

Environmental

Differential analysis of soil using the Orbitrap Exploris GC 240 mass spectrometer and Compound Discoverer software

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Keywords

Orbitrap Exploris GC 240 mass spectrometer, mass resolving power, sensitivity, mass accuracy, Orbitrap technology, gas chromatography, soil, Compound Discoverer software

Goal

To demonstrate the performance of the Thermo Scientific™ Orbitrap Exploris™ GC 240 mass spectrometer for the differential analysis of soil samples. To show the power of Thermo Scientific™ Compound Discoverer™ software for the processing of GC HRMS data and present statistical differences between soils from different locations.

Introduction

Environmental samples, (e.g., soil, sediments, or surface water) can contain a broad spectrum of volatile or semi-volatile contaminants, including polychlorinated biphenyls (PCBs), polychlorinated dibenzodioxins (PCDDs), polyaromatic hydrocarbons (PAHs), brominated flame retardants (BFRs), and pesticides. The combination of gas chromatography (GC) with quadrupole-based mass spectrometers is a common analytical setup for detection of these contaminants. GC-MS quadrupole-based instruments are well known for their robustness and ease of use. However, they have some important limitations for this application. Single quadrupole instruments can perform full scan analysis, but their sensitivity and selectivity in this mode are limited. Triple quadrupole (GC-MS/MS) systems have greater sensitivity and selectivity; however, their advantages are limited to targeted acquisition within a specified compound list.

Creation of targeted methods requires time-consuming optimization and use of analytical standards, which can be very expensive and, on occasion, unavailable. However, the biggest drawback is that only targeted compounds included in the method can be detected, whereas other contaminants present will be overlooked.

High-resolution accurate mass (HRAM) mass spectrometry provides a very sensitive and selective non-target acquisition and surpasses quadrupole instruments in all non-targeted applications. Orbitrap™ MS-based instruments offer unmatched resolving power (up to 240 000 at m/z 200), mass accuracy greater than 1 ppm, wide dynamic range, and high sensitivity. However, to fully realize the benefits of a HRAM system, powerful software is essential to convert high quality data into scientific discovery.¹ Thermo Scientific™ Compound Discoverer™ software is designed to process large non-targeted data sets acquired using high-resolution mass spectrometry instruments, like the Orbitrap Exploris GC 240 mass spectrometer. The software contains a wide range of tools for unknown compound identification and statistical analysis.

In this study, GC-Orbitrap technology and Compound Discoverer software were used to assess the chemical profile of soil sample extracts taken from three locations near Bremen, Germany. Data were acquired in full-scan with electron ionization (EI) mode. Positive chemical ionization (PCI) and negative chemical ionization (NCI) were used to confirm the elemental composition of the molecular ions using accurate mass information, isotopic match (measured versus theoretical), and presence of specific adducts.

Experimental

Sample preparation

Three soil samples were taken from various locations in and near to Bremen in Germany. The samples received the following letter codes: D, L, and M. They were collected in proximity of a motorway junction, close to an airport, and in a stand-alone house neighborhood, respectively. The samples were extracted without any pretreatment. A 2 g portion of soil was weighed in a polypropylene tube followed by the addition of 4 mL of acetonitrile and vortexed for 5 minutes. Acetonitrile is a water miscible solvent, facilitating the extraction of organic contaminants in humid soils. Next, 4 mL of hexane were added and vortexed again in the same manner. Organic contaminants were transferred to the hexane phase through liquid-liquid partitioning between hexane and acetonitrile solvent layers. Subsequently, the tube was centrifuged for 5 minutes at 4,000 rpm with the hexane layer transferred to a GC vial and injected.

In the EI mode, the extracts were analyzed in triplicate in a random order. After every sixth injection, a pooled sample was injected.

The pooled sample contained equal volume of the three soil extracts. The confirmatory injections in the PCI and NCI modes were performed without repetitions.

Acquisition method

The samples were analyzed with an Orbitrap Exploris GC 240 mass spectrometer coupled to a Thermo Scientific™ TRACE™ 1610 gas chromatograph and a Thermo Scientific™ TriPlus™ RSH SMART autosampler. All the instrumental parameters are shown in Tables 1–4.

Table 1. Parameters of the TRACE 1610 GC

TRACE 1610 GC	
Injector	
Injection volume (μL)	1
Liner	Single gooseneck with glass wool Thermo Scientific™ LinerGOLD™ (P/N 453A1925-UI)
Inlet temperature (°C)	300
Inlet module and mode	SSL, Splitless
Splitless time (min)	1
Septum purge flow (mL/min)	5
Oven and column	
Carrier gas, flow rate (mL/min)	He, 1.2
Column	Thermo Scientific™ TraceGOLD™ TG-5SilMS 30 m × 0.25 mm i.d. × 0.25 μm (P/N 26096-1420)
Oven temperature program	
Temperature 1 (°C)	40
Hold time (min)	2
Temperature 2 (°C)	300
Rate (°C/min)	10
Hold time (min)	7
Total GC run time (min)	35

Table 2. Parameters of the Orbitrap Exploris GC 240 mass spectrometer in electron ionization mode

Orbitrap Exploris GC 240 mass spectrometer in EI mode	
Transfer line (°C)	300
Ion source (ionization type)	Thermo Scientific™ ExtractaBrite™ (EI) source
Ion source (°C)	280
Electron energy (eV)	70
Emission current (μA)	50
Acquisition mode	Full scan (FS)
Mass range (m/z)	50–550
Resolving power	120,000
AGC target	Standard
Maximum injection time	Auto
Lock masses	133.01356; 207.03235; 225.04292; 281.05114; 299.06171; 355.06993

Table 3. Parameters of the Orbitrap Exploris GC 240 mass spectrometer in positive chemical ionization mode

