

RESEARCH ARTICLE

Spatial Toxicant–Modality Concordance for Environmental Mass Spectrometry Imaging: A Class-Resolved Instrument-Selection Method for Pollutant Mapping

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Abstract

Environmental toxicology requires spatially resolved chemical evidence because contaminants are retained, transformed and expressed unevenly across tissues, roots, biofilms, sediment interfaces and particle-contact zones. Mass spectrometry imaging (MSI) can provide this evidence only when the ionization modality matches the contaminant class, the spatial scale of interest and the chemical claim being made. This study defines Spatial Toxicant–Modality Concordance (STMC), a class-resolved analytical method for selecting primary and confirmatory MSI platforms for organic, inorganic and particulate pollutants. The calculation uses five instrument routes–MALDI, LDI, SIMS, DESI and LA-ICP-MS–and nine pollutant subclasses: pharmaceutically active compounds, plastic additives, industrial chemicals, personal care products, pesticides, heavy metals, micro- and nanoplastics, particulate matter and engineered nanoparticles. Five modality attributes are scored: spatial granularity, molecular compatibility, quantitative confidence, operational simplicity and contaminant-class concordance. The resulting class scores identify a clear modality switch: MALDI ranks first for organic pollutants at 0.80, LA-ICP-MS ranks first for heavy metals at 0.83, and SIMS ranks first for particulate pollutants at 0.86. LDI provides a matrix-free route for selected surface and low-mass organic questions, whereas DESI is best used for rapid ambient screening. STMC strengthens environmental analytical chemistry by tying pollutant images to the specific molecular, elemental or fragment evidence that each platform can support.

Keywords: analytical chemistry; environmental toxicology; mass spectrometry imaging; MSI instrumentation; MALDI; SIMS; LA-ICP-MS; pollutant localization; microplastics; trace metals

1. Introduction

Environmental contamination is a spatial chemical problem before it becomes a bulk toxicological measurement. Pesticides, pharmaceutical residues, plastic additives, industrial chemicals, personal care compounds, heavy metals, engineered nanoparticles, combustion particles and weathered microplastics enter organisms and environmental matrices through water, soil, air and food-chain transfer. Their distributions are rarely homogeneous. A pesticide may accumulate in a plant cuticle or vascular channel, a pharmaceutical residue may concentrate in a gill or hepatic compartment, a metal ion may bind to mineralized or protein-rich structures, and a particle may remain at an epithelial, biofilm or sediment interface. A bulk concentration value can there-

fore underestimate local exposure where toxic injury begins, while a tissue-averaged response marker can hide microdomains that carry the strongest chemical burden.

Mass spectrometry imaging (MSI) addresses this limitation by preserving spatial coordinates while collecting molecular, elemental or fragment information from a sample surface. Early MALDI-MSI work showed that mass spectra could be transformed into localization maps for biological molecules, and later reviews established MSI as a label-free approach for visualizing molecular distributions in tissues and other structured samples [1–3]. The same principle is now central to environmental toxicology because contaminant exposure and endogenous biochemical disturbance often occur within the same heterogeneous matrix. Spatial MSI can therefore move environmental

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analysis beyond compound presence and toward the more demanding question of where the contaminant resides, which compartment carries the highest burden and whether local chemistry is accompanied by a plausible biological response.

Recent MSI applications cover xenobiotic mapping, plant and microbial systems, food matrices, spatial toxicology and microplastic localization [4–8]. These applications show that MSI is not one instrument class with one evidentiary meaning. MALDI, LDI, SIMS, DESI and LA-ICP-MS differ in ion generation, sample preparation, spatial resolution, analyte coverage, fragmentation behaviour and quantitative potential. A visually convincing ion image can therefore mislead when the selected platform cannot support the chemical claim attached to that image. Strong environmental MSI requires modality selection before acquisition, not interpretive repair after maps have already been produced.

Different contaminant classes impose different analytical requirements. Organic pollutants such as pesticides, plastic additives, pharmaceuticals and industrial compounds require molecular specificity, metabolite or transformation-product awareness, and often simultaneous interpretation of endogenous lipids, metabolites or peptides. Inorganic toxicants require elemental specificity, isotope discrimination and a defensible route to concentration-related inference. Particulate pollutants require surface sensitivity, fine spatial granularity and material-specific evidence because microplastics, nanoparticles and particulate matter may affect tissues through contact zones rather than through uniformly dissolved chemistry. These requirements cannot be satisfied by one universal modality. DESI, SIMS and LA-ICP-MS illustrate this divergence clearly: ambient desorption supports rapid surface screening, secondary-ion methods support high-resolution surface and fragment evidence, and laser-ablation plasma methods support elemental imaging and quantification [9–12]. A platform suited to intact organic molecules may not quantify metals, while a platform optimized for elemental imaging cannot identify intact organic transformation products. Sample preparation and reporting further complicate platform selection. Matrix deposition, washing, drying, laser fluence, ablation geometry, solvent composition, step size, spot size, normalization and registration all influence the interpretability of MSI outputs [13–15]. Environmental samples add further variability because tissues, plant organs, sediment particles, mineral surfaces, polymer debris and biofilms differ strongly in morphology and ionization behaviour. A method-selection procedure is therefore needed to connect contaminant chemistry, sample form, spatial scale and validation requirements before images are interpreted.

