Communication

AIQS-DB: Revolutionizing Simultaneous Analysis of Organic Compounds

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Abstract: This article summarizes studies using the AIQS-DB method to analyze various types of samples for different purposes. This is a method developed to simultaneously analyze nearly 1500 compounds and is widely used worldwide. The method is highly effective for environmental samples such as water, soil, sediment, and air. Recognizing its potential, this article aims to promote the further application and development of AIQS-DB in research related to food analysis and source tracing. Furthermore, if a suitable dataset can be constructed, it could help research quickly and cost-effectively discover the new bioactive compounds from plant medicine.

Keywords: AIQS-DB, GC/MS, LC/MS, simultaneous analysis

1. Introduction

In 2005, Professor Kadodami Kiwao, a distinguished academic at Kitakyushu University, introduced groundbreaking research on AIQS-DB [26], a sophisticated technology that leverages GC/MS analytical instruments to detect hundreds of organic compounds in a single sweep. The development of AIQS-DB marked a significant milestone in the field of analytical chemistry, enabling researchers to identify an unprecedented number of organic compounds with greater efficiency and accuracy than ever before.

At its inception, AIQS-DB boasted a remarkable capacity to identify 672 compounds simultaneously, including 332 types of pesticides, 160 varieties of polycyclic aromatic hydrocarbons (PAHs) and polychlorinated biphenyls (PCBs) composed of carbon and hydrogen, 81 phenols comprised of carbon, hydrogen, and oxygen, and 99 compounds containing nitrogen, sulfur, and phosphorus [26]. However, it was not until 2010 that AIQS-DB was refined and gradually adopted for analyzing diverse sample matrices [20].

Since its inception, AIQS-DB has been widely utilized in numerous studies to concurrently analyze organic compounds in various sample matrices, such as river water samples [1, 4, 5, 25], groundwater samples [9, 27, 39], sediment samples [23, 24, 33], wastewater samples [2, 19, 21], and dust samples [15, 17, 37]. Moreover, AIQS-DB has been adapted for use with other analytical instruments, including LC/MS/MS and LC-TOF/MS, making it an expedient, comprehensive, cost-effective, and scalable approach for identifying organic micro-pollutants [25]. The ability of AIQS-DB to analyze up to 970 compounds simultaneously on GC/MS and 508 compounds on LC-QTOF-MS or LC/MS makes it an ideal tool for non-target analysis across a broad range of sample matrices and applications.

This article provides a comprehensive overview of the wide-ranging applications of AIQS-DB in various fields and highlights its usefulness as a tool for the simultaneous analysis of organic compounds. It aims to promote the use of AIQS-DB, a highly useful product of Professor Kadokami's

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research, and encourages further research on its application to other sample matrices such as food, agricultural products, and plants.

2. AIQS-DB application

AIQS-DB, when used on a GC instrument, is commonly referred to as AIQS-GC, whereas its application on an LC system is known as AIQS-LC [31, 32]. Recently, AIQS-DB has been adopted for Comprehensive Target Analysis, leading to the development of various shorthand terminologies, including Comprehensive Target Analysis with an Automated Identification and Quantification System (CTA-AIQS) [29, 40, 41], target screening analysis (TSA-AIQS) [41], and comprehensive screening method (CSM-AIQS) [35], which are applicable to both GC and LC modalities. In light of its rapid deployment for environmental micro-pollutant screening in emergency scenarios, AIQS-DB has been abbreviated as REPE [41]. The synthesis of research studies revolving around AIQS-DB is presented in Table 1 below.

Table 1. The research used AIQS-DB.