Orbitrap Exploris GC 240 mass spectrometer in PCI mode	
Transfer line (°C)	300
Ion source (ionization type)	ExtractaBrite (CI)
Ion source (°C)	250
CI gas	Methane
CI gas flow (mL/min)	1.0
Acquisition mode	Full scan/ddMS ²
Mass range (<i>m/z</i>)	50–550
Resolving power	120,000
AGC target	Standard
Maximum injection time	Auto
ddMS ² Scans	5
ddMS ² Filters	Dynamic exclusion, Apex detection
ddMS ² Isolation window (<i>m/z</i>)	1.2
ddMS ² HCD collision energies (V)	20; 40; 60
ddMS ² Resolving power	15,000
ddMS ² Scan range	Auto
ddMS ² AGC target	Standard
ddMS ² Maximum injection time	Auto

Table 4. Parameters of the Orbitrap Exploris GC 240 mass spectrometer in negative chemical ionization mode

Orbitrap Exploris GC 240 mass spectrometer in NCI mode	
Transfer line (°C)	300
Ion source (ionization type)	ExtractaBrite (CI)
Ion source (°C)	250
CI gas	Methane
CI gas flow (mL/min)	1
Acquisition mode	Full scan
Mass range (<i>m/z</i>)	50–550
Resolving power	120,000
AGC target	Standard
Maximum injection time	Auto

Compound Discoverer software workflows

Compound Discoverer software contains template workflows for GC EI, as well as GC PCI data. In this study, the EI data were used for statistical analysis and compound identification, whereas the PCI data were used for the confirmation purposes. PCI is an alternative and complimentary form of ionization, which is considered a softer ionization that often gives molecular ion information through mass adduct patterns and lower fragmentation. It is often seen as an important option when an

unknown compound is suspected. Although not mandatory, combination of EI and PCI data is advisable as it increases the confidence of identification due to molecular ion confirmation.

The main features of the EI workflows in Compound Discoverer software are spectral deconvolution, compound identification, and statistical analysis. Compound identification is based on the library search using both high-resolution and nominal mass spectral libraries. The EI workflow (Figure 1) used here was one of the default workflows available in the software. The workflow contained spectral deconvolution and statistical data evaluation (Descriptive Statistics and Differential Analysis visible in the lower part of Figure 1). The template workflows in Compound Discoverer software come with optimized parameters. Thus, the user only needs to select the spectral libraries to be used for identification. The deconvoluted spectra were identified against the NIST™ 2020 (nominal mass) and GC-Orbitrap Contaminants Library (HRAM library).

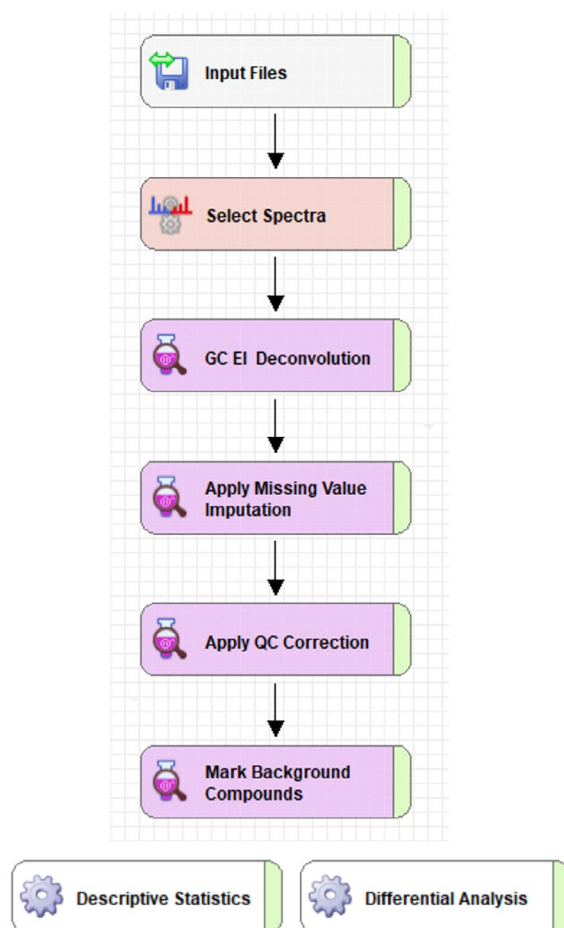


Figure 1. Electron ionization (EI) workflow used in Compound Discoverer software. The node-based structure enables a flexible approach to research data processing.

For various statistical analyses, zero values within the sample set can lead to erroneous results. To avoid this type of error, Compound Discoverer software provides methods for imputing missing chromatographic peak areas for detected compounds across the set of input files. This is the role of the "Missing Value Imputation" node. Additionally, two extra nodes—"Apply QC Correction" and "Mark Background Compounds"—were aggregated to the default nodes present in the workflow. The "Apply QC Correction" node is useful when a long sequence of samples is acquired and compensates for time-dependent batch effects. To use this node, a QC sample is required. To create the QC sample, a small aliquot from each sample must be pooled in one vial. The pooled sample is injected at regular intervals along the sequence, in this case, after every six injections. The "Mark Background Compounds" node is applied to flag compounds that are found not only in the sample but also in the instrumental or matrix blanks. A compound that has

$$\frac{\text{peak area in sample}}{\text{peak area in blank}}$$

below a desired threshold (5 by default) is marked as a background compound and can be hidden in the results table.

Positive chemical ionization

Figure 2 shows the workflow applied for the PCI data processing. The PCI workflows are strongly related to the presence of molecular ion. In this study, the following identification nodes were applied:

- **Predict Composition:** predicts the chemical formulas of the unknown compounds
- **Search ChemSpider™:** enables search in ChemSpider of elemental composition proposed
- **Search mzCloud™:** performs a search in the mzCloud library, which is an exact mass library that contains both MS as well as MS² data
- **Search Mass List:** serves to a databases search (this node is also available for EI workflows)

The task of the "Assign Compound Annotations GC CI" node is to assign and prioritize the annotation coming from the nodes (Predict Composition, Search ChemSpider, Search mzCloud, and Search Mass List). In the software, there is also a node that enables search in Thermo Scientific™ mzVault™ libraries, however in this study it was not employed.