This paper defines Spatial Toxicant–Modality Concordance (STMC) as a class-resolved instrument-selection method for environmental MSI. The research question is specific: can class-weighted modality selection identify the primary and confirmatory MSI route for organic, inorganic and particulate pollutants while preserving the evidentiary boundaries of each instrument class? The analysis uses an instrument table and a pollutant-share table prepared for this manuscript: five MSI routes are compared against nine contaminant subclasses grouped as 51% organic, 27% inorganic and 22% particulate. STMC does not rank one platform as universally superior. Instead, it identifies which modality is defensible for a defined pollutant class and which additional modality is required when spatial localization, chemical identity, quantification and endogenous-response interpretation must be combined.

The analytical sequence in Figure 1 begins with organic, inorganic and particulate contaminant chemistry, applies spatial, molecular, quantitative, operational and concordance attributes, and returns a class-specific instrument route that separates first-line imaging from confirmatory evidence.

The selection chain establishes the paper's analytical boundary. STMC is not a toxicity endpoint model and not an image-classification exercise; it is a measurement-planning method. Its value lies in preventing



A Pollutant classes



B STMC scoring attributes



C MSI modalities

Figure 1: STMC selection chain.

mismatch between contaminant chemistry and measurement chemistry. The organic branch emphasizes molecular and response information, the inorganic branch emphasizes elemental confidence, and the particulate branch emphasizes fine surface localization. This separation is essential because the same visual form of a heat map may represent very different evidence depending on the ionization route.

The modality landscape in Figure 2 shows the practical diversity of the five platforms included in the scoring procedure. The instrument views separate ambient sampling, laser desorption, vacuum surface analysis and elemental ablation, making clear that a spatial image is the end product of distinct physical and chemical processes.

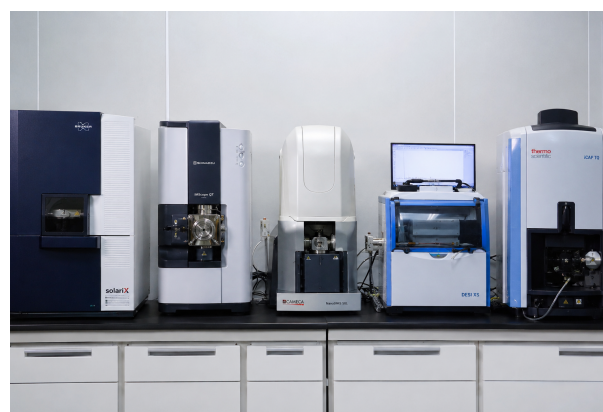


Figure 2: MSI modality landscape.

The instrument comparison supports the need for a class-sensitive method. MALDI and LDI are closer to molecular mapping, SIMS is closer to surface and fragment evidence, DESI is closer to rapid ambient screening, and LA-ICP-MS is closer to elemental quantification. These distinctions justify treating modality choice as an analytical-design decision rather than as a matter of laboratory convenience.

2. Materials and Methods

2.1. Modality table and pollutant classes

The analytical input contains two linked tables prepared for the STMC calculation. The instrument table records MALDI, LDI, SIMS, DESI and LA-ICP-MS with ionization route, representative spatial value, chemical coverage, analytical strengths and limiting conditions. The pollutant table records nine environmental contaminant subclasses: pharmaceutically active compounds, plastic additives, industrial chemicals, personal care products, pesticides, heavy metals, micro- and nanoplastics, particulate matter and engineered nanoparticles. These entries are used as measurement-selection variables rather than exposure measurements, because the objective is to evaluate instrument suitability rather than ecological burden [7].

The nine subclasses were consolidated into three pollutant groups. Organic pollutants include pharmaceutically active compounds, plastic additives, industrial chemicals, personal care products and pesticides. Inorganic pollutants are represented by heavy metals because elemental specificity and quantitative confidence dominate this class. Particulate pollutants include micro- and nanoplastics, particulate matter and engineered nanoparticles because spatial contact, material evidence and surface localization dominate their analytical interpretation. The grouping produces a distribution of 51% organic pollutants, 27% inorganic pollutants and 22% particulate pollutants.

The material basis for the pollutant grouping is illustrated in Figure 3. The visual set clarifies that the three classes are not merely statistical categories: they correspond to different sample forms, preparation requirements and ionization constraints.

The material panels show why one sample-preparation route cannot serve all contaminant classes. Organic extracts and tissue-associated xenobiotics require control of matrix effects and ion suppression, metal and mineral targets require elemental calibration and isotope-aware interpretation, and particulate samples require surface preservation and registration of small deposits. This class separation supports the decision to score modalities by contaminant chemistry instead of assigning a single global MSI rank.

2.2. Class-weighted scoring

Each modality was evaluated by five method-selection attributes. Spatial granularity represented the practical ability to resolve fine pollutant domains, tissue boundaries or particle-contact regions. Molecular compatibility represented the capacity to preserve intact or diagnostically useful molecular information. Quantitative confidence represented the strength of elemental, isotopic or concentration-related inference. Operational simplicity represented the relative preparation burden and matrix dependency. Contaminant-class concordance represented the direct match between the platform and the dominant chemistry of the pollutant class.

The attributes were assigned on a zero-to-one scale from the instrument table. This scale is a comparative device, not a permanent property of any instrument vendor, ionization hardware or mass analyser. Class-specific weights were then applied because each pollutant group requires a different evidence hierarchy. Organic pollutants place the greatest demand on molecular compatibility and class concordance. Inorganic pollutants place the greatest demand on quantitative confidence and class concordance. Particulate pollutants place the greatest demand on spatial granularity and class concordance because the decisive evidence often lies at a small interface or surface deposit. The weighting values are listed in Table 1.

