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Conceptual Review of Urban Molecular Organic Signatures for Environmental Forensics and Net-Zero Transition in Serpong

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ABSTRACT

Non-industrial satellite cities in Indonesia are commonly assessed using conventional air-quality indicators, while molecular-level evidence of diffuse urban organic pollution remains underexplored. This conceptual review examines polycyclic aromatic hydrocarbons (PAHs), volatile organic compounds (VOCs), and phthalates as potential Urban Molecular Signatures (UMS) for environmental forensic research in Serpong and comparable urban areas. A structured narrative-integrative review was conducted covering molecular fingerprinting, GC-MS analysis, pollutant source attribution, environmental forensics, urban metabolism, and Net Zero Emission (NZE) frameworks. The literature indicates that PAHs, VOCs, and phthalates can reflect combustion, traffic, solvent use, household activities, synthetic materials, and urban consumption patterns. However, the integrated application of GC-MS, molecular fingerprinting, environmental forensics, and NZE interpretation remains limited in Indonesia, particularly in non-industrial satellite cities. This study therefore proposes UMS as a conceptual framework for identifying pollutant source pressures. UMS should complement, rather than replace, emission inventories and mitigation assessments by integrating molecular data with activity patterns, emission factors, mobility, household behavior, and policy analysis. Future studies should validate the framework through systematic sampling, GC-MS analysis, diagnostic ratios, multivariate source apportionment, and local emission-activity data.

Contribution to Sustainable Development Goals (SDGs):

SDG 11: Sustainable Cities and Communities

SDG 15: Life on Land

1. INTRODUCTION

1.1. Research Background

Nowadays, urban expansion can no longer be described solely in terms of economic growth; instead, a city should be viewed as a growing, increasingly complex metabolic system. This system

generates various chemical footprints associated with transportation, domestic energy use, synthetic materials, consumption patterns, land cover change and other human activities [1].

In this context, urban pollution extends beyond conventional gaseous and particulate pollutants such as polycyclic aromatic hydrocarbon (PAHs), volatile organic compounds (VOCs), and phthalates, which are increasingly detected in urban



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environments and have become major risk to human health and the environmental [2]. Figure 1 shows sources of pollution in urban areas such as Serpong City. Meanwhile, although identifying pollution in heavily industrialized zones presents major challenges, these challenges may be even bigger in non-industrial areas. Generally, in non-industrial urban areas, pollution is generally diffuse, derived from multiple sources, and characterized by complex mixture, making it difficult to access using conventional air pollution monitoring approaches. Stout and Wang [3] argued that approaches such as environmental forensics and molecular fingerprinting are needed to characterize the complexity of mixed pollution sources in non-industrial urban areas. Therefore, researchers have increasingly recognized the potential of these approaches and are optimistic about using

Urban Molecular Signatures (UMS) to characterize urban activities through their distinctive molecular fingerprints or signature features.

Simultaneously, global initiatives to reduce carbon emissions and achieve Net Zero Emissions (NZE) highlight the need to connect pollution science to the transition toward lower-emission systems. Although most NZE models continue to rely on macroscopic carbon inventories, they almost entirely excludes molecular pollutants data from emission mitigation planning [4]. Molecular signature could serve as an initial framework for linking household level of sources of pollution and emission with efficient, context specific energy transition pathways. [2][3][4]

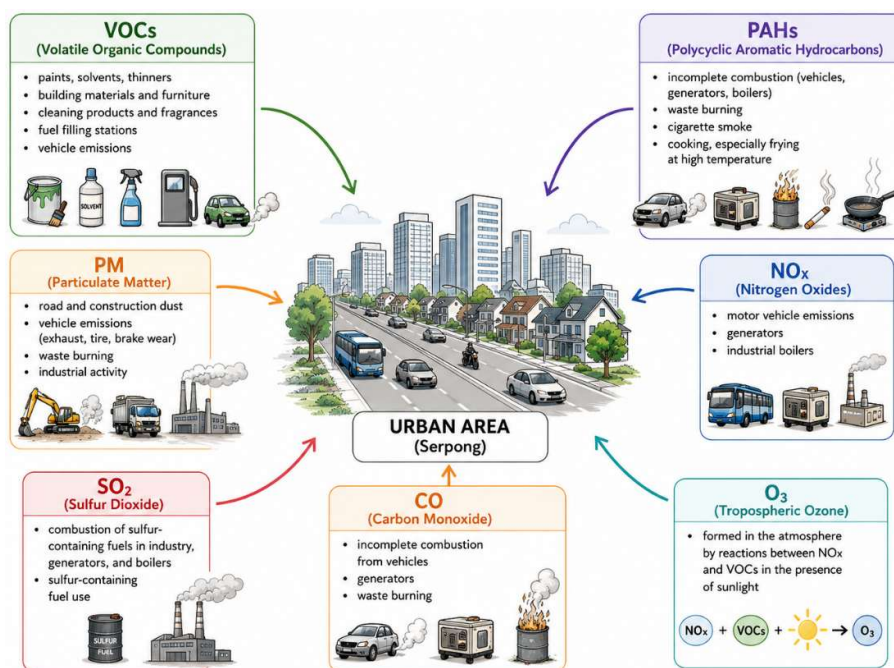


Fig. 1.
model for
pollution in
Serpong City

1.2. Research Gap in Indonesia

In Indonesia, study of molecular-level organic pollution and environmental forensics remain limited. Most research, surveys, and monitoring activities have focused on industrial areas, macro-scale emission indicators such as PM_{2.5}, NO_x, SO₂, the atmospheric deposition of inorganic compounds, or conventional air quality monitoring [5]. Several studies have provided important baseline data but have not specifically investigated highly distinctive molecular urban pollutants or their source-specific fingerprints. In Indonesia, studies of organic pollutants have generally focused on heavily contaminated areas [6]. However, studies on molecular urban pollution at non-industrial satellite urban areas are still limited. In a report by Ratnaningsih et al. [7] reported the occurrence of PAHs in the ambient air of Serpong and Jakarta; however, their study did not integrate these compounds into an urban molecular fingerprint framework, source attribution,

model. Therefore, as a modern rapidly satellite city, Serpong was selected as the primary study area. The city is characterized by rapid urban expansion and increasing material and energy consumption associated with suburban housing, domestic chores, and transportation. Izzatuljannah and Zakiah [8] reported that transportation emissions, limited green space availability, and other anthropogenic urban activities were major contributions to pollution in South Tangerang, demonstrating that urban areas without substantial industrial activity may still exhibit complex pollution dynamics.

This pollution pattern shows that urban areas with no industrial activities can still carry complex pollution dynamics.

The essential need in this study is integrative study from Indonesia that is combined: organic pollution analysis with Gas Chromatography-Mass Spectrometry (GC-MS), urban molecular fingerprints as urban chemical fingerprint" or "city-scale molecular fingerprint, distribution of source-based environmental forensics,

and conversion of this parameter into the Net Zero Emission (NZE) model. This gap is very significant because the pollution data provided in the study that is unintegrated and synthesized often produces problem diagnosis and fails to provide alternative solutions for substitution emission and end-of-pipe. Therefore, this study elaborates on integration of the three domains of NZE environmental forensics UMS as an agenda for research frontiers. This is intended for those in both industrial and non-industrial urban areas, particularly Serpong, which is a high priority for scientific research in Indonesia.