Year	Instrument	Compound number	Matrix	Main objective	Ref
2023	GC/MS	58/949	Wastewater, treated water	Assessment of the influencing factors of ozonation performance in removing CoC in a wastewater discharge.	[14]
2023	LC-QTOF-MS	125/484	River water	Analytical method development for LC-QTOF-MS	[25]
2023	GC/MS; LC/QTOF-MS	144/969; 69/421	River water	Development of AIQS-DB for passive sampling as CC and POCIS	[1]
2022	GC/MS	288/n.a	PM 2.5	Comprehensive analysis	[15]
2022	LC-QTOF-MS	57/508	Indoor dust	Comprehensive analysis and health risk assessment	[16]
2022	GC/MS	97/886	Indoor air and dust samples	Comprehensive analysis and health risk assessment	[37]
2022	GC/MS; LC/MS	133/969	Dust samples	Comprehensive analysis and health risk assessment	[17]
2022	GC/MS	32/886	Wastewater treatment effluent	Profiling of organic pollutants	[18]
2022	GC/MS	109/~1000	Flood sediment or soil samples	Risk assessment	[32]
2022	LC-QTOF-MS	20/296 pesticides	Surface water samples in agriculture area	Comprehensive and agrochemical analysis	[40]
2021	LC-QTOF-MS	22/187	Particle samples	Risk assessment	[10]
2021	GC/MS; LC/QTOF-MS	78/970 2/501	Sediment	Comprehensive analysis	[29]
2021	LC-QTOF-MS	19/107	Particle samples	Comprehensive analysis and risk assessment	[30]
2021	GC/MS; LC/QTOF-MS	474/970	Wastewater eluted by fire extinguishing activities and river water	Comparison with GC-QTofMS	[31]

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2021	GC/MS	136/948	River water	Analytical method development	[35]
2021	GC/MS; LC/QTOF-MS	131/948 311	River water	Screening and ecological risk	[38]
2020	LC-Q/TOF-MS	85/484	River water	Comprehensive survey	[11]
2019	GC/MS	195/942	Indoor dust	Comprehensive analysis	[3]
2019	GC/MS	118/970	Particle samples	Target screening analysis	[8]
2019	GC/MS	167/942	Passive air sampling	Comprehensive analysis and health risk assessment	[12]
2019	GC/MS	105/942	Road dust samples	Comprehensive analysis and health risk assessment	[13]
2019	LC-Q/TOF-MS	201/484	Wastewater of a Sewage Treatment Plant	Comprehensive Target Analysis	[21]
2019	GC/MS	63/937	Tsunami sediment samples	Comprehensive screening and risk assessment	[41]
2018	GC/MS	127/940	Surface river water	Comprehensive screening and risk assessment	[4]
2018	GC/MS; LC/QTOF-MS	165/1153	River water	Comprehensive screening and risk assessment	[5]
2018	GC/MS	196/943	Municipal wastewater	Comprehensive analysis	[19]
2018	GC-MS LC-MS	109/1250	Wastewater	Assessment of the efficiency of wastewater treatment system	[2]
2018	GC-MS	Used for only PAH and OCP	Soils and Sediments	Analytical method development	[34]
2017	GC-MS	277/940	Floodwater	Comprehensive analysis	[7]
2016	GC-MS LC-MS	78/1300	Groundwater	Comprehensive screening	[27]
2016	GC-MS LC/QTOF-MS LC-MS	80/1300	Groundwater	Comprehensive screening	[39]
2015	GC-MS LC-MS	227/1300	River water	Water monitoring	[28]
2015	GC-MS	74/940	Groundwater	Comprehensive screening	[9]
2014	GC-MS	185/940	River sediment	Comprehensive screening	[6]
2014	GC-MS	195/940	Sediment	Comprehensive screening	[33]
2014	GC-MS	95/940	River water	Comprehensive screening	[36]
2013	GC-MS	184/888	Sediment	Comprehensive screening	[23]
2012	GC-MS	914	Sediment	Analytical method development	[24]
2011	GC-MS	114	N.a	Verification of analytical method	[42]
2010	GC-MS	95/940	River water	Comprehensive screening	[20]
2009	GC-MS	188/882	River water	Comprehensive screening	[22]

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2005	GC-MS	13/672 56/672 150/672 150/672	River water Soil Spinach Orange	Analytical method development	[26]

