time and intensities are acquired. Each pair (mass and retention time) is specific to a compound.



Each lighting point represent a detected compound. In this example over 100,000 are detected in one environmental sample.

b. Data processing

In order to identify compounds in samples, 3 types of screening are used. Each of them have a level of confidence different on the compound identification.



Does the compound X is in my sample??

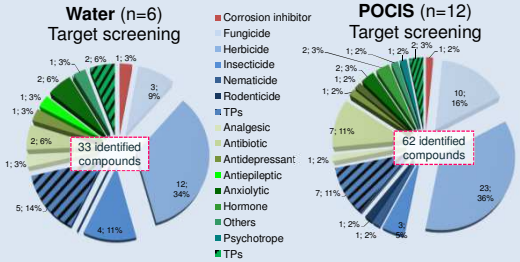
The difference between target/suspect = information I have on compound

Which is in my sample??

All compounds present in sample

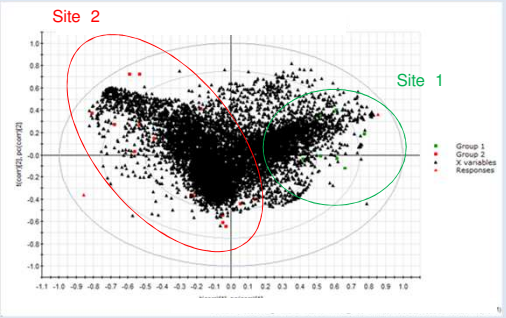
3. What kinds of results

Information about the content, or lack of content, of compounds in sample. This research is based on list of target compounds with theoretical and experimental data (retention time, accurate mass, isotopic pattern and fragment) from analytical instrument



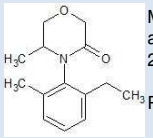
Soulier, C., et al. (2016), Sci Total Environ, http://dx.doi.org/10.1016/j.scitotenv.2016.01.056

Of all the signals present in samples it can be interesting to preselect relevant compounds from statistics. This differentiates both or several sites, source of pollution, etc. And the identification is made only on the specific compounds.



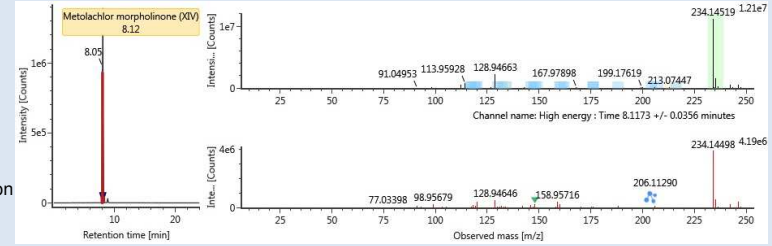
One application of suspect screening is the identification of transformation products in sample from in silico modeling tools (transformation of parent compounds) or common fragments. Another application is the search of compounds from public database (literature or on-line).

Metolachlor morpholinone, Transformation products of metolachlor



Monoisotopic accurate mass: 233,141 6uma

Positive ionization



4. Conclusions

HRMS is a complementary technique compared to those applied routinely in analytical laboratories. All information present in sample are acquired and stored. In this way data can be used over and over again because data processing depends on needs and objectives.

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