2. CONCEPTUAL BACKGROUND/SCIENTIFIC BASIS OF URBAN MOLECULAR SIGNATURE (UMS)

2.1. *Role of Polycyclic Aromatic Hydrocarbon as Markers of Urban Molecular Signatures*

Polycyclic aromatic hydrocarbon (PAHs) are one of the categories of organic pollutants that are most widely used as molecular markers in urban pollutant analysis. This is because these cases are closely related to combustion activities and human-made pollutants [9]. In urban environments, PAHs usually arise from several pyrogenic sources such as vehicle emissions, biomass combustion, heating and cooking at home, as well as wear and tear on asphalt and tires [10]. Traffic emissions, particularly from diesel engines and gasoline, are often called as dominant sources of PAHs in a city, because those emissions tend to release high molecular weight combustion derivatives. PAH ratios and profiles associated with biomass combustion suggest additional molecular sources, as evidenced by the dominance of specific compounds. As markers of urban molecular signatures, PAHs provide insight into urban emissions. This is essential because they serve as markers of emission sources [3]. One of the oldest and probably most popular techniques in environmental forensics is the use of PAH homolog ratios to identify emission sources, particularly to differentiate among petrogenic, pyrogenic, traffic, and biomass combustion emissions. For instance, ratio of Fluoranthene/(Fluoranthene + Pyrene) or Flu/(Flu + Pyr) is used to identify the dominance of emission from fossil fuel combustion compared with emission from biomass combustion; and ratio of Anthracene/(Anthracene + Phenanthrene) or Ant/(Ant + Phe) is used to identify emissions from combustion sources compared with petrogenic emissions [11]. The ratio of BaA/(BaA + Chr) and IcdP/(IcdP + BghiP) are also commonly used to identify the dominance of emission from vehicles, as well as emission from coal and biomass combustion [12].

The importance of a diagnostic ratio approach is particularly evident in the study of molecular signatures of urban pollutants, as it helps identify sources within complex pollutant mixtures. Several researchers have shown that it is important to use diagnostic ratios alongside multivariate analysis because these ratios may change due to atmospheric transformation [12]. However, the combination of PAH fingerprints and multivariate analysis remains one of the main strategies applied in contemporary environmental forensics. Stout and Wang [3] emphasized the persistent characteristic of PAHs in environment and their unique distribution associated with certain pollutant sources which are also considered as an indicator. For PAHs, this means they can be used to correlate exposure and to track emission sources and timelines. PAHs are also important in non-industrial urban drainage systems such as Serpong, as well as

in industrial areas. As vehicle and residential emissions are main contributors to PAH emissions, PAH emission fingerprints have the potential to determine pattern of emissions distribution that are commonly undetected by PM_{2.5} standards or other criteria gaseous pollutant emission measurements. The use of PAHs in the study of markers of urban molecular signature, somehow focuses on interpretation of urban emissions systems, that move beyond simple process of urban air quality assessment. For molecular studies that discusses urban organic infrastructure, PAHs serve as classical pollution fingerprints and a key chemical medium for understanding the transition of urban emissions toward sources attribution and emission tracking models for Net Zero Emission (NZE).

Volatile Organic Compounds (VOCs) and Its Use in Describing Urban Emissions Patterns

While polycyclic aromatic hydrocarbons (PAHs) occasionally function as markers of combustion sources and pollutant accumulation occasionally, VOCs offer advantages as indicators of urban combustion sources due to their ability to detect rapidly changing emissions. They also show a stronger response to changes in human activities[13]. In urban systems, VOCs include various compounds, such as aromatic hydrocarbons categorized as BTEX (benzene, toluene, ethylbenzene, and xylene), and other VOCs including acetaldehyde, ketones, alcohols, and oxygenated VOC (OVOC). BTEX compounds and OVOCs indicate different emission sources and their chemical transformation in the atmosphere [14]. Essentially, VOCs represent the urban emission system and provide real-time depiction of the dynamic characteristics of urban structure emissions; they reflect changes in the transportation system, VOC emissions resulting from the use of homemade solvents, and VOC emissions associated with household energy consumption, while also consistently characterizing the urban pollutant system. In urban areas, most BTEX emissions arise from vehicle fuel combustion and evaporation, with BTEX from fuel splash typically containing benzene and toluene [13]. Because BTEX ratio observes most significant emissions, including vehicle, light industry, and use of domestic or commercial solvents, BTEX tends to be prioritized in source attribution study. VOCs are strongly influenced by evaporation and solvent use, including emissions from paints, cleaning products, and newer consumer products, making them important determinant of urban pollution. As reported by Atkinson and Arey [14], the complex characteristics of VOCs arise from various emission sources and their involvement in photochemical reactions occurring in the atmosphere, which generate not only tropospheric ozone but also secondary organic aerosol.

The particular advantage of the VOC approach in environmental forensics is the ability to interpret sources and photochemical aging through molecular ratios. Response from toluene and benzene (T/B) ratio separates traffic emissions from emission domination of industry source and solvents, while xylene ratio towards ethylbenzene (X/E) is often considered as photochemical aging because xylene is more reactive than those two compound [13,15]. Regarding the molecular footprints of urban areas, this ratio plays an important role in determining emission sources and pollutant transformations in urban ecosystems. VOCs have sensitivity and capability that make them some of the primary tracers used to differentiate the spatial and temporal emission characteristics of urban areas. In particular, because Serpong is a non-industrial urban ecosystem, VOCs are essential, as their emissions are more closely tied to daily air

exchange across its various parts. In this case, VOCs reflect the chemical processes occurring in urban ecosystems rather than merely serving as air pollutants and support the hypothesis of urban molecular signatures.

2.2. *Phthalates and Domestic Pollutant as Markers of Urban Modernity*

In the studies of urban molecular pollution over the last twenty years, it has been found that domestic pollutants such as phthalate have shifted from being considered secondary pollutants to becoming a major focus in studies of urban lifestyle related emission, i.e. emission related to consumption, synthetic materials, and modern domestic practices [16]. Due to its various uses, phthalates which are used as plasticizers in PVC, consumer products, packaging, vinyl flooring, various cosmetics and household products, migrate into the environment through dust-borne emissions, urban runoff, damage and leaching from those materials [16]. Among these compounds, the phthalates most commonly found in traffic dust, aerosol, wastewater, and urban sediment were di-(2-ethylhexyl) phthalate (DEHP), dibutyl phthalate (DBP), diisobutyl phthalate (DiBP) and benzyl butyl phthalate (BBP) which are recognized as chemical indicator of modern urban lifestyles and manifestation of modern urban metabolism [17]. The occurrence of these compounds is associated with patterns of plastic consumption, house dust, domestic emission, and modern urban synthetic materials patterns. Unlike conventional pollutants that are associated mainly with industrial areas or emission from combustion, phthalates represent pollutants arising from daily activities and expand the range of urban emission sources to include consumption-based activities.

Using urban molecular footprints as a framework for defining the chemical identity of a city helps to explain how urban molecular footprints and urban emissions can be considered chemical indicators of consumption behavior that characterize a city. In a modern environment, many semi-volatile chemicals, including phthalate, dominate human exposure through multiple pathways involving both indoor and outdoor areas; phthalates present in urban dust can be used to represent urban emissions and urban environmental pressure. Therefore, phthalates have become a key element in the environmental molecular forensics of urban areas. In non-industrial cities like Serpong, this group of compounds is very important because it represents the dominance of domestic emissions sources. In low density urban areas dominated by domestic activities, phthalates may also indicate environment pollution associated with urban lifestyles consumer product use, and synthetic materials, thereby helping to characterize the urban environment of a city. Thus, their presence provides evidence that urban lifestyles can also be sources of organic pollution. Besides, it helps to explain that pollution in urban environments can also arise from urban consumption systems. In this case, phthalates are urban pollutants that represent the chemical characteristics of modern urban lifestyles. Therefore, they play an important role in the environmental forensics of urban modernity. Figure 2 showing the conceptual framework for UMS.

3. LITERATURE SEARCH STRATEGY AND REVIEW METHODOLOGY

This study was designed as a narrative–integrative review and conceptual framework paper, rather than a bibliometric review,

systematic review, or meta-analysis. This approach is appropriate for synthesizing fragmented evidence across related fields and developing a new conceptual perspective, particularly when the target topic is still emerging and the available literature is limited [18,19].

A full PRISMA-based systematic review was not adopted because direct studies on Urban Molecular Signatures (UMS) in Serpong or comparable non-industrial Indonesian cities remain very limited. Few peer-reviewed studies currently integrate GC–MS-based organic pollutant analysis, molecular fingerprinting, environmental forensics, and Net Zero Emission transition modeling in such urban settings. Therefore, this review employed a structured narrative strategy, supported by PRISMA-style screening logic, to improve transparency without claiming to be a full systematic review [20].