The weighting matrix makes the calculation interpretable before the scores are obtained. Organic pollutants receive a molecular bias, inorganic pollutants receive an elemental-quantitative bias and particulate pollutants receive a spatial-surface bias. The common 0.30 concor-

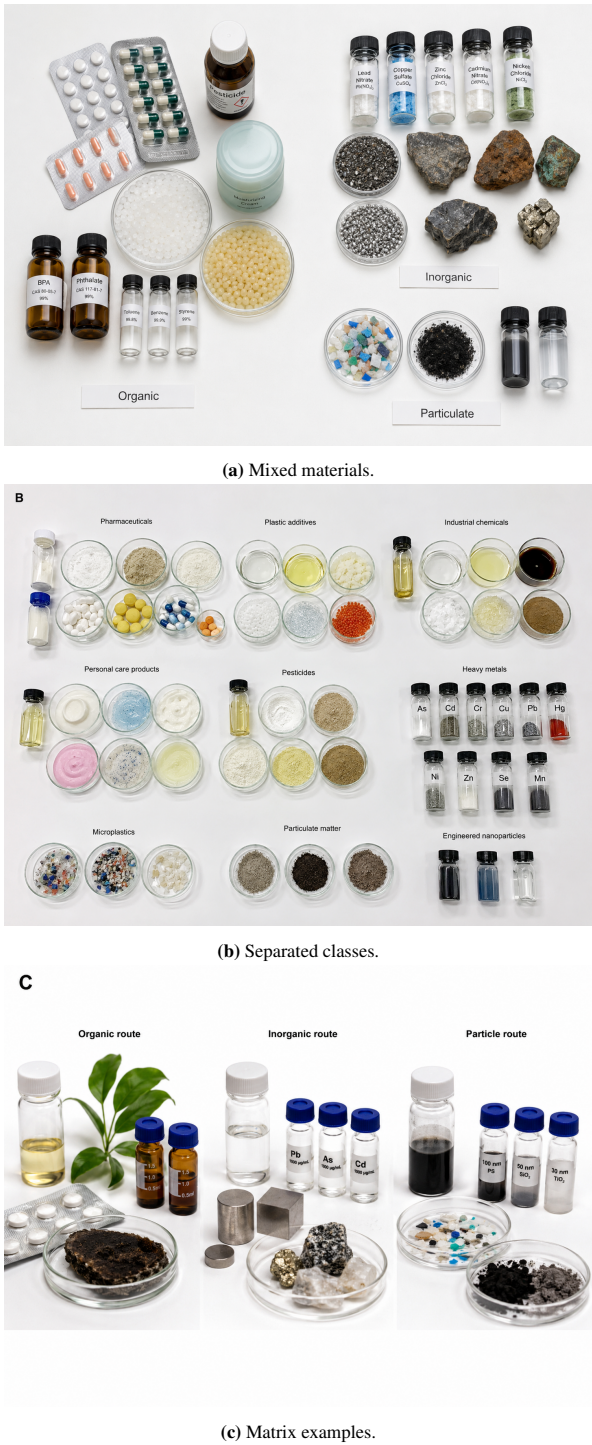


Figure 3: Material classes.

Table 1: Class-specific STMC weights.

Pollutant class	Spatial	Molecular	Quantitative	Simplicity	Concordance
Organic pollutants	0.20	0.30	0.10	0.10	0.30
Inorganic pollutants	0.25	0.10	0.30	0.05	0.30
Particulate pollutants	0.35	0.10	0.20	0.05	0.30

dance term ensures that a modality is not rewarded only for technical performance; it must also match the chemistry of the target class. This choice is important for environmental analytical chemistry because high resolution or high sensitivity alone does not make a platform appropriate for every contaminant.

2.3. Pollutant shares and map agreement

The pollutant shares were retained as percentages so that the final interpretation reflected the relative prominence of the nine subclasses. The pollutant groups are shown visually in Figure 4. This separation is placed before the scoring results because organic, inorganic and particulate pollutants make different demands on MSI evidence.