N.a: Not available

Among the studies conducted, four studies have focused on the development of analytical methods, primarily using GC/MS instruments. The first study published in 2005 analyzed only 672 compounds, and showed potential for application to environmental matrices such as river water, soil, and food samples such as spinach and oranges [26]. In 2011, Terumi Miyazaki et al. tested the accuracy of the AIQS-DB method [42], focusing on 114 compound groups of organochlorine pesticides and PAHs. The results showed a high level of accuracy. In 2012, GS. Kadokami published another study that expanded the AIQS-DB parameters to analyze up to 914 compounds and applied it to sediment analysis [24]. The maximum number of compounds that can be analyzed using AIQS-DB is 970 [8, 29, 31]. The application of AIQS-DB on LC/MS and LC-TOF-MS was first published in 2016 by Xuehua et al., with a range of over 300 compounds [39]. LC/MS and LC-TOF-MS are less frequently used than GC/MS, but up to 508 compounds have been constructed using these methods [16]. In total, both methods can analyze 1,478 compounds.

The number of compounds detected depends on the sample matrix. For example, in wastewater matrices analyzed by GC/MS in Japan, Ryo Omagari was able to detect the presence of 474 compounds in the influent wastewater soluble fraction [31]. In dust samples collected in Vietnam, Le Quang Huong et al. identified 288 compounds [15], and Trinh Thu Ha et al. identified 277 compounds in flood water samples [7]. Almost 200 compounds can be detected in sediment samples [6, 23, 33]. For samples analyzed by LC, around 201/484 compounds can be detected in wastewater samples [21]. AIQS-DB on LC/MS and LC-TOF-MS is often able to identify fewer compounds, which may be why studies using AIQS-LC are less common than those using AIQS-GC. The number of identified compounds demonstrates that AIQS-DB is very useful for simultaneous determination of pollutants in the environment.

In the nearly 20 years since GS. Kadokami's study was published, AIQS-DB has only been applied in studies of environmental samples collected in a few countries, such as Australia [1, 2], China [18, 19, 20, 27], Japan [23, 33, 36], Malaysia [17], Serbia [4], and Vietnam [3, 5-10, 12]. The application of AIQS-DB in environmental studies should be expanded to more countries.

3. Summary of AIQS Mechanisms, Instrumental Conditions

The AIQS-DB method, described by Ryo Omagari et al. in their research, utilizes retention times, mass spectra, and internal standard calibration curves stored in a database to identify and quantify chemical compounds [26, 31]. To achieve accurate results, the GC-MS instrument must be adjusted to specific conditions. The AIQS-GC and AIQS-LC methods were validated through the analysis of procedural blanks, duplicate samples, and certified reference materials. The beauty of the AIQS theory lies in the fact that if the measurement equipment conditions remain constant, the retention times and calibration curves of chemicals remain unchanged, thereby eliminating the need for standard chemical preparation. During AIQS analysis, the target ion's peak in a sample is located, and the target is identified by assessing the similarity between actual and predicted values using the extracted spectrum. Based on the accuracy of identification, the target is then given a rating of 1-5 stars. The AIQS-DB method holds great promise for revolutionizing the analysis of organic compounds.

Studies using the AIQS-DB method were all conducted using the GC or LC methods developed by GS. Kadokami. Therefore, publications only present quality assurance and quality control procedures. Analytical conditions for GC/MS and LC-TOF-MS instruments are briefly presented, while detailed equipment conditions are discussed below.

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Table 2. Summary of GC-MS and LC-TOF-MS conditions.