The literature search used Scopus, Web of Science, ScienceDirect, SpringerLink, ACS Publications, and Google Scholar. Keywords included combinations of “urban molecular signature,” “molecular fingerprinting,” “environmental forensics,” “organic pollutants,” “PAHs,” “VOCs,” “BTEX,” “phthalates,” “GC–MS,” “source apportionment,” “urban metabolism,” “exposome,” “urban pollution Indonesia,” “Serpong,” and “Net Zero Emission.” The synthesis was organized into three levels: studies directly related to Serpong and Indonesian urban pollution; studies on molecular fingerprints and environmental forensics in urban environments; and broader conceptual literature on urban metabolism, exposome science, and NZE transition. This structure enabled the review to identify a clear research gap and to ground the proposed UMS framework in peer-reviewed scientific evidence.

The limited number of direct studies on Serpong should not be interpreted as a limitation of the review design only, but also as one of the main scientific gaps identified by this study. The absence of integrated studies combining GC-MS, molecular fingerprinting, environmental forensics, and NZE transition in non-industrial Indonesian urban areas provides the rationale for proposing UMS as a new conceptual framework.

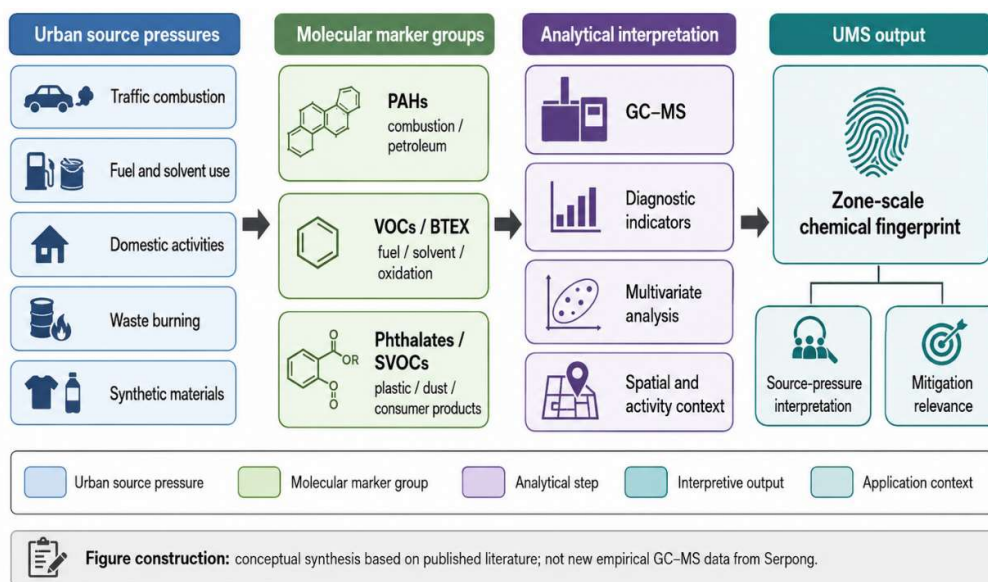
4. URBAN MOLECULAR SIGNATURES (UMS): CONCEPT AND DEVELOPMENT

4.1. *Definition of Urban Molecular Signatures (UMS)*

Urban Molecular Signatures (UMS) is the newest concept in environmental chemistry related to urban areas which have unique molecular compositions that describe primary anthropogenic activities through organic pollutant fingerprints and their transformations in ecosystems. In simple terms, UMS can be described as the chemical characteristics of a city resulting from various emission sources, the process by which pollutants are transported, transformed, and accumulated in the urban environment, the movement of pollutants in the atmosphere, chemical reactions caused by sunlight hitting suspended particles, and the accumulation of organic chemicals as community by-products [1]. Unlike conventional methodologies that consider pollutants in urban environments as a chemical code that communicates the characteristics of the urban environment from this perspective, not only does a city have an emissions profile, but it also has unique fingerprints. UMS considers pollutants in urban environments as chemical code that communicates urban environment characteristics. From this perspective, not only does a city have emissions profiles, but it also has unique molecular

fingerprints. UMS draws on principles from advances in several fields that were previously developed simultaneously or independently, such as molecular fingerprinting, environmental metabolomics, the urban chemical exposome, and source signature analysis. Molecular fingerprinting relies on identifying constituent patterns in organic materials to differentiate sources of organic materials and pollutants [3]. Environmental metabolomics then develops this idea by describing the environment as a network of constant movement and molecular signals [21]. On the other hand,

urban exposure science characterizes the urban environment as a large, complex, and heterogenous chemical exposure system that leaves pollution exposure footprints on the communities in urban environments. The combination of these ideas has created UMS as a framework that not only identifies pollutants but also manages them to reveal deeper patterns in how urban metabolic structure, human activities, and pollution affect the environment.



Supporting references: Yunker et al. (2002); Atkinson & Arey (2003); Weschler & Nazaroff (2008); Hopke (2016).

Figure 2. Proposed conceptual framework linking urban activities, molecular organic pollutants, environmental forensics, and future NZE-related research. The diagram summarizes how diffuse urban activities may generate PAHs, VOCs, phthalates, and other organic molecular markers that can be analyzed using GC-MS, diagnostic ratios, and multivariate source-attribution tools. The final NZE-related component is presented as a future research direction rather than as a validated carbon-accounting model. The framework is synthesized from literature on molecular fingerprinting, environmental forensics, source apportionment, and urban emission-transition studies.

The primary contribution of this framework is a change in focus from individual pollutants as chemical constituents to their collective recognition, i.e. as chemical fingerprints of an urban environment. In this framework, one sees beyond the concentration of individual compounds or homologous distributions and compounds, molecular ratios, transformation pathways, and relationships among the compounds. This framework conveys the focus that is needed in modern urban chemical systems, particularly in urban environments with various pollution sources, widespread emissions, and a complex anthropogenic environmental systems. In this sense, UMS represents conceptual change from pollutant monitoring into a systemic conceptual framework in urban environments.

4.2. From Single Pollutant into Mixed Signature

The evolution of the UMS concept reflects a fundamental shift in environmental pollution studies from an individual-pollutant approach to a mixed-signature approach. Single pollutant studies in pollution research focuses on the determination of single pollutants, such as certain PAH, benzene, or PM_{2.5}, and their comparison with standard or regulatory threshold. Even though this is an essential approach to evaluating compliance, it is often insufficient to solve more challenging urban pollution issues because emission sources in urban areas to operate and provide pollutants as mixtures. In

modern urban studies, pollution indicates a mixture of compounds that correlate with various urban purposes, UMS paradigm is related to mixed patterns, source fingerprint, atmosphere transformation, and relationship within urban systems [1]. This approach relates to urban system connectivity and the chemical patterns that emerge from it. This is an interesting observation since mixed pollutants provide source fingerprints that cannot be easily identified through individual compound patterns.

This idea supports advances in mixed toxicology and the environmental exposome, and shows that the urban environment involves mixed exposures rather than a single pollutant [22]. In this case, mixed signatures becomes more important than the classic methods because they help capture emissions fingerprints, describe transformation dynamics in atmosphere, and examine the suitability of emissions structures for the social structure and cities ecology, which have not yet been explored. Stout and Wang [3] stated that a fingerprint-based approach to mixed pollutants is more beneficial to environmental forensics than single-pollutant identification, since it enables a more reasonable reconstruction of pollution sources. By using this approach, UMS can be understood as an effort to support the claim that contemporary cities are hybrid chemical systems whose inherent complexity cannot be captured by a single metric. In urban systems science, a mixed-signature

approach is more accurate for assessing urban pollution than classic observational paradigms.