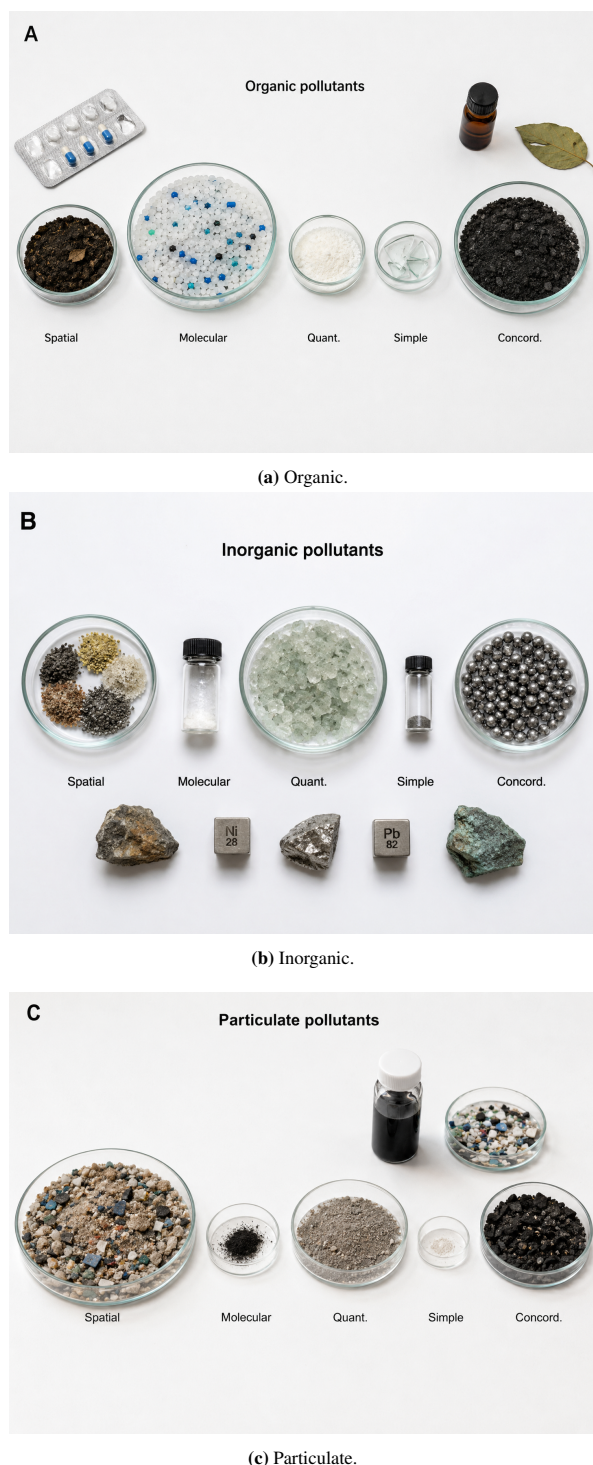


Figure 4: Pollutant classes.

The class view defines the analytical burden of the study. Organic subclasses dominate numerically, but the inorganic and particulate groups carry high evidentiary demands because metal quantification and particle localization cannot be inferred from organic molecular

images. STMC therefore treats the 51% organic share as a strong driver of molecular-imaging need without allowing it to erase the 27% elemental and 22% particulate requirements.

For paired pollutant and endogenous-response images, STMC applies a map-agreement rule. The pollutant-associated ion map and response-marker map are normalized within a common sample mask, registered to the same region and interpreted according to whether high-intensity pollutant domains coincide with high-intensity response domains. Positive spatial agreement identifies candidate microdomains for confirmatory tandem MS, accurate-mass review, isotope-pattern checking, standards, histology or orthogonal chromatography. Spatial separation is not treated as a failed result; it may indicate detoxification, compartmentalization, delayed response, sample-preparation bias or an inappropriate response marker. The rule is therefore a prioritization step, not proof of causality.

3. Results and Discussion

3.1. Instrument-performance matrix and measurement meaning

The modality attributes are summarized in Table 2. The table is the analytical core of STMC because it shows that the five modalities occupy different evidence regimes. MALDI provides broad tissue-scale molecular coverage and is therefore suited to organic toxicants and endogenous-response chemistry. LDI offers a matrix-free laser-desorption route that is useful when low-mass interferences or surface-active compounds are central. SIMS provides the finest spatial value and strong surface sensitivity, making it especially relevant to particles, interfaces and fragment-based material evidence. DESI provides an ambient and operationally simple screening route, but its coarser spatial resolution limits claims at fine tissue or particle boundaries. LA-ICP-MS provides the strongest elemental and isotopic pathway, particularly for heavy metals and metal-containing particles, but it does not preserve intact organic molecular information.

The matrix demonstrates that modality choice must be tied to the claim being made. MALDI and LDI are defensible when the question concerns organic localization or response chemistry; SIMS is defensible when spatial precision and surface evidence dominate; DESI is defensible when rapid ambient screening is more important than fine spatial detail; and LA-ICP-MS is defensible when elemental concentration and isotope-supported interpretation are required. This interpretation also explains why multimodal acquisition is often necessary: no single row in the table provides molecular coverage, elemental quantification and particle-interface localization at the same time.

The readout context in Figure 5 links physical sample presentation with spectra and spatial visualization. It shows the visible result of the instrument chain, but STMC interprets that output through instrument attributes rather than through image appearance alone.

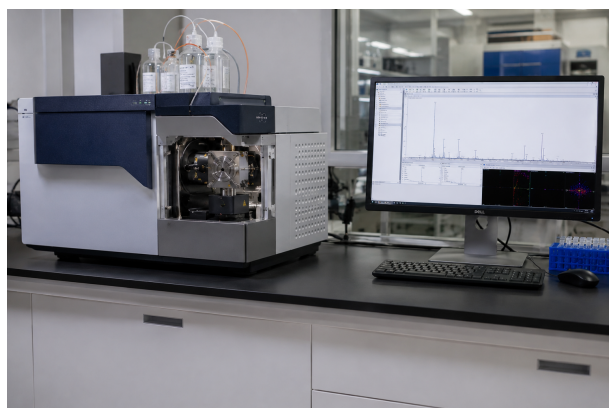
The readout view emphasizes that a map becomes analytically meaningful only when the chemical basis of the signal is identified. A bright region in a MALDI image, a SIMS fragment map and an LA-ICP-MS elemental map may all appear as similar intensity distributions, but their chemical defensibility is not equivalent. This is why STMC uses modality attributes before interpreting pollutant maps.

The primary workstation contexts are separated in Figure 6. The panels distinguish soft molecular imaging, laser-desorption analysis and surface-focused acquisition.

The workstation grouping clarifies the measurement consequence of the score matrix. MALDI should be planned with matrix selection, crystal uniformity and ion-suppression control in mind. LDI should be planned around laser fluence, surface energy and fragmentation risk. SIMS should be planned around field size, vacuum compatibility, ion-beam effects and fragment interpretation. These practical differences are not secondary details; they determine whether an environmental

Table 2: MSI modality attribute matrix.

