EVALUATING THE REMOVAL OF CONTAMINANTS OF EMERGING CONCERN IN DRINKING WATER AND WASTEWATER TREATMENT SYSTEMS

Report to the
WATER RESEARCH COMMISSION

by

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EXECUTIVE SUMMARY

BACKGROUND

Humanity faces a pressing challenge with water quality, compounded by increasing demand due to population growth, urbanization, and industrialization, while the supply diminishes due to contamination and resource exhaustion. Particularly acute in regions naturally scarce in water, such as parts of South Africa, this issue threatens food security and public health. South Africa anticipates a water supply deficit by 2025, necessitating rigorous management and control of water quality. Consequently, the country has embarked on large-scale efforts to reclaim and reuse wastewater to enhance water sustainability. However, the presence of contaminants of emerging concern (CECs) in treated wastewater poses serious health risks, emphasizing the urgency of identifying and assessing these contaminants.

Traditional water quality assessment methods focus on individual priority substances but fail to address the complex mixture of potentially toxic pollutants found in water systems. A holistic approach integrating chemical analysis with *in vitro* or *in vivo* toxicity tests is essential for a more realistic understanding of water quality and associated risks. Bioassays complement chemical analysis for monitoring water quality as they can detect both unknown and known chemicals that are biologically active in water or other environmental samples. Moreover, bioassays account for the effect of mixtures and groups of chemicals that exert their action through the same mode of action. Additional advantages of using effect-based methods (EBMs) include the use of small amount of sample, short exposure time, and their applicability to wide range of matrixes such as surface water, borehole water, wastewater, and sediments. Overall, EBMs are helpful for measuring the effects of mixtures of chemicals and detecting their potential toxicity to non-target organisms and humans, lowering the risk of neglecting transformation products, mixture effects, and hazardous unknown chemicals, identifying hot spots for contaminants, and linking chemical with ecological status. While this approach is gaining traction globally, its application in South Africa remains limited.

This project was part of a collaborative Water Research Commission project that explores the integration EBMs and chemical analysis to assess the efficiency of CEC removal in drinking water and wastewater treatment plants. Combining EBMs with chemical analysis offers a more holistic evaluation of water quality, helping to identify potential health risks and optimize treatment processes for cleaner, safer water. This report only focuses on the use of chemical analysis to characterise the CECs in source water, and their removal in drinking water and wastewater treatment systems. Additionally, this study also characterises the impacts of wastewater discharge on surface waters and determining the potential impacts of such discharges.

RATIONALE AND SCOPE OF THIS PROJECT

The rationale for this project stemmed from the recognition that the overexploitation of freshwater resources poses a significant threat to the welfare of humankind, as highlighted in various studies. To address this challenge, seawater desalination and the reuse of treated wastewater have emerged as promising strategies to meet increasing global water demands. However, treated wastewater, which is a significant component of water reuse strategies in Southern Africa, contains various contaminants of emerging concern (CECs), including agricultural and industrial chemicals, pharmaceuticals, and personal care products. These contaminants pose risks to ecosystems and human health, necessitating thorough assessment and monitoring.

Chemical analysis methods, particularly chromatography-based techniques such as High-performance liquid chromatography (HPLC) and Gas Chromatography (GC) coupled with mass spectrometry, have been instrumental in detecting and quantifying. However, relying solely on chemical analysis for water quality monitoring has limitations, including the inability to account for the toxic effects of (un)known chemicals,

mixtures, and compounds present below detection limits. To address these limitations, integrating biological tools with chemical analysis through EBMs has been advocated. EBMs, particularly bioassays, offer a comprehensive approach to assess water quality by measuring the effects of chemical contaminants on ecotoxicological endpoints.