4.3. UMS in Non-Industrial City

The UMS concept has developed rapidly, but its applications are focused on megacities, industrial corridors, harbor areas, and areas with significant traffic, which are considered organic pollution hotspots [1]. Cities with significant industrial and transportation activities become primary sites of UMS because they exhibit strong, clear pollution signals. However, UMS has been applied less frequently in non-industrial satellite city, or newly developed suburbs that are surrounded by commercial or light industrial activities but have no substantial industrial activity. Serpong represents a new type of urban pollution that is scientifically interesting. Unlike in industrial cities, the emissions system in this area is likely affected by suburban domestic emissions, suburban commuter traffic, energy-related pollutants from household use, and pollution from synthetic materials and modern consumption. Even though these pollutants are widespread and diffuse, they are often unmeasured under conventional pollution paradigms but are compatible with the UMS paradigm. Therefore, molecular signatures from non-industrial urban areas may indicate comparable pollution levels, but their sources, compositions, and emission patterns likely differ in dominance. This idea is important because it challenges the traditional notion that the absence of industrial activity in a geographic area implies relative cleanliness in molecular pollution studies. According to the UMS framework, urban systems including contemporary satellite city can develop unique chemical fingerprints that reflect their local emission structures [1]. In Indonesia, this indicates a significant research void since most pollution-related studies focus on industrial area or large scale pollution assessments, and studies of molecular pollution fingerprint in non-industrial urban areas are nearly nonexistent. Therefore, implementing UMS in an area like Serpong is highly significant as a local case study. Besides, it may significantly expand the coverage of urban environmental chemical study in Indonesia.

4.4. UMS in Connection with Current Environmental Frameworks

Rather than serving a traditional pollution-monitoring role, Urban Molecular Signatures (UMS) is proposed as an integrative framework for urban environmental geochemistry. Although it frequently treats them as distinct variables, routine monitoring is still crucial for assessing specific pollutants including PM, NO_x, SO₂, PAHs, VOCs, and other criterion pollutants. Organic pollutants, on the other hand, are interpreted by UMS as a composite molecular fingerprint that represents material consumption, urban activity, atmospheric transformation, emission sources, and spatial heterogeneity. This viewpoint is in line with current molecular-marker research demonstrating that dissolved organic matter and urban organic aerosols can encode chemical signatures associated to land use and source specificity (Wang et al., 2020; Salvador et al., 2022; Hu et al., 2022).

Because UMS use diagnostic chemicals, compound distributions, and multivariate patterns to infer mixed pollutant sources, it is strongly associated with environmental forensics and molecular source apportionment. Although their interpretation must account for weathering and atmospheric changes, PAH markers have

frequently been used to differentiate petroleum, combustion, traffic, coal, and biomass-burning inputs. While phthalates and other semi-volatile organic compounds reflect synthetic materials, consumer goods, indoor dust, and household exposure pathways, volatile organic compounds (VOCs) are also significant because they contribute to atmospheric oxidation, ozone formation, and secondary organic aerosols [23–26].

UMS is unique in that it defines an urban system's chemical identity in addition to source identification. It uses the "signature" logic of urban metabolism, environmental metabolomics, exposome science, and environmental forensics to molecular contaminants in urban environmental media. This framework is helpful in Serpong because, despite the absence of dominant point-source industrial emissions, commuter traffic, household activities, waste burning, consumer goods, synthetic materials, and urban runoff can all leave a detectable molecular fingerprint in a non-industrial satellite city. Therefore, the systematic integration of various markers into a spatially explicit urban chemical fingerprint—rather than the identification of individual molecular markers—is what makes UMS new. Because it addresses PAHs, VOCs, phthalates, and other organic pollutants as an interpretable molecular assemblage representing urban activity structure, source contributions, environmental transformations, and potential mitigation pathways, UMS is unique. Table 1 below showing the comparison between UMS and existing environmental frameworks.

5. ENVIRONMENTAL FORENSIC FOR URBAN POLLUTANT SOURCE CONTRIBUTION

5.1. Environmental Forensic Evolution

Initially, environmental forensics was only related to the methodology used to track industrial pollutants. Nowadays, the focus of this discipline has undergone a paradigm shift following new findings on pollution. Environmental forensics methodology has become a key component of post-oil-spill analyses and investigations into the dynamics of hydrocarbon contamination, particularly for determining environmental liability obligations and ensuring industrial safety with regard to pollution [3]. The primary function of this discipline is to determine the cause of pollution through chemical analysis, differentiate the origins of oil pollution as either petrogenic or pyrogenic, and observe the temporal progression of pollution within the scope of legal regulations and industrial politics. Nevertheless, as related environmental challenges emerge, environmental forensics as a discipline have extended its scope from pollution identification to the characterization of pollutants based on variables in the atmosphere and the contour of industrial ecosystem. As the years have passed, the field of environmental forensics has developed significantly; it now addresses source attribution, contamination fingerprinting, pollution chronology, and contaminant migration analysis [3,4]. Modifying environmental forensics tools to deal with pollution issues that involve fragmented emissions, mixture, and transport under various physical conditions is very valuable, since urban pollution rarely comes from a single source. This shifts environmental pollution forensics from investigating where emissions originate to investigating how emissions vary cyclically across various physical conditions, thereby elucidating the environmental chemistry of pollution in the surrounding environment.

Stout and Wang [3] also explained that the true potential of environmental forensics can be seen from the combination between analytical chemistry, multivariate statistics, and the interpretation of environmental processes which helps reconstruct complex pollution. This applies to urban pollution, where the capture, mixing, and overlap of emissions from transportation, domestic

sources, surface runoff, and diffuse pollutant sources create analytical challenges for conventional pollution monitoring. Environmental forensics has transformed from a mere tools for attributing pollution source to an advanced method for analyzing urban chemical metabolism.

Table 1. Comparison between UMS and existing environmental frameworks.

Framework	Main focus	Typical data or markers	Similarity with UMS	Difference from UMS	Contribution of UMS
Conventional pollutant monitoring	Regulatory assessment of pollutant concentration	PM, NO _x , SO ₂ , CO, O ₃ , PAHs, VOCs, metals	Measures pollutants in urban environments	Often parameter-based and does not fully resolve mixed molecular fingerprints	Interprets pollutants as an integrated molecular pattern of urban activities
Environmental forensics	Identification of pollution sources and contamination history	Molecular fingerprints, diagnostic ratios, biomarkers, isotopes, GC-MS data	Uses chemical evidence for source attribution	Usually applied to specific contamination cases, spills, or liability questions	Extends forensic interpretation to diffuse non-industrial urban emissions
Molecular source apportionment	Quantifying contributions from different sources	PAH ratios, VOC ratios, PCA, HCA, PMF, receptor models	Separates overlapping sources using chemical profiles	Often focuses on source percentages rather than urban chemical identity	Uses source profiles to define a city- or zone-scale molecular signature
Environmental metabolomics	Molecular response of organisms or systems to environmental stress	Metabolites, biomarkers, omics-based molecular profiles	Uses molecular patterns as system-level indicators	Primarily biological-response oriented	Adopts the “signature” logic but applies it to urban pollutant mixtures
Exposome framework	Total environmental exposure across human life	External and internal exposure markers, pollutants, lifestyle factors	Recognizes complex mixed exposure	Human-exposure centered, not necessarily source-attribution centered	Links urban pollutant mixtures with local anthropogenic activities and exposure pressure
Urban metabolism	Material and energy flows in cities	Energy, water, waste, carbon, material-flow inventories	Views the city as a system with flows and transformations	Usually macro-scale and not compound-specific	Adds molecular-resolution evidence to urban metabolism interpretation
NZE and emission inventory models	Carbon accounting and decarbonization scenarios	Energy use, carbon factors, sectoral emissions, technology scenarios	Supports transition and mitigation planning	Often lacks molecular evidence of actual local emission behavior	Provides molecular-informed evidence for local mitigation priorities

5.2. GC-MS in Environmental Forensics

Gas Chromatography-Mass Spectrum (GC-MS) is considered as one of the most important technologies in environmental forensics science and is often credited with the primary advancement of this discipline because of its ability to analyze complex mixtures of organic compounds, identify and characterize individual organic compounds within mixtures at trace concentrations [27]. The inherent advantage of GC-MS is its ability to separate and characterize complex mixtures, since these tasks cannot be accomplished using standard field techniques. The ability of GC-MS to detect numerous pollutants at trace levels, identify mixture patterns, and determine unique chemical fingerprints explains why GC-MS is crucial in environmental forensics [3,27]. In the field of urban organic pollution, GC-MS enables a significant shift from conventional monitoring to forensic investigation. While conventional monitoring only offers aggregate concentration of pollutants or the environmental quality status, GC-MS provides potential to analyze the mixture composition of pollutants, homologous series distribution, source marker distributions, and molecular patterns that are suitable for source attribution [3,27]. GC-MS plays an important role in urban molecular fingerprints and environmental forensics since it can identify urban fingerprints from traffic emissions, domestic combustion, plastic combustion, pollutant, plastics, and other materials related with modern consumption. This tool is very sensitive and selective. Thus, it can analyze otherwise undifferentiated mixtures more effectively. These molecules can have a very wide range, and GC-MS is the best standard for environmental forensics study. For those who study urban pollution, GC-MS is used for advanced laboratory

analyses. It is not intended solely for the direct analysis of individual compounds, but also for conceptual source attribution based on direct molecular evidence from pollution that is analyzed through urban pollution. The concept of unique urban molecular signature from GC-MS in environmental forensics can be seen in Figure 3.