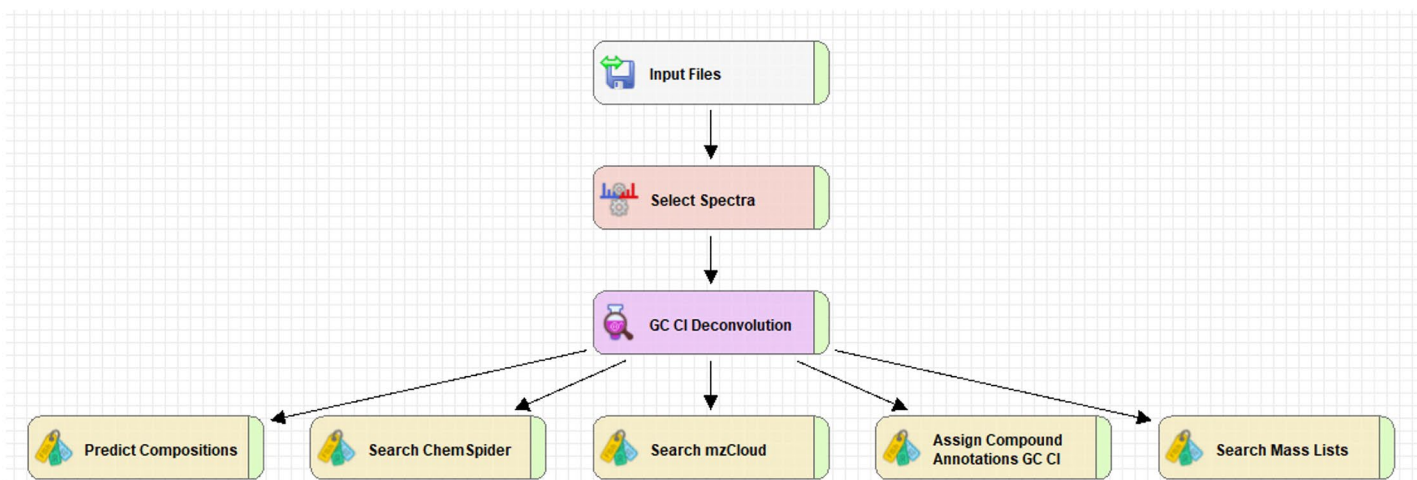


Figure 2. Positive chemical ionization (PCI) workflow used in Compound Discoverer software. Detection of the molecular ion is the focus in this workflow to confirm identification of compounds or to propose an elemental composition of an unknown.

Data evaluation - statistical tools and unknown compound identification

The first objective was to identify if there was any significant difference between the three soil samples at locations D, L, and M. This was achieved through a PCA plot of the replicate injections of each sample. Figure 3 shows the PCA plot that demonstrates that there are clear differences between the samples and good agreement of the replicate injections. The following steps then help identify which peaks contribute to the differences so that a compound identification can be proposed. As an example, Figure 4 shows a volcano plot for the samples D and L. The volcano plot is a type of scatter plot for replicate data where the x axis represents the log₂ of the fold change between two sample groups (generated ratio), and the y axis represents the negative log₁₀ of the p-value (test of significance) of the fold change. In other words, when a point (compound) is more on the right (positive values on x axis), the peak area of that compound is much higher in the sample D than in the sample L. Whereas, points that are higher on the graph are statistically more significant.

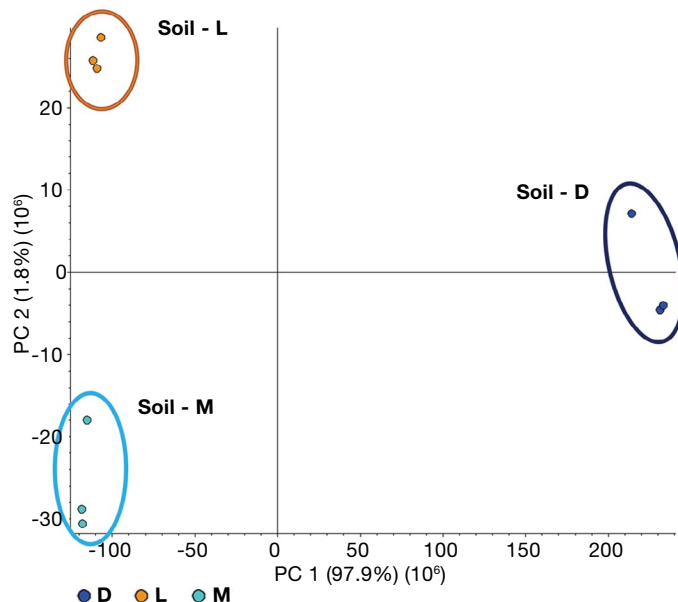


Figure 3. PCA score plot of the volatile compounds that differentiate the three soil samples from different locations. A complete separation between the sample groups was observed and good agreement between replicate injections.