The primary focus of this report is on the chemical analysis aspect of the project, which entails various stages including water sampling, sample preparation/extraction, solvent exchange and chemical analysis using various techniques for assessing water quality. This component aims to complement *in vitro* and *in vivo* bioassays by providing valuable insights into the composition of intricate chemical mixtures present in water samples. To enhance the effectiveness of assessments, we explored the use of passive sampling techniques, which offer advantages such as in-situ collection of target analytes without disturbing the bulk solution. The utilization of passive samplers, in conjunction with bioassays, represents a promising approach for conducting comprehensive evaluations of water quality. To comprehensively assess the performance of various treatment technologies across a spectrum of water sources, we included conventional drinking water, direct and indirect water reuse, desalination, as well as both industrial and domestic wastewater. This comprehensive approach aimed to capture the breadth of water sources subject to treatment processes. Each water type presents unique challenges and considerations, ranging from contamination profiles to regulatory requirements, thereby necessitating a holistic assessment approach.

METHODS

Water samples were collected from various key points to comprehensively assess water quality. Samples were obtained from a conventional drinking water treatment plant, desalination plant, direct and indirect potable water reuse plants, domestic and industrial wastewater treatment facilities, as well as from upstream and downstream locations of the respective effluent receiving rivers and dams utilized as sources for drinking water treatment plants. Both grab sampling and composite sampling methods were employed at each designated sampling site to ensure representative sampling. Consideration was given to the hydraulic retention time of each treatment plant during the collection of influents, intermediate treatment steps, and effluent water samples. To maintain sample integrity, collected samples were promptly placed in ice-filled coolers for transportation to the laboratory, where they were processed and subjected to chemical analysis and effect-based assays within a 48-hour timeframe. In addition to traditional sampling methods, various passive sampling techniques such as Membrane Assisted Passive Sampler (MAPS), Chemcatcher, and Polar Organic Chemical Integrative Sampler (POCIS) were investigated for routine monitoring of emerging contaminants in aquatic systems. Extracts from passive sampling devices were utilized for extensive chemical analyses.

The effectiveness of different Dispersive Liquid-Liquid Microextraction (DLLME) and Solid Phase Extraction (SPE) methods was evaluated using synthetic mixtures in laboratory settings. A mixture encompassing a range of environmentally relevant chemicals with diverse physicochemical properties was prepared for this purpose. Various sorbents for SPE, including Hydrophilic-Lipophilic Balance (HLB), and mixed-mode anion and cation exchange (MAX and MCX), were tested and optimized to maximize recovery efficiency. The extraction method demonstrating the highest recovery rate for a maximum number of components in the mixture was selected for the extraction of real water samples for both bioassays and chemical analysis. Chemical analysis was performed using state-of-the-art liquid chromatography-mass spectrometry (LC-MS) or gas chromatography-mass spectrometry (GC-MS) depending on the analytes of interest. Advanced instruments including UHPLC-QTOF-mass spectrometry (Bruker, Germany), LC Q Exactive HRAM spectrometry (ThermoFisher Scientific, Germany), GC-QTOF-mass spectrometry (Leco, USA), and ICP MS (PerkinElmer, UK) were employed for both target and non-target analysis of chemical pollutants in the water samples.

RESULTS AND DISCUSSION

The drinking water samples collected from the four drinking water treatment technologies assessed (i.e. conventional, desalination, direct and indirect drinking water plants) met the regulated levels in the SANS 241 drinking water quality standard for various parameters: pH at 25°C of ≥5 to ≤ 9.7, conductivity at 25°C of ≤ 170 (mS/m), total dissolved solids of ≤ 1200 ng/mL, and operational turbidity of ≤ 1. These parameters were monitored by the drinking water treatment plants. Similarly, the microbiological determinants were monitored by the treatment plant laboratories and did not exceed the standard limits as per regulation. It should be noted that the analysis of the disinfection by-products (DBPs) was not conducted for this study because of the volatile nature of many DBPs.

In this report, we focus on the analysis of contaminants of emerging concerns. To comprehensively assess the presence of organic chemicals across various treatment technologies, we conducted a non-targeted chemical analysis. Identified compounds may not necessarily be under consideration for future development or regulatory standards, but they serve as site-specific indicators of source and product water composition and treatment efficacy. Chemical analysis of source water through the entire water cycle was conducted to assess the performance of various water drinking water treatment technologies. These treatment technologies included conventional drinking water treatment, direct and indirect water reuse as well as desalination processes. In general, source water exhibited a relatively higher abundance of chemical contaminants, compared to the product water meaning in all treatment technologies there were some levels of reduction in the abundance of chemicals from source water through intermediate stages to the final produce water. In some cases, the intermediate and product water showed a comparable abundance of chemical contaminants.