5.3. Ratio Diagnostic Integration and Multivariate Analysis

Molecular diagnostic ratios have become a fundamental applied technique within environmental forensics for mapping pollution sources. Nowadays, modern approaches and research emphases in this type of study indicate that the interpretation of complex pollution sources cannot be derived from a single or two molecular ratios. Overlapping emissions in urban environments require techniques that produce more complex result, and advanced multivariate statistical analyses [11,12]. Diagnostic ratio such as Flu/(Flu+Pyr), Ant/(Ant+Phe), or various VOC ratios function as initial metrics of source attribution and have become the subject of various studies, although their source signature may appear diffuse, semi-transparent, or direct [12]. Therefore, recent technical environmental forensic analyses apply diagnostic ratio combined with multivariate techniques, such as Primary Component Analysis (PCA), Hierarchy Cluster Analysis (HCA), Positive Matrix Factor (PMF), and newer machine learning-based sources to identify complex pollutant sources [4,28]. (Figure 2). This combination has enabled them to identify overlapping sources, that is very important in urban areas where vehicle emissions, domestic combustion, blocked

emissions, and modern consumption source are collaborating and creating single pollution footprint.

For instance, PCA is a method for categorising compounds based on their covariance structure and is commonly used to identify dominant sources in a given molecular dataset, whereas HCA is useful for mapping fingerprint similarities across locations and sources [28]. The PMF method is more advanced in estimating the contributions of different sources to a pollutant mixture. The newest advances in machine learning method focuses on identifying complex patterns that is usually difficult to observe and capture using traditional statistical source identification methods, thereby increasing the accuracy of source classification [4]. Integrating this knowledge increases the value of the method by interpreting pollution not just in terms of individual sources but in terms of the overall structure of emission systems. When analyzing urban molecular signatures, the integration of chemical fingerprints, diagnostic ratios, and multivariate analysis helps establish urban space as a complex chemical system with different emission patterns, not just a system from various pollution source. Stout et al. [29] implied that the modern environmental forensics science paradigm is established based on these techniques and approaches since they generate credible and robust solutions that are applicable to real world conditions, regardless of the complexity of the issues. In the case of non-industrial pollution in urban areas, such as Serpong, indirect emission pathways and source systems that cumulatively contribute to the issue become more relevant due to the complexity of emissions, which are not easily differentiated using standard approaches.

5.4. *Environmental Forensics in Indonesia: Focus on Industrial Study*

Indonesia has focused on environmental forensics for the past 20 years and has emphasized studies that investigate and analyze highly polluted industrial areas, particularly studies on petroleum and oil pollution, manufacturing and industrial waste, polluted sediments, heavy metal contamination, and hydrocarbon pollution in industrial zones and coastal areas. The initial approach to environmental forensics sought to identify pollution sources, hold perpetrators accountable, and address industrial pollution in affected areas. Most studies in Indonesia use chemical fingerprints especially towards pollution sources that can be identified, such as industries, harbors, or petrochemical activities [3,6]. These studies use hydrocarbon biomarkers, PAH profiles, or sediment contaminant distributions to differentiate between petrogenic and pyrogenic sources. Even though this approach is useful, these studies examine the most prominent pollution case rather than urban systems with diffuse pollution and multiple sources. In Indonesia, the number of studies applying chemical fingerprints to urban pollution is limited. Most studies remain focused on measuring macroscopic parameters such as pollutant concentrations, deposition, and PM_{2.5}, rather than on implementing molecular fingerprinting approaches [5,30]. Many studies that explored organic compounds, such as PAHs, did not examine pollutant concentrations and distributions using chemical fingerprints. For instance, Ratnaningsih et al. [7] studied PAHs in Jakarta and Serpong and correlated them with vehicle emissions, but they did not use chemical fingerprinting methods, diagnostic ratios, or multivariate analyses to identify pollution sources. Many international environmental forensics

studies have used these methods, including GC-MS and chemical fingerprinting [4,28].

This limitation shows that the purpose of environmental forensics in Indonesia has focused primarily on analyzing the environmental impacts of industrial pollution rather than comprehending the urban pollution system. A modern forensics framework to analyze urban pollution is needed to examine contemporary metropolitan areas. Modern urban pollution is a complex mixture created by emissions from various sources, such as urban traffic, pollution, industrial activities, urban runoff, residential pollution, synthetic material usage, alienation from nature, and others [1]. Therefore, expanding the scope of environmental forensics from industrial pollution to urban pollution, and then to molecular forensics, is important for the development of environmental research in Indonesia. This is particularly relevant to urban areas like Serpong, as they may represent a transition from industrial pollution forensics to non-industrial urban forensics systems. This transition will have a positive impact on other environmental forensics fields and forensics science more broadly by supporting emissions assessment, risk assessment, the development of forensic evidence strategies, and the evaluation of evidence for emission transitions toward Net Zero Emission (NZE).

6. INTEGRATION OF UMS WITH NZE MODEL: INTO MOLECULAR INFORMED DECARBONIZATION FRAMEWORK

6.1. *From Environmental Forensics into Molecular-based NZE*

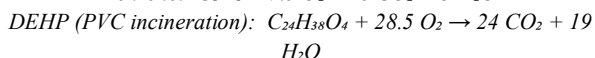
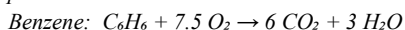
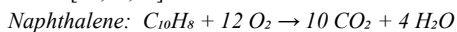
For several decades, studies on pollution and decarbonization were pursued primarily along two distinct scientific pathways. Environmental chemistry, and more recently, environmental forensics have examined issues such as identification, attribution, contaminant transport dynamics, and health and ecosystem related risks [3]. Net Zero Emission (NZE) studies tend to focus on pollution and carbon measurement, energy systems, low emission technologies, and decarbonization transition pathway [31,32]. Even though emissions examined from both branches are anthropogenic, the interaction between the two fields is minimal. Therefore, most NZE strategies depend on sector specific assumptions and large scale emissions estimates, and do not fully integrate molecular data that capture real urban emissions behavior. However, organic pollutant signature shows most potential as indicator that represent emission more accurately than an aggregate carbon balance. For instance, the distribution patterns of PAHs, VOCs, and local contaminants not only indicate the presence of pollutants but also reveal the characteristics of emission structures, emission intensity, and the anthropogenic activities underlying it [1]. In this case, there is a new paradigm called organic molecular-based decarbonization which utilizes evidence provided by urban molecular signature and environmental forensics as a scientific basis for designing NZE strategies. In this paradigm, evidence of pollution is no longer used as a diagnostic element but remains an active element in interventions for mitigation and transition planning.

Principally, this methodology creates a series of relationship connecting molecular signature, source identification, emissions behavior, the description of transition scenarios, and the development of NZE pathway. In urban systems, this is

particularly relevant because urban emissions typically comprise numerous small, dispersed sources that are difficult to quantify with top-down emission inventories. Within this scope, pollution observation is transitioning toward evidence-based transition planning, in which urban environmental chemistry serves not only as a means of addressing pollution issues, but also as a starting point for developing decarbonization solutions. This is one of the primary innovations integrating Urban Molecular Signatures (UMS) and NZE.