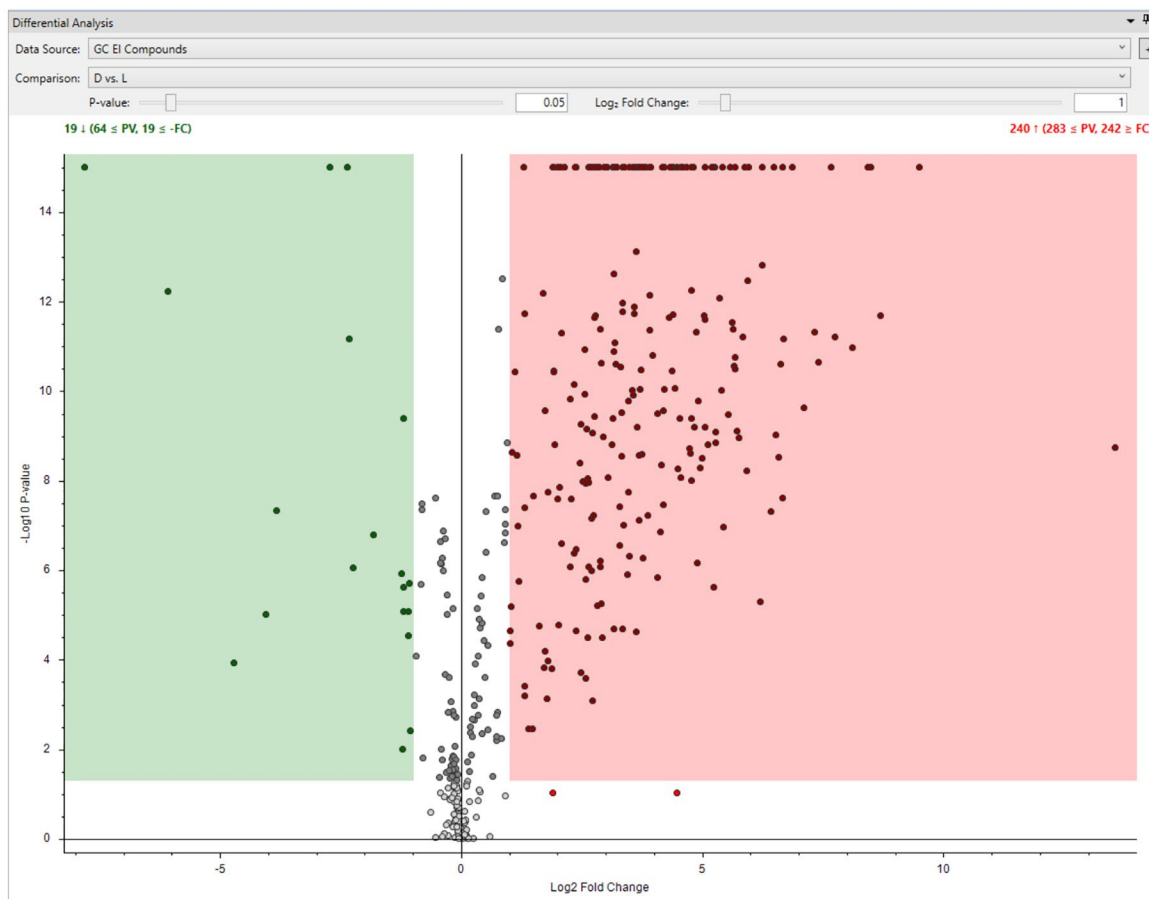


Figure 4. V-plot scatterplot showing the statistical significance (P value) versus magnitude of change (fold change) when comparing the soil sample D (right) versus the soil sample L (left). The main chemical components that are responsible for sample diversity between two sample groups are located in the upper right and left sides of the plot.

In Figure 4, it can be easily recognized that sample D contained more characteristic compounds than sample L, possibly due to a higher content of the organic fraction. Double-clicking on any of the points (features) takes the user to the results table, where the compound details can be checked (Figure 5). The table contains library search results (name, formula, search index, reverse search index, etc.) as well as information about peak areas. Moreover, each of the rows contain related tables where the user can check the details of NIST identification.

In the discussed samples, the majority of detected compounds were related with the presence of the soil organic matter. Nevertheless, a deeper insight revealed some typical contaminants. Pyrene is an interesting example. Figures 6a and 6b show pyrene identification details. This compound was present in all three analyzed soils; however, its signal was the highest in the sample M. In the EI workflow, pyrene was identified, achieving a search index of 897 and reversed search index of 932. Pyrene and other polyaromatic hydrocarbons produce a stable and intense molecular ion, which is not very common in EI. The molecular ion presence is mentioned in the results table. In Figure 6a, a comparison between the deconvoluted spectrum and spectrum present in the library can be seen.

The identification of pyrene was confirmed in the CI mode, where all the annotation sources suggested its presence. As discussed, the CI identification is based on the presence of the molecular ion. In contrary to the electron ionization, the chemical ionization is a softer ionization process, allowing for easy identification of the molecular ion due to reduced fragmentation. Information on the molecular ion allowed the Compound Discoverer software to predict the molecular formula for our unknown compound (Figure 6b). That prediction was verified by the evaluation of the isotopic profile and search for alternative adducts (Figure 6b). The obtained molecular formula ($C_{16}H_{10}$) was assigned to pyrene by the following nodes: "ChemSpider Search", "MassList Search", and "mzCloud Search". During the data acquisition, full scan MS was combined with a data dependent MS^2 (ddMS²). This means that after each full scan MS, there was a series a MS^2 scans. The five most abundant ions from each MS spectrum

were fragmented, each in a separate fragmentation event. In this manner, high quality MS^2 spectra were obtained. Thus, the "mzCloud Search" involved the MS^2 data as well.

Pyrene was not the only polyaromatic hydrocarbon detected. The samples also contained fluoranthene and perylene. The peak areas of these compounds were the greatest in the sample M. That sample was collected in a stand-alone house neighborhood, and many of the houses situated there have a fireplace. This could be the reason of the elevated amount of PAHs.

In addition to the Volcano Plot, Compound Discoverer software offers other tools for data visualization. Box Whisker Charts can be used to easily visualize the pyrene peak areas in the investigated samples. As mentioned above, the peak areas in the sample M were higher than in the samples L and D. This is clearly visible in Figure 7. Moreover, the figure reveals the relations between the samples D, M, and L were the same in EI and CI. This is a strong suggestion that the peaks belong to the same compound.