When compared to indirect and conventional drinking water technologies, the source water (wastewater effluent) for the Direct water reuse technology showed a relatively higher chemical load, with conventional treatment exhibiting the lowest load. This suggests a higher risk associated with direct wastewater reuse and underscores the need for advanced treatment technologies to effectively treat this complex water matrix. Notably, distinct groupings indicating a different chemical profile of direct source water compared to conventional and indirect source water were observed. The variation within these groupings exceeded 20% of the sum of the t principal components exhibiting the most variation. Despite several reports suggesting marine environments as major reservoirs for various chemicals, the LC-MS results obtained from the desalination plant samples showed none of these chemical groupings. Instead, only substances classified as fumigants, industrial surfactants, and plasticizers were noted. These compounds likely originated from the biocides and other chemicals used in the desalination treatment process. Furthermore, principal component analysis (PCA) separated the sampling approaches into distinct groupings. The scores and loading plots of the sampling approaches showed a significant difference in classes of compounds accumulated by the three sampling techniques.

The chemical characterization of wastewater discharges into receiving surface waters yielded significant insights into various parameters and contaminant profiles. Across different sampling points, the pH of water samples ranged from 6.38 to 7.95, which falls within the acceptable health risk range of 6.50 to 8.50. Notable disparities were observed in influent pH between domestic and industrial wastewater treatment plants. WwTP1, which receives both domestic and industrial waste, exhibited acidity with a pH of 6.38, but secondary treatment raised the pH to 7.35. Conversely, WwTP2, dealing solely with domestic waste, showed higher influent pH values. In comparison to the Department of Water Affairs (DWAF) published wastewater discharge range (5.5 to 9.5), all measured pH values at influent, effluent, upstream, and downstream sites were within acceptable limits. Electrical Conductivity (EC) ranged from 220 to 1268 µS/cm, with elevated levels in WwTP2 effluent and WwTP1 anoxic samples, indicating high objectionable levels of dissolved salts. Although WwTP1 influent exceeded the target limit, secondary treatment reduced EC concentrations. Total Dissolved Solids (TDS) concentrations ranged from 120 to 634 ppm, complying

with regulatory guidelines, and signifying acceptable TDS levels in the water. Turbidity levels ranged from 0.1 to 51 NTU, with influent samples exhibiting higher turbidity, exceeding domestic use standards but effluent meeting discharge standards set by the Department of Water Affairs (DWA). A total of 1560 organic compounds were identified, with approximately 54% detected exclusively in domestic WwTP2 samples and 46% in industrial WwTP1 samples. Endogenous metabolites were the most detected, followed by pharmaceuticals like antiretroviral drugs (ARVs) and non-steroidal anti-inflammatory drugs (NSAIDs). Industrial contaminants such as glycol dimethyl ether and 3,3'-dimethoxybenzidine were also identified. Effluents from both industrial and domestic WwTPs emerged as the main source of downstream surface water contamination by these compounds. The reduction in detected compounds downstream suggests the efficacy of wastewater treatment processes. However, non-formal settlements near domestic WwTPs and overflows at wastewater treatment plants, leading to raw sewage discharge into receiving rivers, contribute to upstream contamination.

GENERAL

A passive sampling approach was employed to evaluate both the desalination treatment technology and the impacts of treated wastewater discharge on a receiving river. In the desalination plant, samplers were deployed in the source and product water storage tanks, while for the impacts of discharge experiments, samplers were placed at the effluent channel, upstream and downstream of the receiving river. Three types of passive samplers were investigated namely: Polar organic Integrative Passive Samplers (POCIS), Membrane Assisted Passive Sampler (MAPS) and Chemcatcher. For each passive sampler, two types were fabricated for deployment at each sampling site, one sampler for toxicity profiling and the other sampler for chemical analysis. Prior to deployment, the passive samplers meant for chemical analysis were spiked with performance reference compound (PCR), and the ones intended for toxicity profiling were not spiked with PRCs. Laboratory and field blanks were also fabricated as part of quality assurance. Laboratory blanks remained in the laboratory and were used to account for any contamination during the processing and analysis of the samplers.