Modality	Ionization mode	Spatial value	Coverage	Main limitation
MALDI	Laser-assisted soft ionization	20–50 μm	Metabolites, peptides, oligosaccharides, lipids, polymers and several pollutant classes	Matrix selection and crystal deposition affect repeatability; quantitative imaging is difficult
LDI	Laser desorption without added matrix	20 μm	Metabolites, oligosaccharides, lipids, organic pollutants and selected trace-metal-related signals	Neutral compounds and large biomacromolecules are difficult; photofragmentation may occur
SIMS	Ion-beam hard ionization	0.1 μm	Elements, trace metals and fragments of small molecules or polymeric materials	Strong fragmentation, chemical noise, small field area and non-ambient operation
DESI	Ambient electrospray-derived desorption	100 μm	Polar metabolites, lipids and organic pollutants	Lower spatial resolution and sensitivity; weaker for non-polar and high-mass molecules
LA-ICP-MS	Laser ablation with atomizing plasma	30 μm	Elements and isotopes, especially trace metals	Requires matrix-matched standards and does not preserve intact molecular information

**Figure 5:** Instrument readout.

MSI map can support a pollutant-specific conclusion.

Complementary modality stations are shown in Figure 7. The station group places molecular, surface and elemental routes beside one another.

The station-level comparison strengthens the case for registered evidence layers. Organic toxicant maps, particle-interface maps and elemental maps can be brought into a common interpretation, but they should not be collapsed into one evidentiary category. A spatial toxicology conclusion is strongest when each modality contributes the type of evidence it is suited to provide.

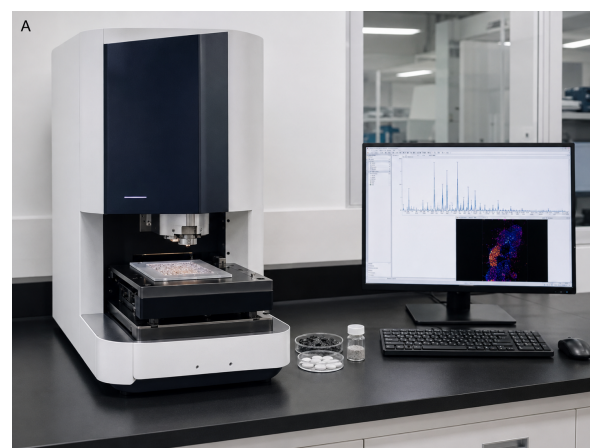
3.2. Pollutant distribution and method-selection pressure

The pollutant distribution is listed in Table 3. Organic subclasses form the largest share of the analytical set, with pesticides as the largest single subclass at 17%. This distribution favours molecular MSI because organic toxicants and transformation products require chemical specificity beyond elemental presence. Heavy metals form a large separate share at 27%, which prevents the study from treating elemental imaging as a minor add-on. Particulate pollutants form a 22% aggregate share but impose strong spatial and material constraints because their toxicity may depend on contact, surface chemistry and local retention.

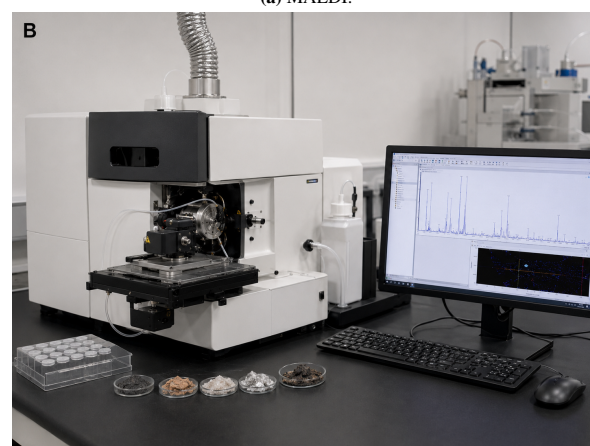
The pollutant-share table shows that analytical importance is not determined only by percentage. Organic contaminants dominate the number of subclasses, but a 27% heavy-metal share can determine whether LA-ICP-MS is required, and a 22% particulate share can determine whether SIMS must be included. The result is a three-pressure measurement problem: molecular identification, elemental confidence and particle-interface localization all remain necessary even when one class is numerically larger than the others.

3.3. Class-specific STMC outcomes

The class-specific scores are presented in Table 4. MALDI produced the highest score for organic pollutants, with a value of 0.80. This



(a) MALDI.

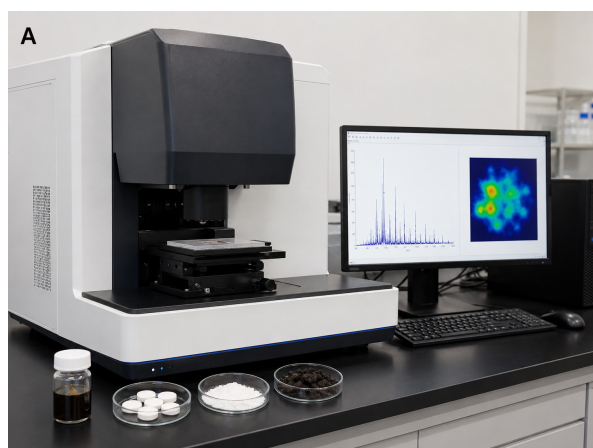


(b) LDI.