Item	GC-MS specification [26, 29 40,	LC-TOF-MS specification [25, 29]
Company	Shimadzu	Sciex, Agilent, Shimadzu
Column	DB-5 MS (30×0.25×0.25)	ODS (2.1×150×3) at 40°C
Temperature program/ Gradient	2 min at 40°C, 8°C/min to 310°C, 5 min at 310°C;	A95:B5 (0′) - A5:B95 (30′-50′) Flow Rate: 0.3 mL/min
Injection:	250°C/*splitless*	
Transfer line	300°C	
Ion source	200°C	
Carrier gas/Mobile phase	He	H2O (A): CH3OH (B) + 5mmol CH3COONH4
Linear velocity	40 cm/s, constant	
Ionization	EI	ESI-Positive at 3500V
Mode	SIM/SCAN (400-600 aum)	SCAN (m/z 50-1000

4. Prospects

The advantage of AIQS-DB is that it can simultaneously analyze up to 970 compounds on GC/MS equipment and 508 compounds on LC-QTOF-MS or LC/MS equipment. When combining the analysis results from AIQS-DB with multivariate statistics such as PCA or LDA, the geographical origin of the sample can be traced. Origin tracing studies have been developed for over 15 years. The types of samples used in origin tracing studies include food samples, agricultural products, rice samples, wine samples, meat samples, etc. The analysis techniques used in origin tracing are also diverse, such as GC/MS, LC/MS, ICP/MS, Isotope, FTIR, etc. The methods can be accurate concentration analysis, semi-quantitative analysis, or even just intensity signal analysis. All are methods that analyze multiple elements and compounds. Therefore, the AIQS-DB method is very suitable for application in origin tracing studies.

AIQS-DB is a highly promising technology that has the potential to revolutionize the way we determine food geographical origin traceability and identify bioactive compounds in plant medicine. The method combines retention times, mass spectra, and internal standard calibration curves registered in a database to identify and quantify chemical substances with high accuracy and reliability.

One of the major advantages of AIQS-DB is that it requires minimal preparation of standard chemicals, as the retention times and calibration curves remain constant if the measurement conditions are consistent. This saves time and resources, while ensuring that results are consistent and reproducible.

In terms of food geographical origin traceability, AIQS-DB can be used to accurately identify the geographic origin of food products based on the chemical composition of the sample. This can be especially important for products with geographical indications, such as wines, cheeses, and meats, where consumers rely on the origin to determine the quality and authenticity of the product. With AIQS-DB, we can ensure that the geographical origin of a product is accurately determined, which can help to prevent fraud and protect the reputation of the product.

AIQS-DB is also highly useful in the field of plant medicine, where it can be used to identify bioactive compounds that have therapeutic properties. Traditional methods of identifying bioactive compounds can be time-consuming and require a significant amount of resources. With AIQS-DB, we can quickly and accurately identify bioactive compounds, allowing us to develop more effective treatments and therapies for various medical conditions.

Overall, the potential applications of AIQS-DB are numerous and diverse. By providing accurate and reliable results with minimal preparation of standard chemicals, this technology has the potential to transform the way we determine food geographical origin traceability and identify bioactive compounds in plant medicine, leading to improved quality control and better health outcomes.

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5. Conclusion

Clearly, the application of AIQS-DB is very wide-ranging and has great potential to be applied in many fields because AIQS-DB can simultaneously analyze up to 1500 compounds. This is the largest chemical analysis database system in the world. However, until now, the number of studies applying AIQS-DB is still quite low, with only about 40 studies. Therefore, this article is eager for research applying AIQD-DB to be further developed and applied for various purposes such as in food analysis and source tracing. Moreover, developing a suitable dataset could potentially reduce the time and cost for discovering new bioactive compounds in plant medicine.

Author Contributions: For research articles with several authors, a short paragraph specifying their individual contributions must be provided. The following statements should be used "Conceptualization, X.X. and Y.Y.; methodology, X.X.; software, X.X.; validation, X.X., Y.Y. and Z.Z.; formal analysis, X.X.; investigation, X.X.; resources, X.X.; data curation, X.X.; writing—original draft preparation, X.X.; writing—review and editing, X.X.; visualization, X.X.; supervision, X.X.; project administration, X.X.; funding acquisition, Y.Y. All authors have read and agreed to the published version of the manuscript." Please turn to the CRediT taxonomy for the term explanation. Authorship must be limited to those who have contributed substantially to the work reported.

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