The linkage between UMS and NZE should be interpreted as indirect and supportive rather than direct. PAHs, VOCs, and phthalates do not measure carbon neutrality or CO₂-equivalent emissions. These compounds are better understood as molecular indicators of source pressures, such as combustion, traffic, solvent use, domestic consumption, degradation of synthetic materials, or waste burning. Their potential relevance to NZE planning depends on integration with conventional carbon-accounting data, including activity data, emission factors, energy use, mobility patterns, waste-management information, socioeconomic conditions, and policy feasibility. Therefore, this review does not propose molecular signatures as standalone NZE indicators. Instead, UMS is proposed as a conceptual framework that may complement future emission-inventory and mitigation studies by identifying dominant local source pressures. Quantitative translation of molecular fingerprints into carbon-reduction metrics is outside the scope of this review and should be addressed in future empirical research. **oward a Quantitative Molecular–CO₂ Linkage: A Conceptual Indicator Framework**

Although the qualitative rationale linking PAHs, VOCs, and phthalates to combustion-derived CO₂ emissions is well supported in the literature, a more explicit quantitative framing strengthens the conceptual contribution of this review. At the molecular level, PAHs, VOCs, and phthalates are frequently co-emitted with CO₂ because they share the same combustion or thermal-degradation pathways. Complete combustion of representative marker compounds illustrates this shared origin, as shown below for naphthalene, benzene, and DEHP during PVC incineration [36,38,39].



Field-based evidence supports this common-source relationship: ambient VOC concentrations have been shown to correlate strongly with CO₂ ($R = 0.8$) in source-apportionment studies of combustion-dominated urban air [37], approximately 56.7% of global PAH emissions are attributed to fuel combustion [36], and PVC-based materials associated with phthalate plasticizers carry among the highest carbon footprints of common plastics, at 7.83 kg CO₂-eq per kg [39,40].

Building on this mechanistic and correlative evidence, this review proposes a Molecular-Informed Emission Pressure Index (MEPI) as an illustrative, hypothesis-generating indicator rather than a validated carbon-accounting tool:

$$MEPI = (w_{pah} \times N_{pah}) + (w_{voc} \times N_{voc}) + (w_{phth} \times N_{phth})$$

where N_j is the normalized signal intensity of pollutant group j (0–1 scale), obtained either from concentration data relative to a local reference value, $N_j = \min(A_j / A_{ref,j}, 1)$, or from category-based activity proxies, $N_j = s_j / s_{max}$, following standard min–max normalization practice used in comparable environmental index construction. The weight w_j reflects each group's literature-supported

association with combustion-derived CO₂ co-emission ($\sum w_j = 1$); in the absence of Serpong-specific calibration data, weights should initially be treated as equal ($w_j \approx 0.33$) and refined once local GC–MS and activity data become available.

A second, complementary expression translates anticipated reductions in molecular marker intensity into an indicative CO₂ co-benefit estimate for future mitigation scenarios:

$$\Delta CO_2_{est} = \sum_j (\Delta M_j \times k_j)$$

where ΔM_j is the estimated reduction in group- j marker intensity following a specific intervention (e.g., reduced waste burning, mode shift away from private vehicles, or substitution of PVC-based consumer products), and k_j is a stoichiometry- and literature-derived conversion coefficient, illustrated for example by the combustion relationships above and by reported emission factors such as 0.87 kg CO₂e per kWh for grid-based electricity consumption or 7.83 kg CO₂e per kg for PVC-based material streams [39–42].

Both expressions are conceptual and intended to guide future empirical calibration rather than to serve as validated carbon-accounting outputs. Neither MEPI nor ΔCO_2_{est} should be interpreted as a direct measurement of carbon neutrality or as a substitute for activity-based emission inventories. Their value lies in providing a transparent, falsifiable structure through which future field-based GC–MS data, diagnostic ratios, and household-activity data from Serpong can be formally linked to NZE-related decision-making, addressing the quantitative gap between molecular evidence and carbon-accounting frameworks.

6.2. Urban Molecular Fingerprints as Parameter in NZE Model

Standard NZE models use energy consumption, carbon intensity, emission factors, technology penetration, and policy scenarios as parameters. Even though these factors are important in modeling emissions scenarios, most of them not represent actual emissions systems based on environmental chemistry evidence. Here, urban molecular signatures can provide new contributions. In the context of a molecular-based NZE approach, the formation of molecular signatures can be seen as a proxy to support the identification of change in dominant emissions sources and prioritize the need for transition interventions. A pyrogenic PAH signatures can demonstrate the contribution of traffic as a sources of pyrogenic pollution, and this can reveal the need to implement complementary mobility electrification and decarbonized transportation mode shift approaches [9,11]. Therefore, PAH signatures can do more than describe traffic pollution; they can also indicate the need for specific changes in the transportation sector. Similarly, inefficient energy consumption, emissions from combustion, and domestic activities can be represented by VOC emissions from households and correlated with household energy scenarios [14]. Specifically among Ontario residents, VOC emissions from households influenced by phthalate and other pollutants that reflect modern pattern of consumption. Based on this idea, a three layers conceptual framework for molecular-based NZE has been proposed in this study. The first layer is the molecular evidence layer, which uses GC–MS fingerprints, diagnostic ratios, PCA, and dominant-source categories to classify emission sources. The second layer is the transition interpretation layer, in which provides source pressure fingerprints, emission behavior proxies, and intervention points. The third layer is the NZE scenario layer,

in which the information determines whether the transition pathways are gradual, medium, or aggressive. This framework essentially combines molecular chemical evidence with transition modeling that is nearly completely unexplored.

Although this review proposes a conceptual linkage between Urban Molecular Signatures (UMS) and future Net Zero Emission (NZE)-related studies, this linkage should not be interpreted as a quantitative carbon accounting or emissions inventory framework. PAHs, VOCs, phthalates, and other organic molecular markers cannot be directly converted into carbon-neutrality indicators, CO₂-equivalent emissions, or decarbonization metrics without additional empirical data. In this framework, molecular signatures are treated only as source-pressure indicators that may help identify dominant urban activities, such as traffic combustion, fuel evaporation, solvent use, domestic activities, synthetic-material use, and waste burning.

6.3. Household Scale NZE Model: Bottom-up Approach based on Molecular Evidence

One of the primary contributions of the molecular-based decarbonization approach is the potential to create an NZE model at the household level. Thus far, most NZE strategies have been designed using a top-down approach based on national energy sectors or city inventories. Nevertheless, various studies have shown that significant contributions originate from household electrical consumption, direct and indirect emissions, private transportation, fuel use, and the material footprint of consumption

[31]. In urban molecular pollution, households are examined not only as exposed entities but also as emitting entities. This argument helps formulate a household-based NZE using pollutant fingerprints. This model can integrate household energy profiles, mobility patterns, plastic and waste related behaviors, and local molecular pollutant indicators as input variables. These variables can be connected through scenario layers to prioritize transition interventions. For instance, if traffic fingerprint is the most dominant, priority can be given to transportation decarbonization; if domestic energy inefficiency represented by household VOC emissions is more dominant, interventions should be prioritized along this pathway; and if plastic derivative pollution is dominant, priority can be given to intervention throughout circular consumption pathway. Compared to a conventional emissions calculator, this approach enables practitioners to create models that combine various levels and intervention ranges. This range covers behavior intervention continuity, low-cost efficiency, partial electrification, other technology efficiency intervention, and deep decarbonization. These interventions may range from modest to radical. Most importantly, practitioners must iteratively incorporate these pathways to achieve a net-zero trajectory that reflects long-term goals while also providing a realistic transition framework with practical steps and immediate action. The conceptual model for integration of UMS, environmental forensics, and NZE context is shown in Figure 4.