The field blanks were used to account for contamination during transport to and from study sites, exposure to airborne contaminants during the deployment and retrieval periods, and contamination from storage, processing, and analysis. Field blanks were stored in airtight containers and transported to the field sites in insulated containers filled with blue ice. At the study sites and during the deployment and retrieval operations, the lids of field blank airtight containers were opened to allow for exposure to the surrounding air. All samplers were deployed in a stainless-steel canister for a period of 14 days. Grab samples of water were collected at deployment and retrieval of passive sampling devices using 1L amber glass bottles considering the hydraulic retention time of the treatment process.

Desalination results indicated that membrane-assisted samplers predominantly accumulated fumigants, while POCIS and SPE extracts contained industrial chemicals like Amino-PEG3-C2-acid. MAPS accumulated mainly non-ionizable compounds at pH 6.8 which become ionized at higher pH levels, while POCIS-HLB samplers accumulated polar organic compounds. Passive sampling devices detected more compounds than grab sampling. A target list of compounds was compiled via robust non-target analysis/identification using mass spectrometry data. Accurate masses of compounds absent in procedural blanks were extracted, and possible molecular formulas were generated. Online databases like KEGG, CHEBI, HMBD, and FOR-IDENT were used for annotation. Screening parameters included mass accuracy, isotopic fit, signal-to-noise ratio, and MS/MS information. Suspect compounds were verified using spectral libraries and in silico fragmentation platforms. Calibration levels for quantitation followed EPA Method 1694 and 1699, with none of the compounds exceeding reportable limits.

CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE RESEARCH

Overall, the study highlights the effectiveness of various treatment technologies in providing safe drinking water, identifies potential risks associated with direct wastewater reuse, underscores the specific contamination patterns associated with desalination processes, and emphasizes the challenges posed by overflows at wastewater treatment plants, leading to raw sewage discharge into receiving rivers. Additionally, the use of advanced analytical techniques and passive sampling approaches enhances our understanding of contaminant profiles and distribution in water systems. Based on the limitations encountered in the current study, it is recommended that future research undertakings focus on addressing key gaps and enhancing the robustness of the findings. We recommend allocating resources and time to conduct fully-fledged quantitation experiments of the lists of contaminants identified in this work, adhering to established standards and protocols such as EPA Method 1694 and 1699. This includes the incorporation of isotopically labelled compounds as surrogates and internal standards to ensure accurate quantitation, as well as the implementation of rigorous quality control and assurance workflows to validate analytical measurements and ensure data reliability. Additionally, we recommend prioritizing the evaluation of passive sampling approaches and utilizing extracts from the sampler to evaluate a battery of bioassays targeting various toxicological pathways. We believe these future studies can contribute significantly to our understanding of the environmental implications of wastewater treatment processes and facilitate the development of sustainable water management strategies.