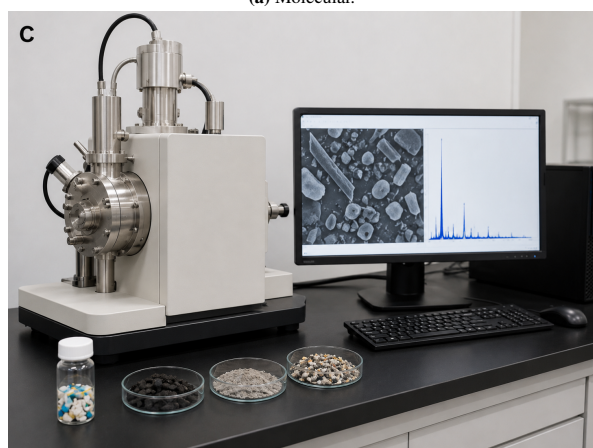


(c) SIMS.

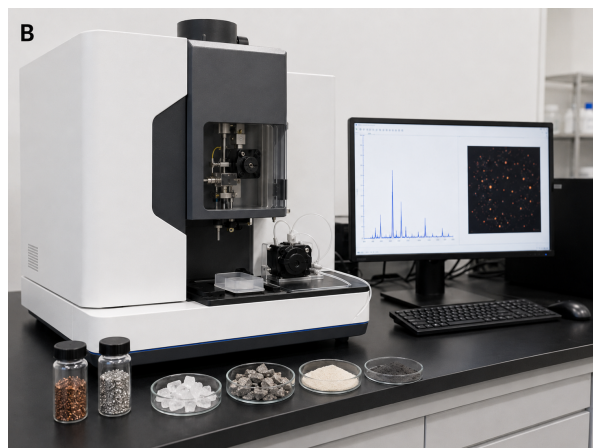
Figure 6: Primary workstations.



(a) Molecular.



(b) Surface.



(c) Elemental.

Figure 7: Complementary stations.

result follows from its molecular breadth, tissue-scale spatial utility and compatibility with endogenous response mapping. LDI followed at 0.71, indicating that matrix-free acquisition is valuable when low-mass background, surface chemistry or matrix interference is a concern. DESI scored 0.55 for organic pollutants, which supports its use as a fast ambient screen but not as a universal replacement for higher-resolution molecular MSI. SIMS and LA-ICP-MS are not primary organic-pollutant routes, although SIMS can be valuable when organic residues are bound to particles or surfaces.

For inorganic pollutants, LA-ICP-MS achieved the highest score, 0.83. This outcome is analytically expected because heavy-metal studies require elemental specificity, isotope-aware interpretation and stronger

Table 3: Pollutant shares for STMC.

Broad class	Subclass	Share (%)
Organic	Pharmaceutically active compounds	8
Organic	Plastic additives	10
Organic	Industrial chemicals	13
Organic	Personal care products	3
Organic	Pesticides	17
Inorganic	Heavy metals	27
Particulate	Micro- and nanoplastics	5
Particulate	Particulate matter	5
Particulate	Engineered nanoparticles	12

concentration-related confidence than soft-ionization MSI can usually provide. SIMS followed at 0.78 because of its fine spatial granularity and surface-sensitive elemental information. MALDI and LDI remained secondary for inorganic pollutants because their main strength is molecular imaging, not elemental quantification. DESI scored poorly for inorganic pollutants because elemental mapping is outside its central analytical role.

For particulate pollutants, SIMS produced the strongest score, 0.86. The result is driven by its fine spatial scale, surface sensitivity and fragment-level material evidence. LA-ICP-MS ranked second, 0.74, because it is important for metal-containing nanoparticles and elemental particulate matter. LDI showed intermediate utility, 0.64, particularly where carbon-rich surfaces or matrix-free laser desorption are relevant. MALDI and DESI were weaker as primary particulate methods, although MALDI remains useful for evaluating whether particle-rich regions are associated with nearby lipid or metabolite changes.

Table 4: Class-specific STMC scores.

Modality	Organic	Inorganic	Particulate	Aggregate score
MALDI	0.80	0.46	0.52	0.65
LDI	0.71	0.55	0.64	0.65
SIMS	0.52	0.78	0.86	0.66
DESI	0.55	0.23	0.23	0.39
LA-ICP-MS	0.40	0.83	0.74	0.59

The score table answers the research question in quantitative form. STMC does not identify a universal winner. Instead, it identifies a modality switch across pollutant classes: MALDI leads organic mapping, LA-ICP-MS leads inorganic mapping and SIMS leads particulate mapping. The narrow whole-set range among SIMS, MALDI and LDI is also meaningful. Similar aggregate values arise from different strengths, so the final selection must follow the contaminant class and the intended analytical claim rather than the overall score alone.

The quantitative-readout context is shown in Figure 8. Its placement after the score table reinforces that quantitative claims must be tied to the modality with suitable chemical evidence.

The readout image links the numerical rankings to practical reporting. Heavy-metal maps require standards, calibration strategy and isotope-aware interpretation; organic maps require annotation confidence and, where possible, tandem MS or accurate-mass support; particulate maps require evidence that the imaged signal corresponds to a material fragment or elemental component. The visual emphasis on readout therefore strengthens the central argument that map appearance alone is insufficient.

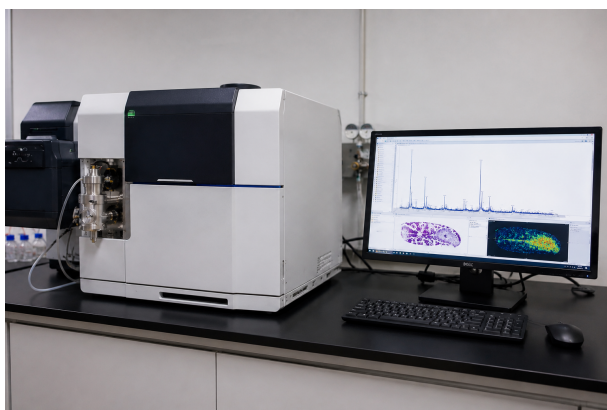


Figure 8: Quantitative anchor.