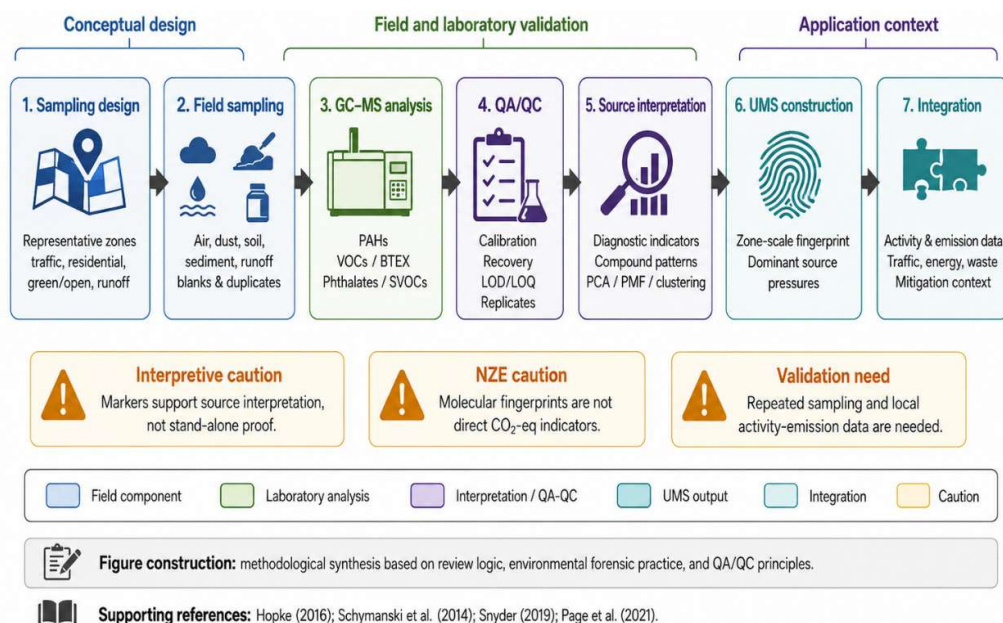


Figure 3. Conceptual structure of a prospective urban molecular fingerprint. The figure illustrates how different urban activities may contribute to distinct but overlapping molecular marker groups, including PAHs from combustion and traffic-related sources, VOCs from fuel evaporation, solvents, and household activities, and phthalates from synthetic materials and consumer products. The diagram is conceptual and intended to show the proposed UMS logic; it does not represent measured molecular data from Serpong.

6.4. *Serpong as a Proposed Prospective Living Laboratory Pilot Model for Molecular-Informed NZE*

In this case, the presence of a molecular-based NZE approach could potentially support the development of living laboratory concepts in Serpong. There are many non-industrial urban areas that are dominated by household emissions, high levels of commuter mobility, and rapid suburban expansion. Serpong offers perfect concepts to investigate pollutant fingerprints, comprehend emissions behavior, and conduct transition trajectory simulations [8]. Unlike industrial cities or national models which usually form the foundation of NZE studies, Serpong provides a spatial context that is closer to household emissions, thus it can serve as proof of concept for an urban molecular forensics approach, household transition simulation, and local-scale NZE framework. The uniqueness of this scale is important because most NZE-related studies have been designed at a macro scale, and most satellite cities dominated by households have not yet been explored. Therefore, it can be concluded that Serpong can be considered not only a case study but also a research model for implementing an integrated framework of environmental chemistry and emissions transition.

6.5. *Integration Potential of AI, Machine Learning (ML), and Predictive Environmental Forensics for NZE*

The evaluation of this framework lies in the integration of AI and ML to create a foundation for predictive environmental forensics within the NZE scope. Ditzler et al. [28] examined the use of multivariable analytics and pattern recognition to explain pollutant sources and create opportunities for designing AI based predictive systems. The combination of molecular fingerprints and household mobility and behaviour data indicates that machine learning models could adaptively estimate source contribution, reduction elasticity, and probabilistic NZE pathways. This opportunity arises from the potential to support a transition from static models to dynamic ones. In the long term, this integration could evolve into an urban molecular digital twin for decarbonization planning, particularly through its predictive ability to stimulate the behaviour of urban emission systems in relation to molecular data.

6.6. *Knowledge Gap and Future Research Agenda*

The existence of the NZE approach, along with molecular techniques, introduces several research opportunities. First, the number of empirical studies that indicate the relationship between pollutant fingerprints and NZE parameters remains limited. Second, there is still limited research on the standardization of parameters that allows molecular signatures to be translated into transition variables, with much debate still occurring in advanced countries. This also applies to their implementation in the Global South including Indonesia. Therefore, the basic urban molecular signatures dataset, a molecular signature-based household emissions model, a pilot study in a satellite city like Serpong, the integration of a GC-MS-forensics-NZE model, followed by the development of an AI-based transition-predictive model, will strengthen this emerging subfield of urban environmental chemistry which promotes the relationship between pollution and sustainability transitions.

The primary conceptual advancement of this framework is that it positions pollution data not only as a diagnostic tool but also as a component of transition. In previous paradigms, pollutant measurement, risk assessment, and diagnosis were the end points of a study. Meanwhile, in the new paradigm, pollutant measurement, source attribution, transition scenario construction, and NZE pathway assessment become the new end points. This represents a paradigm shift since it allows environmental chemistry to be involved in the sustainability transition science rather than merely serving as contamination science. In this cycle, the primary innovation from the UMS-environmental forensics-NZE framework is its strategy for integrating molecular evidence with transition modeling, through which pollution data can help explain recent and past scenarios, and contribute to the future formulation of evidence-based decarbonization strategies.

7. WHY IS SERPONG SCIENTIFICALLY INTERESTING?

Serpong is a rapidly developing area and a modern non-industrial satellite city. Even though this area is experiencing rapid urbanization, there are still no published studies on its molecular environmental chemistry and forensics. Industrial areas generally have clearly defined emission sources, whereas rapidly developing urban areas have multiple, more complex sources. Common sources found in urban areas include emissions from increased vehicle use, domestic activities, land use changes, and the increased use in synthetic materials. Rapid development and the existence of complex pollution and emissions sources have become the reason why Serpong is considered a suitable area for examining urban molecular features. Another reason is the rapid pace of its development. As a satellite city of Jakarta, Serpong has developed horizontally and structurally, and population mobility to and from Serpong has increased. Urban development affects changes in the abundance and types of organic pollutants, their distribution, emerging emission patterns, and land-use changes. Serpong is a suitable area for examining urban molecular features because transportation and urban development are primary sources of air pollution there. In addition, the unique combination of diverse non-industrial emissions sources provides an opportunity to generate significant scientific values. Organic pollution related to industrial and manufacturing locations has become the purpose of many studies. However, contemporary urban emissions, particularly those in Serpong, can also be tracked through city traffic, household heating, household fuel combustion, and solid waste degradation, as well as through the generation of PAH, VOC, and phthalates. Ratnaningsih et al. [7] observed the example of traffic-based emissions as primary contributor of PAH in Serpong and found that non-industrial pollution pressure is quite significant. Urban spaces with similar conditions experience traffic emissions as a primary source of organic pollution pressure.

Serpong deserves greater attention because of its potential for testing the UMS theory. The UMS hypothesis posits that an urban area has a distinctive molecular signature reflecting its primary anthropogenic activities and pollution sources [1]. In Serpong, this signature can be considered hybrid UMS derived primarily from traffic, household, lifestyle, and industrial emissions. This hypothesis helps to develop the existing framework by raising theoretical questions about modern, affluent suburban areas that are often assumed to be relatively free of molecular pollutants.

Another aspect that strengthens the research potential of Serpong is its role as a living laboratory for pollution and Net Zero Emission (NZE) transition.