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LIST OF ABBREVIATIONS

ACR	Acute-to-chronic ration
AGC	Automatic Gain Control
ARGs	Antibiotic resistance genes
ARVs	Antiretroviral drugs
BEQ	Bioanalytical equivalent concentrations
BNR	Biological nutrient removal
CCT	Chlorine contact tank
CEC	Contaminants of emerging concern
CHEBI	DBPs Disinfection by Products
DDA	Data dependant analysis
d-DwTP	Direct drinking water plant
DLLME	Dispersive Liquid-Liquid Microextraction
DRC	Dynamic reaction control
DWAF	Department of Water Affairs
EBMs	Effect-based methods
EBT	Effect-based trigger
EC	Electrical Conductivity
EFS HRAM	Environmental Food Safety High Resolution Accurate Mass
EPA	Environmental Protection Agency
EQS	Environmental quality standards (EQS) or guideline values (GV).
GAC	Granular activated carbon
GC	Gas Chromatography
GC-MS	Gas chromatography-Mass spectrometry
GC-QTOF MS	Gas Chromatography – Quadrupole Time of Flight Mass spectrometry
GV	Guideline values (GV).
HCD	High energy collision dissociation
HLB	Hydrophilic-Lipophilic Balance
HPLC	High-performance liquid chromatography
ICP MS	Inductive Coupled Plasma Mass spectrometry
ind-DwTP	Indirect drinking water plant
KED	Kinetic energy discriminator
KEGG	Kyoto Encyclopaedia of Genes and Genomes
LC-MS	Liquid chromatography-Mass Spectrometry
LLE	Liquid-liquid extraction
MAPS	Membrane Assisted Passive Sampler
MAX	Mixed-mode Anion exchange
MCX	Mixed-mode Cation Exchange
MIT	Maximum injection time
NIST	National Institute of Standards and Technology
NOAEL	No observed adverse effect levels
NOEC	No observed effect concentrations
NSAIDs	Non-steroidal anti-inflammatory drugs
PCA	Principal Component Analysis
PES	Polyether sulphone
POCIS	Polar Organic Chemical Integrative Sampler
REP	Relative effect potencies
S/N	signal-to-noise

SANS	South African National Standard
SDB	Styrene Divinyl Benzene
SIMONI	Smart Integrated Monitoring
SPE	Solid Phase Extraction
SPME	Solid phase microextraction
SSD	Species sensitivity data
STD	Standard
TB	Tuberculosis
TDS	Total Dissolved Solids
TOrC	Trace organic compounds.
TWA	Time-weighted averaged
UHPLC-QTOF MS	Ultra High-performance Liquid chromatography – Quadrupole Time of Flight
UNISA	University of South Africa
UP	University of Pretoria
US	United States
WHO	World Health Organisation
WRC	Water research commission
WwTP	Wastewater Treatment Plant

1 BACKGROUND

1.1 INTRODUCTION

The contamination of aquatic environments by a diverse array of anthropogenic compounds is increasingly prevalent, leading to the presence of complex contaminant mixtures that pose significant threats to aquatic ecosystems (De Baat et al., 2020). Micropollutants, also known as trace organic compounds (TOrC) or contaminants of emerging concern (CEC), have been identified as key contributors to water quality degradation (Dopp et al., 2019). These micropollutants elicit adverse biological effects in organisms, necessitating improved assessment methods to accurately evaluate their impact on aquatic ecosystems (Dopp et al., 2019). CECs enter the aquatic environment following various routes such as discharge of treated or untreated wastewater into receiving water bodies, industrial effluents, hospital effluents, leakage or overflow of municipal sewers, landfill leachate and runoff from agricultural and urban areas where effluent and/or sludge from wastewater treatment is used for irrigation activities. Among the abovementioned sources, wastewater treatment plants (WWTPs) are of particular concern since they constantly introduce CECs into the aquatic environment (Tran et al., 2018).

Traces of emerging contaminants have been reported in the aquatic environment such as surface water and wastewater of which all of them can be a source of potable or non-potable water reuse. Studies of sources of drinking water have detected CECs of wastewater origin such as caffeine, atrazine, codeine, carbamazepine, dieldrin, metolachlor, de-sulfinyl fipronil and metformin in samples collected from sources of drinking water located downstream of treated wastewater release locations (Glassmeyer et al., 2005). In South Africa, studies such as that of Wanda et al. (2017), Yahaya et al. (2019) as well as Agunbiade F.O and Moodley B. (2015) have demonstrated the occurrence and distribution of emerging contaminants such as caffeine, galaxolide, bisphenol A, 2-nitrophenol, aspirin, nalidixic acid and bezafibrate in different aquatic environments such as a river, dam, and wastewater. In addition, antimicrobial drug resistance and antibiotic resistance genes (ARGs) have been recognized as an international threat associated with the presence of emerging contaminants in the environment, particularly antimicrobial drugs (Kumar and Pal, 2018). Wastewater treatment plants are known to offer environments conducive to the growth and proliferation of microorganisms as well as the dissemination of ARGs (Krzeminski et al., 2018).