3.4. Class route interpretation and measurement planning

The aggregate scores place SIMS, MALDI and LDI in a narrow overall band, with SIMS at 0.66 and MALDI and LDI at 0.65. This result should not be interpreted as equivalence. SIMS reaches its score through particulate and inorganic strength; MALDI reaches its score through organic molecular imaging; and LDI reaches its score through matrix-free utility across selected organic and surface contexts. LA-ICP-MS scores lower overall, 0.59, because it is specialized for elemental evidence, not because it is weak for the class it is designed to address. DESI scores 0.39, confirming that it is better treated as a screening or triage modality than as a complete environmental MSI solution.

These results support a tiered measurement route. Organic-dominant studies should begin with MALDI when the objective is xenobiotic localization, transformation-product mapping or endogenous biochemical response. LDI should be added when MALDI matrix peaks, low-mass interference or surface carbon chemistry create interpretive risk. DESI can be used for preliminary screening of polar compounds or fragile surfaces, but positive regions should be confirmed by higher-resolution or more chemically specific modalities before microdomain conclusions are made.

Metal-dominant studies should use LA-ICP-MS as the quantitative anchor. SIMS should be added when finer interface information or surface-localized elemental evidence is required. MALDI or LDI should be applied to adjacent or serial sections only when the aim is to connect metal accumulation with lipids, metabolites or peptides. This arrangement separates elemental certainty from biochemical interpretation while retaining the possibility of spatial registration.

Particulate studies should begin with SIMS when particle identity, polymer fragments, small deposits or surface interfaces are central. LA-ICP-MS should be included when particles contain metals or when elemental co-localization may distinguish engineered nanoparticles, mineral particles or metal-bearing particulate matter. MALDI should serve as a response-mapping layer rather than as the primary detector of particles. The resulting route treats particle localization, material confirmation and biological response as complementary evidence streams.

The tiered route is summarized in Figure 9. The visual route separates organic, metal and particle questions before image interpretation begins.

The route diagram converts the scores into measurement decisions. Its main implication is that the leading modality changes with the contaminant class, and the confirmatory modality changes with the evidentiary requirement. A study can therefore justify why a molecular platform, elemental platform or surface-sensitive platform was selected rather than merely naming the available instrument.

Route-specific readouts are shown in Figure 10. The three panels

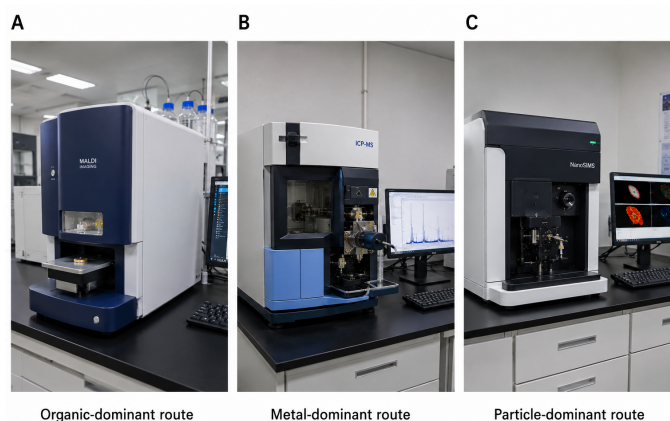


Figure 9: Class-specific routes.

translate the measurement route into spatial outputs for organic, metal and particulate contexts.

The route maps show how STMC protects interpretation from overextension. A MALDI organic map can support organic localization and response chemistry but cannot be used as evidence of metal burden. An LA-ICP-MS metal map can support elemental localization and concentration-related interpretation but cannot identify intact organic pathways. A SIMS particle map can identify surface fragments or localized deposits, but intact molecular mechanisms require additional evidence. The method therefore assigns a defined role to each image rather than treating all spatial readouts as equivalent.

3.5. Implications for analytical reporting

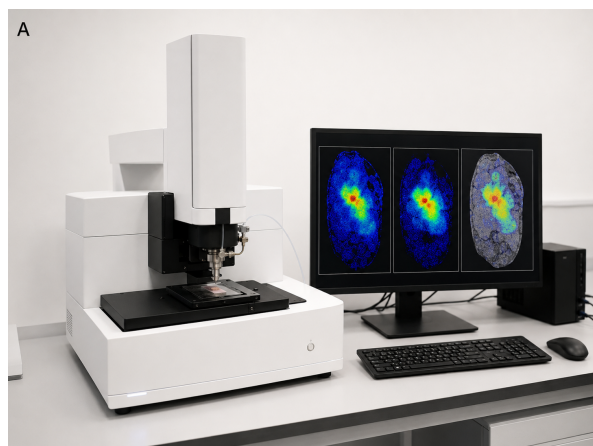
The reporting consequence of STMC is straightforward: environmental MSI manuscripts should justify modality selection before presenting pollutant maps. A complete report should state the pollutant class, expected spatial scale, sample form, ionization route, validation strategy, quantitative ambition, map-normalization procedure, spatial-registration procedure and criteria for ion assignment. This expectation is consistent with broader MSI reporting guidance and data-standardization work, including the need to document acquisition geometry, spot size, step size, sample preparation and image-processing decisions [14, 15].