Another interesting contaminant discovered in the investigated samples was a PCB containing six chlorine atoms. Sample D showed the highest levels of contamination; however, the analyte was also present in the two remaining soil samples. Thanks to the presence of six chlorine atoms, the isotopic pattern is very characteristic and can aid in the confirmation of the molecular formula. Figure 8a shows a comparison between the experimental spectrum and the theoretical isotopic pattern of an ion with elemental composition corresponding to a hexachlorinated PCB. As can be seen, the match is nearly perfect. Unfortunately, polychlorinated biphenyls do not ionize easily in positive chemical ionization mode. However, PCBs with six or more chlorines show excellent response with negative chemical ionization. Presence of an ion corresponding to $C_{12}H_4Cl_6$ was also confirmed in the NCI data. Figure 8b shows the acquired spectrum and theoretical isotopic pattern of $C_{12}H_4Cl_6$ in the negative ionization mode. To specify which PCB congener was present in the sample, the knowledge about the retention index would be very helpful.

Checked	Tags	Name	Calc. MW	RT [min]	Reference m/z	Avg TIC	NIST Lib Hit Formula	NIST Theo. Mol. Mass	NIST Observed Mol. Mass	# Usable QC	RSD QC Areas [%]	RSD Corr. QC Areas [%]	Total Score	HRF Score	SI	Group Areas	Group CV [%]	Ratio	Log2 Fold Change	
<input checked="" type="checkbox"/>		Glutinol	424.37060	33.300	259.24210	11531224	C30 H50 O	426.38562		8	11		2	95.4	99.3	783	1.65e5	2.21e5	0.651	0.112
<input checked="" type="checkbox"/>		Vitamin E	430.38113	29.770	165.09097	41002533	C29 H50 O2	430.38053	430.38058	8	26		8	97	98.9	871	1.39e5	7.50e5	5.52e5	11
<input checked="" type="checkbox"/>		D-Friedoolean-14-en-3-one	424.37060	31.999	204.18723	57941738	C30 H48 O	424.36997	424.37006	8	9		2	96.6	99.8	833	1.21e5	2.54e5	1.76e5	5
<input checked="" type="checkbox"/>		Lup-20(29)-ene-3-one	424.37076	32.844	107.08556	24447923	C30 H48 O	424.36997	424.37021	8	9		4	96.5	99.2	842	1.16e5	4.33e5	1.19e5	3
<input checked="" type="checkbox"/>		Benzene, 1,3-bis(1,1-dimethylethyl)-	190.17201	12.120	176.15134	60043400	C14 H22	190.17160	190.17166	8	7		2	96.6	98.5	838	9.17e7	1.33e8	1.10e8	4
<input checked="" type="checkbox"/>		D-Friedoolean-14-en-3-ol	426.36832	32.335	287.23654	17583323	C30 H50 O	426.38562	426.38577	8	12		3	96.4	99.6	829	8.36e7	1.34e8	8.12e5	6
<input checked="" type="checkbox"/>		Lupcol	426.36623	33.161	91.05423	59034145	C30 H50 O	426.38562	426.38568	8	14		3	91.9	98.6	624	6.60e7	9.22e5	2.54e5	8
<input checked="" type="checkbox"/>		Sigmastane, 3-one, (3a)	414.38623	32.640	217.15872	9512695	C29 H50 O	414.38562	414.38568	8	12		3	94.8	99.6	750	6.99e7	3.74e5	2.11e5	8
<input checked="" type="checkbox"/>		Peak@33.209	275.20117	33.205	105.06938	44114470				8	14		5							
<input checked="" type="checkbox"/>		Sigmasta-3,5-dien-7-one	410.35492	33.222	159.08044	20613877	C29 H46 O	410.35432	410.35437	8	17		7	91.4	97.5	618	8.16e7	3.77e5	1.78e5	7
<input checked="" type="checkbox"/>		Oxalic acid, allyl nonyl ester	125.13303	12.395	57.06978	65913653	C14 H24 O4	256.16691		8	7		2	96.6	99.5	840	5.08e7	5.26e7	5.21e7	5
<input checked="" type="checkbox"/>		Sigmasta-3,5-dien-7-one	410.35498	33.209	324.18726	29980675	C29 H46 O	410.35432	410.35443	8	12		4	89.3	96.8	527	5.02e7	9.79e5	4.72e5	8
<input checked="" type="checkbox"/>		1-Nonene, 4,6,8-trimethyl-	124.12514	15.215	71.08553	64880697	C12 H24	168.18725		8	8		2	96.6	99.5	850	4.83e7	8.00e7	4.89e7	8
<input checked="" type="checkbox"/>		γ-Sitosterone	412.37064	33.792	124.08827	11399267	C29 H48 O	412.36997	412.37009	8	16		3	95.6	99.0	800	4.62e7	7.35e5	8.56e5	7
<input checked="" type="checkbox"/>		Peak@33.795	106.07827	33.795	124.08826	21011495				8	16		3							
<input checked="" type="checkbox"/>		d-Friedoolean-14-en-3-ol, acetate, (β)-	468.39664	33.558	191.14307	89111568	C32 H52 O2	468.39618	468.39602	8	15		4	92.0	93.5	774	4.14e7	3.22e7	2.07e7	4
<input checked="" type="checkbox"/>		1-Nonene, 4,6,8-trimethyl-	154.17218	19.905	71.08553	53485473	C12 H24	168.18725		8	8		2	96.1	99.5	813	4.12e7	4.23e7	4.17e7	4
<input checked="" type="checkbox"/>		γ-Sitosterol	414.38614	31.951	329.32028	24311664	C29 H50 O	414.38562	414.38559	7	20		6	91.8	98.2	625	4.01e7	2.82e5	8.44e5	8
<input checked="" type="checkbox"/>		1-Nonene, 4,6,8-trimethyl-	101.00157	17.600	71.08553	60834492	C12 H24	168.18725		8	8		3	95.8	99.0	700	3.66e7	1.60e7	1.60e7	4

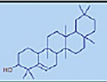
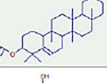
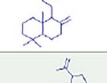
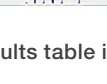