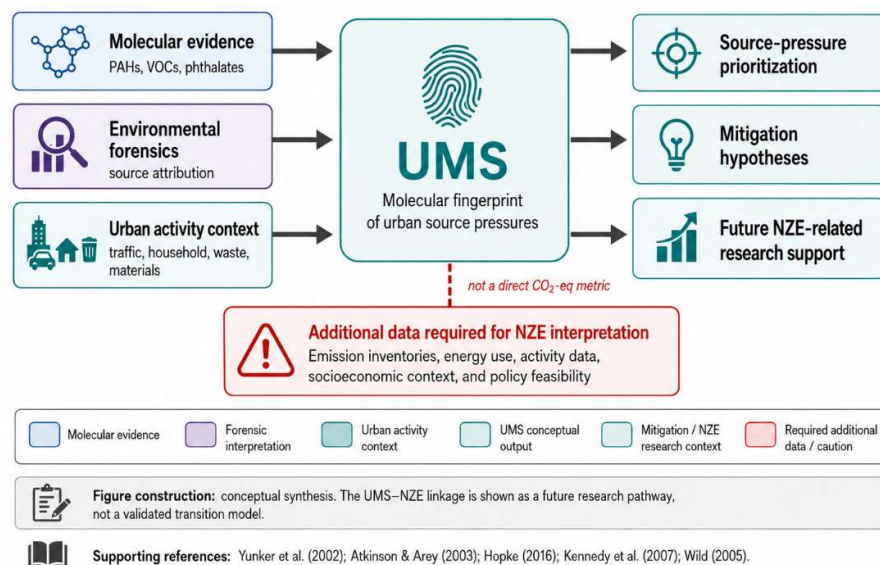


Figure 4. Conceptual integration of Urban Molecular Signatures (UMS), environmental forensics, and NZE-related research. Molecular evidence, source attribution, and urban activity data are synthesized into UMS to identify source pressures and support mitigation hypotheses. UMS is not a direct CO₂-equivalent metric and requires additional emission, energy, socioeconomic, and policy data to interpret NZE.

Considering that many emissions are associated with household routines and daily mobility, particularly in Serpong, households may be major contributors to pollution, and such data may be a good initial point for pollution modeling. The integration of pollution modeling and NZE transition remains underrepresented, especially in Indonesian cities. More importantly, Serpong holds a prominent position in the national research landscape. Most recent publications in Indonesia emphasize macroscopic parameters, such as PM_{2.5}, inorganic deposition, or industrial hotspot [5]. There are almost no studies that take an interdisciplinary approach, combining GC-MS, molecular fingerprinting, environmental forensics, and NZE models in non-industrial urban areas. Therefore, Serpong has the potential to become not only an important research location but also a representative case study for advancing urban environmental research in Indonesia.

8. SCOPE OF EVIDENCE, CONCEPTUAL BOUNDARIES, AND FUTURE VALIDATION

This review distinguishes between established scientific knowledge, the proposed conceptual framework, and future research needs. Established methods such as GC-MS analysis, PAH indicators, VOC characterization, phthalate detection, and multivariate source apportionment are widely used to identify organic pollutants and support environmental forensic interpretation of combustion, traffic, petroleum, solvent, domestic, and mixed contaminant sources [11,33,34].

However, the integration of UMS with NZE planning is proposed here as a conceptual framework rather than an experimentally validated model. Molecular signatures may help identify dominant urban source pressures, such as traffic

combustion, household activities, synthetic-material use, and waste burning, but they cannot independently determine NZE pathways without additional data on energy use, emission factors, household behavior, technology adoption, socioeconomic conditions, and policy feasibility.

For Serpong, this review does not claim that a complete UMS profile has already been established. Instead, Serpong is used as a prospective case study of a rapidly developing non-industrial satellite city, where commuter traffic, domestic emissions, consumer products, synthetic materials, and urban runoff may generate distinct molecular patterns. Future work should validate this framework through systematic sampling, GC-MS analysis, diagnostic and multivariate source apportionment, and integration with household-scale activity and emission data.

9. CHALLENGES AND LIMITATIONS OF UMS-BASED ENVIRONMENTAL

Although UMS may help interpret complex mixtures of urban organic pollutants, it should be treated as a complementary framework rather than a stand-alone forensic or transition-planning tool. PAH indicators, VOC profiles, phthalates, GC-MS data, and multivariate source-apportionment methods can support source interpretation, but each has methodological limitations. PAH diagnostic ratios, for example, are useful as preliminary indicators of petrogenic, pyrogenic, traffic, coal, or biomass-burning inputs, but they may be altered by weathering, degradation, transport, and overlapping source profiles. Therefore, PAH ratios should be used alongside compound distributions, spatial context, and multivariate analyses rather than as definitive source markers [11,34].

VOC-based interpretation is also uncertain because VOCs are highly reactive, volatile, and sensitive to meteorology,

photochemical aging, indoor–outdoor exchange, fuel evaporation, solvent use, traffic density, and household activities. In non-industrial urban areas, these sources are often diffuse and episodic, making simple source classification unreliable. Similarly, phthalates and other semi-volatile organic compounds may indicate synthetic materials, plasticizers, consumer products, and indoor dust exposure, but their distribution is influenced by indoor partitioning, surface interactions, and human activity patterns. Reliable UMS interpretation therefore requires repeated sampling, QA/QC control, meteorological information, and integration with receptor or multivariate models [23,33].

Analytical standardization is another major challenge. GC–MS results can vary with sampling media, extraction protocols, clean-up methods, instrument configuration, calibration standards, detection limits, and data-processing procedures. Targeted GC–MS is useful for quantifying selected PAHs, VOCs, phthalates, and other known compounds, but may miss unknown or emerging pollutants. Non-targeted screening can broaden compound detection, but the confidence in identification depends on spectral libraries, reference standards, instrument resolution, and expert validation. UMS studies should therefore report blanks, duplicates, calibration curves, surrogate recovery, detection limits, quantification limits, and uncertainty ranges, especially when comparing results across sites or studies [35].

In developing-country contexts, UMS implementation may also be constrained by the cost of GC–MS instruments, certified standards, high-purity solvents, trained analysts, instrument maintenance, and long-term monitoring. For Indonesia, early UMS studies should therefore begin with realistic pilot designs using selected robust markers, such as priority PAHs, BTEX compounds, and major phthalates, before expanding toward broader molecular inventories. Importantly, molecular signatures should not be treated as direct Net Zero Emission indicators. They may help identify dominant urban source pressures, but NZE planning still requires emission inventories, energy-use data, household behavior, socioeconomic information, technology-adoption scenarios, and policy feasibility assessments. Thus, for Serpong, UMS remains a prospective framework that requires systematic field sampling, GC–MS validation, source apportionment, spatial analysis, and integration with local activity-emission data before it can be used as a practical tool for molecular-informed urban mitigation. Molecular signatures should not be treated as direct indicators of NZE. They may support the identification of dominant urban source pressures, but NZE-related planning requires integration with emission inventories, activity data, energy-use information, household behavior, socioeconomic context, technology-adoption scenarios, and policy feasibility analysis.

10 CONCLUSION

This review positions Urban Molecular Signatures (UMS) as a conceptual framework for interpreting complex mixtures of organic pollutants in non-industrial urban environments. Previous studies have widely used PAHs, VOCs, phthalates, GC–MS analysis, diagnostic indicators, and multivariate source-apportionment methods to identify traffic, combustion, petroleum, solvent, domestic, synthetic-material, and other diffuse urban pollution sources. These approaches provide a scientific basis for using molecular evidence not only to detect

pollutants, but also to interpret the chemical expression of urban activities.

However, this manuscript does not present new GC–MS data or empirically derived molecular fingerprints from Serpong. Therefore, Serpong is not treated as a completed UMS case study but as a prospective context for developing molecular forensic research in Indonesian non-industrial satellite cities. The proposed UMS–environmental forensics–NZE linkage should also be understood as a future-oriented conceptual pathway, not as a validated transition model. Molecular signatures may help identify dominant urban source pressures, but NZE-related planning still requires integration with emission inventories, energy-use data, household activity patterns, socioeconomic information, and policy feasibility.

Overall, this review identifies a research gap and proposes a structured direction for future field-based studies. For Serpong and similar urban areas, future work should combine systematic sampling, GC–MS analysis of organic molecular markers, diagnostic and multivariate source apportionment, spatial interpretation, and local activity-emission data. Only after such empirical validation can UMS be evaluated as a supporting tool for molecular-informed urban mitigation and NZE-related planning.

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