The final evidence view is shown in Figure 11. The two panels connect spectral evidence with registered spatial output.

The evidence panels identify the minimum interpretive chain expected from an STMC-guided study. A pollutant map should be accompanied by a stated modality rationale, a spectral or elemental basis for the signal, a validation route appropriate to the class and a registration statement when endogenous-response maps are compared. This structure helps distinguish a spatially persuasive visualization from a chemically defensible conclusion.

3.6. Limitations and appropriate use

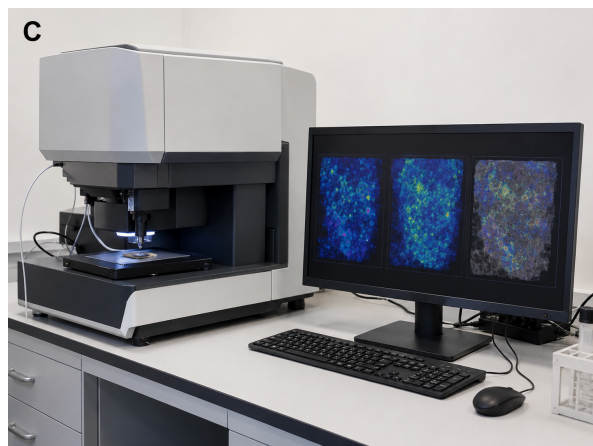
STMC is a rule-based method and should be adjusted when laboratory-specific performance values are measured. Instrument configuration, mass analyser type, ion optics, desorption geometry, sample preparation, matrix effects, calibration standards, isotope dilution, tandem MS capacity and imaging geometry can change the practical suitability of a modality. The pollutant groups are intentionally broad; a fluorinated surfactant, an organophosphate pesticide, a cadmium ion, a titanium dioxide nanoparticle and an aged polyethylene fragment require different preparation and validation even when grouped under organic, inorganic or particulate labels. STMC also does not replace confirmatory



(a) Organic route.



(b) Metal route.



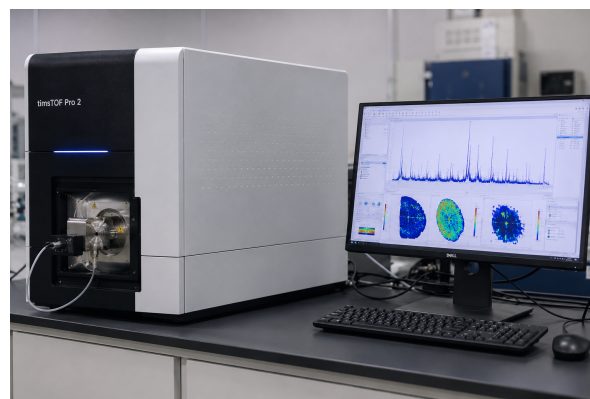
(c) Particle route.

Figure 10: Route-specific readouts.

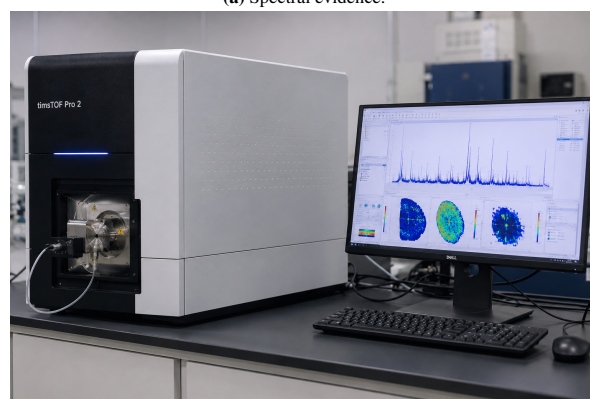
identification by accurate mass, tandem mass spectrometry, isotope patterns, reference standards, orthogonal chromatography, histology or controlled exposure studies. Its appropriate use is measurement planning, modality justification and reporting discipline.

4. Conclusion

The research question asked whether class-weighted modality selection can identify defensible primary and confirmatory MSI routes for organic, inorganic and particulate environmental pollutants while preserving the evidentiary limits of each instrument class. The an-



(a) Spectral evidence.



(b) Registered map.

Figure 11: Evidence outputs.

swer is affirmative. STMC shows that modality suitability changes with contaminant chemistry and with the type of evidence required. MALDI is the strongest first-line route for organic xenobiotics because it combines tissue-scale imaging with broad molecular compatibility and endogenous-response interpretation. LA-ICP-MS is the most defensible route for heavy metals because it provides elemental and isotope-aware evidence with stronger quantitative potential. SIMS is the leading route for particulate pollutants because it offers fine spatial granularity, surface sensitivity and material-fragment information. LDI is best positioned as a matrix-free complement for low-mass and surface-sensitive organic questions, while DESI is best positioned as a rapid ambient screen rather than as a general environmental MSI platform.

The main conclusion is not that one instrument should replace the others, but that environmental MSI should be planned as a class-specific evidence chain. Organic localization, elemental quantification, particle-interface mapping and biochemical-response assessment require different measurement routes and should be presented as registered but distinct evidence layers. The STMC calculation therefore provides a reproducible analytical-instrumentation method for reducing modality mismatch, strengthening spatial toxicant interpretation and making environmental MSI reports more chemically specific. In practical terms, the paper recommends MALDI-led designs for organic-pollutant questions, LA-ICP-MS-led designs for metal questions, SIMS-led designs for particulate questions and multimodal confirmation whenever a manuscript claims both pollutant localization and biological response.

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