Checked	Structure	Name	CAS Num	Formula	Total Score	HRF Score	RHRF Score	SI	RFI	Elements Found [%]	Molecular Weight	Theo. Mol. Mass	Observed Mol. Mass	ΔMass [Da]	ΔMass [ppm]	M+ In Lib	M+ found	Selected	Library	Library Hit key	Library ID Number
<input checked="" type="checkbox"/>		Glutinol	545-24-4	C30 H50	95.4	99.3	99.9	783	803	100.0	426.38617	426.38562				Yes	No	True	mainlib	mainlib267653	267653
<input checked="" type="checkbox"/>		(3S,6R,8aR,12bS,14aR)-4,4,6b,8a,11		C32 H52	95.0	99.3	99.9	763	828	100.0	468.39673	468.39618				Yes	No	False	mainlib	mainlib267347	267347
<input checked="" type="checkbox"/>		1-Naphthalenopropanol, α-ethyldec	72360-94	C20 H36	93.6	97.7	99.9	727	765	100.0	292.27662	292.27607				Yes	No	False	mainlib	mainlib153426	153426
<input checked="" type="checkbox"/>		Lup-20(29)-en-3-one	1617-70-	C30 H48	93.0	99.3	99.4	663	667	100.0	424.37052	424.36997	424.37006	0.00009	0.21	Yes	Yes	False	mainlib	mainlib106262	106262

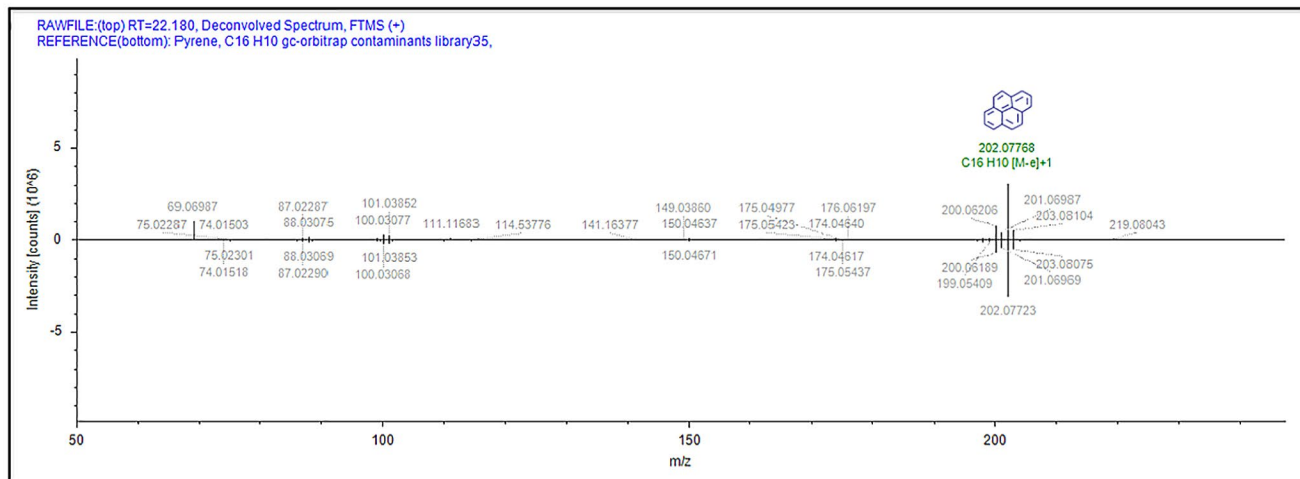
Figure 5. Results table in Compound Discoverer software showing a list of detected compounds with information on identification criteria

Checked	Name	Calc. MW	RT [min]	Reference m/z	Avg TIC	NIST Lib Hit Formula	NIST Theo. Mol. Mass	NIST Observed Mol. Mass	# Usable QC	RSD QC Areas [%]	RSD Corr. QC Areas [%]	Total Score	HRF Score	SI	RSI	Group Areas
<input checked="" type="checkbox"/>	Pyrene	202.07823	22.180	200.06206	3131930	C16 H10	202.07770	202.07768	8	10	3	95.6	94.2	897	932	68.165 9.965 2.4566

A

Checked	Structure	Name	CAS Num	Formula	Total Score	HRF Score	RHRF Score	SI	RSI	Elements Found[%]	Molecular Weight	Theo. Mol. Mass	Observed Mol. Mass	ΔMass [Da]	ΔMass [ppm]	M+ In Lib	M+ Found	Selected	Library	Library Hit key	Library ID Number
<input checked="" type="checkbox"/>		Pyrene	129-00-0	C16 H10	95.6	94.2	95.1	897	932	1000	202.07825	202.07770	202.07768	-0.00002	-0.10	Yes	Yes	True	gc-orbitrap contaminants library	gc-orbitrap contaminants library35	35

B



C

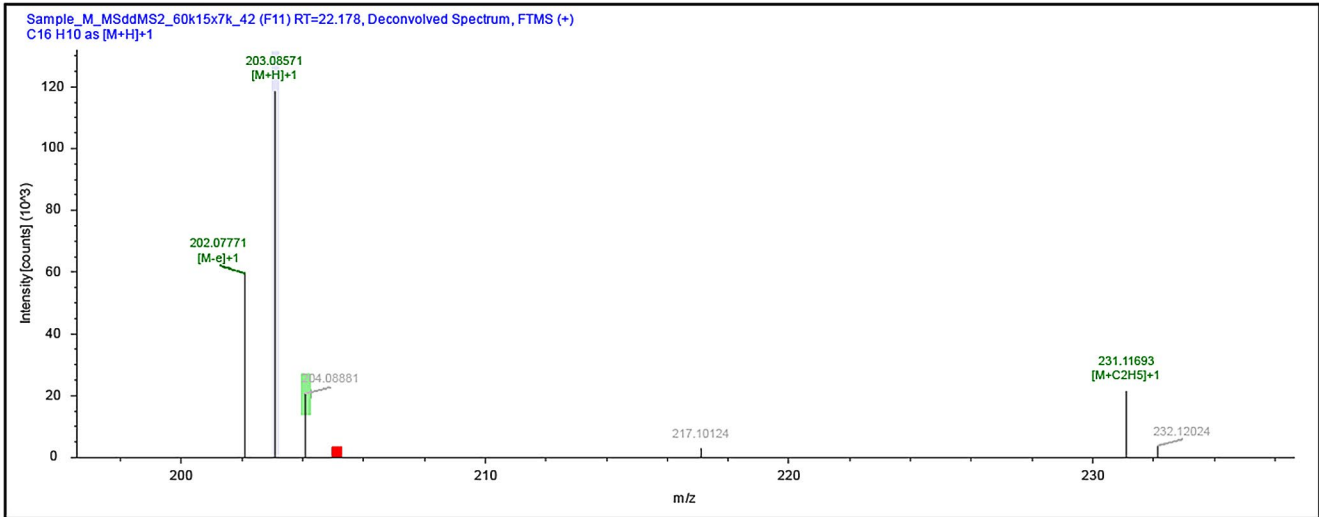
Figure 6a. Identification of the peak at 22.18 minutes as pyrene. Table data (A) showing search index (SI) at 897 and reverse SI (932). The compound molecular mass was detected with excellent mass accuracy of 0.1 ppm (B). The spectrum mirror plot (C) comparison to the library is displayed in Compound Discoverer software to support the proposed identification.

#	Checked	Tags	Name	Formula	Annot. Source	ΔMass [ppm]	Calc. MW	RT [min]	# ChemSpider Results	# mzCloud Results	mzCloud Best Match	mzCloud Best Sim. Match	Reference m/z	Arg TIC	Mass List Matches	# Adducts	MS2	MS Depth	Group Areas
1	<input checked="" type="checkbox"/>		Pyrene	C16 H10		0.00	202.07843	22.178	13	11	633	83.8	202.07771	74966		3		2	43.54 1.454


D

#	Tags	Checked	Compound Match	Formula	Molecular Weight	ΔMass [Da]	ΔMass [ppm]	RDSE	H/C	Rank	# Matched Iso.	# Missed Iso.	# Matched Frag.	SFit [%]	Pattern Cov. [%]	MS Cov. [%]	MSMS Cov. [%]
1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	C16 H10	202.07825	-0.00005	-0.23	12.0	0.6	1	3	0	3	74	100.00	100.00	88.58
2	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	C8 H11 F5	202.07809	0.00011	0.55	1.0	1.4	2	2	0	3	60	99.70	98.34	88.58
3	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	C8 H14 N2 O2 S	202.07760	0.00060	2.99	3.0	1.8	3	2	1	3	34	95.23	98.34	88.58
4	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	C8 H16 N2 P2	202.07887	-0.00067	-3.31	3.0	2.0	4	2	0	1	60	99.03	98.34	10.20


E



F

#	Tags	Checked	Compound Match	Structure	Name	Formula	Molecular Weight	ΔMass [Da]	ΔMass [ppm]	Match	Best Match	Best Sim. Match	Type	mzCloud ID
1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>		Pyrene	C16 H10	202.07825	-0.00005	-0.23	69.1	69.1	68.6	Identity	Reference:3062

G

#	Checked	Tags	Compound Match	Structure	Name	Formula	Molecular Weight	ΔMass [Da]	ΔMass [ppm]	CSID	# References
1	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>		Pyrene	C16 H10	202.07825	-0.00005	-0.23	29153	3214

H

#	Tags	Checked	Compound Match	Name	Formula	Molecular Weight	ΔMass [Da]	ΔMass [ppm]	Reference List Name	CAS
1	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Fluoranthene	C16 H10	202.07825	-0.00005	-0.23	GC Orbitrap Contaminants	206-44-0
2	<input type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	Pyrene	C16 H10	202.07825	-0.00005	-0.23	GC Orbitrap Contaminants	129-00-0

I

Figure 6b. Identification and confirmation of pyrene through positive chemical ionization (PCI) section (D). Elemental composition proposal for molecular ion 0.23 ppm mass accuracy (E) with annotated spectrum (F). Library search results for the elemental composition proposed in mzCloud (G) and Chemspider (H). Mass List (I). All results combine to provide high confidence in compound identification.

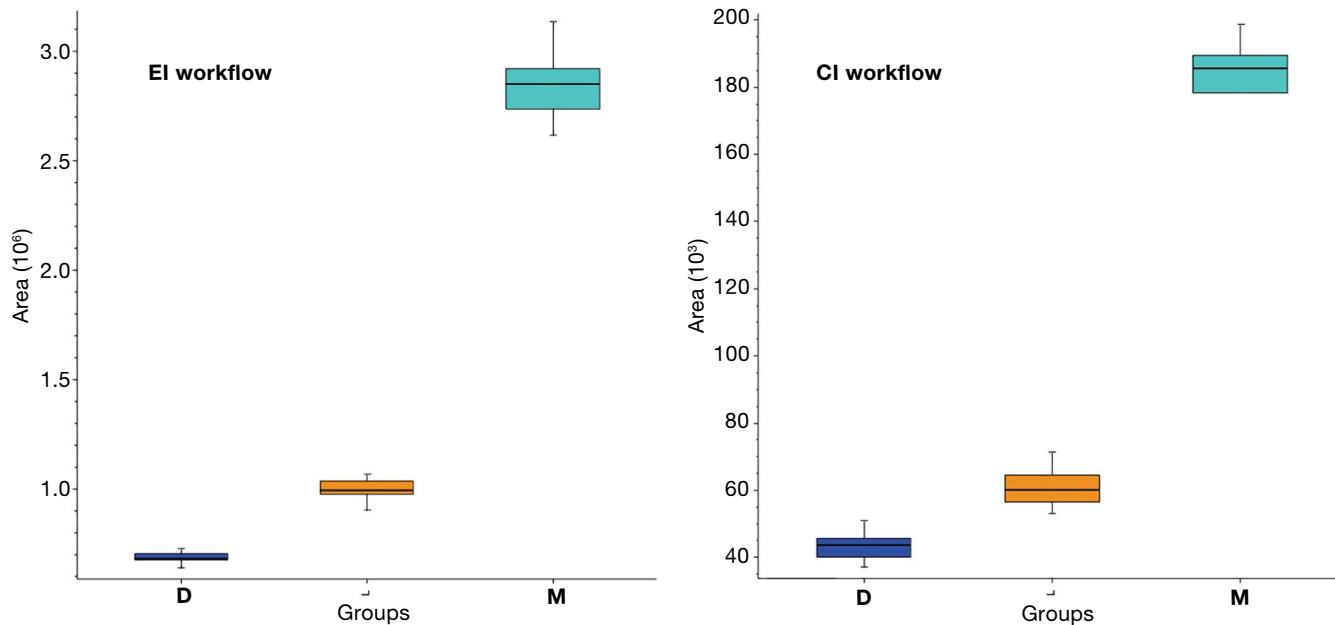


Figure 7. Box plot view from Compound Discoverer software showing how pyrene peak area varies across the three soil samples. The response was significantly higher in sample M.

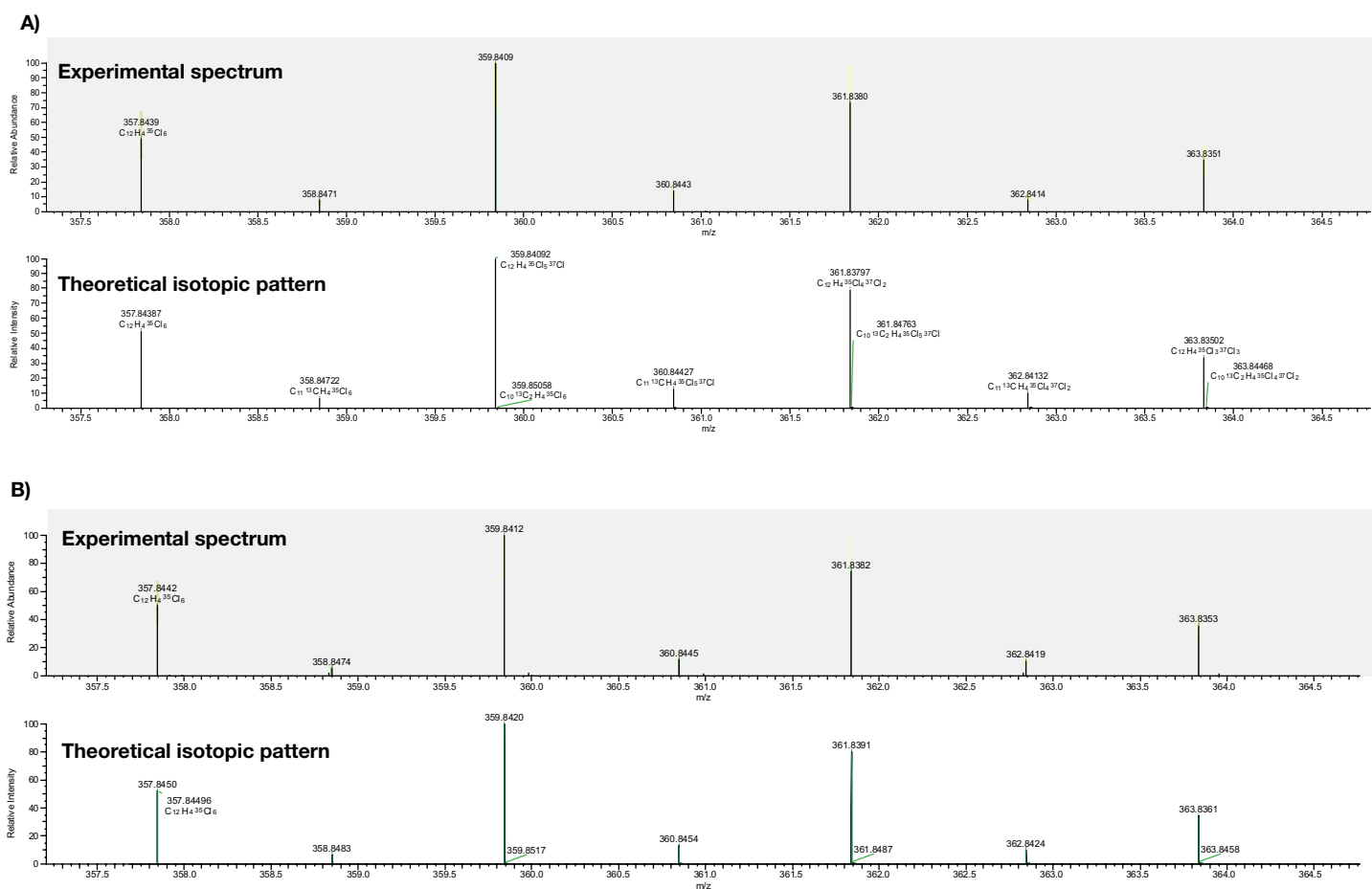


Figure 8. Comparison between experimental and theoretical isotopic pattern for C₁₂H₄Cl₆ in EI (A) and in NCI (B)

Conclusion

The Orbitrap Exploris GC 240 mass spectrometer in combination with Compound Discoverer software is an excellent tool for environmental sample analysis. Even in such a complex matrix as soil, the software detected and identified untargeted contaminants. The identification in EI was confirmed in CI. Moreover, the statistical analysis and graphical visualization tools facilitated the results interpretation. Differential analysis (Volcano Plot) was useful in the global comparison between two selected

samples, whereas Whisker Charts allowed presentation of a particular compound peak area across all samples. The high quality data obtained from the Orbitrap Exploris GC 240 mass spectrometer enabled the sensitive detection and confident identification of compounds in this study.

Reference

1. Thermo Fisher Scientific Technical Note 10730: Mass resolving power of 240,000: for confident compound identification, 2021. <https://assets.thermofisher.com/TFS-Assets/CMD/Technical-Notes/tn-10730-gc-ms-power-confident-compound-identification-tn10730-en.pdf>

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