For that reason, multi-drug-resistant pathogens are evolving at an alarming rate. In 2017, WHO reported annual death of about 250, 000 people by drug-resistant Tuberculosis (TB), demonstrating antibiotic-resistant infections being the greatest risk to human health (Krzeminski et al., 2018). In Europe, antimicrobial resistance is associated with mortality of 25,000 annually and 23,000 people in the US (Sachdeva et al., 2017). Although there is no quantitative data in Africa, the effect of antimicrobial drug resistance on public health is expected to be immense (Ekwanzala et al., 2018). Thus, a comprehensive assessment and monitoring of such water are vital as it gives the health risks associated with the exposure to such contaminants.

Various analytical methods have been developed and used for contaminant identification and quantification (Rasheed et al., 2018; Huckins et al., 2006; Nyoni et al., 2017). Attributed to their higher selectivity, sensitivity, and efficiency, chromatography-based techniques mainly High-performance liquid chromatography (HPLC) and Gas Chromatography (GC) hyphenated to mass spectrometry (HPLC/GC-MS) or tandem mass spectrometry (HPLC/GC-MS-MS) have been the most commonly used techniques for the detection and determination of CECs (Martín-Pozo et al. 2018; Lorenzo et al., 2018; Cahill et al., 2004). HPLC is generally used for non-volatile and polar compounds, while GC is applied for compounds that are intrinsically volatile or can be converted to volatile through derivatizations (Lorenzo et al., 2018). These techniques have enabled researchers to perform targeted analysis as well as to detect other micropollutants which would have gone undetected using the targeted methods, with the help of suspect screening and screening for unknowns (Assress et al., 2019; Newton et al., 2018; Alygizakis et al., 2018). Current water

quality monitoring and management are mostly based on chemical analysis of selected priority substances, whose levels should not be above recognized environmental concentrations that are linked to known detrimental effects (van der Oost et al., 2016; WHO, 2017). However, there is an increase in awareness that the use of chemical analysis alone for water quality monitoring does not take into consideration the effect of unknown chemicals, mixtures, transformation products, and chemicals present at below their detection limit (Escher et al., 2018; Brack et al., 2019). In addition, new compounds are constantly released to the aquatic environment which necessitates updating the priority list continuously. The current approach of water quality assessment is inadequate to evaluate the possible harmful effects that chemical pollution has on human health and/or aquatic organisms and to devise mitigation steps to minimize the impacts of chemical contamination (Brack et al., 2019; van der Oost et al., 2016).

Recently, the need for integrating biological tools with chemical analysis (targeted and untargeted) has been highlighted by several researchers and regulatory bodies (Connon et al., 2012; Wernersson et al., 2015; Schulze et al., 2017). To this end, effect-based methods (EBMs) have been found to be useful in establishing cost-effective and rational water quality monitoring programs, improving the environmental significance of the assessment, and linking chemical and ecological information (Connon et al., 2012). EBMs are bioanalytical methods that employ the response of in vitro (cellular) bioassays and/or in vivo (whole organism) to detect and measure the effects of chemical contaminants on ecotoxicological endpoints of concern (Escher et al., 2018). EBMs determine particular biological effects of complex chemical mixtures in an environmental sample without the need for prior knowledge of the chemical composition (Houtman et al., 2018). Furthermore, EBMs are risk-scaled, with potent compounds having a greater contribution to the mixture effect than chemicals with lower potency at similar concentrations (Escher et al., 2018; Leusch et al., 2018). Depending on the monitoring approach employed, effect-based methods are classified into three major groups: bioassays, biomarkers and ecological indicators (Milinkovitch et al., 2019).

Bioassays involve in vitro and/or in vivo test batteries to measure the toxicity of environmental under controlled laboratory experimental conditions. These include tests that signify different pathways of cellular toxicity such as cell viability, adaptive stress reactions, receptor-mediated responses, and xenobiotic metabolism, as well as early-life in vivo assays suggestive of apical effects (Jiang and Li, 2019; Wernersson et al., 2014). Biomarkers use biological responses at the individual or sub-individual levels observed in organisms exposed in the field. They incorporate several subtle physiological/biochemical parameters to measure geno-toxicological, endocrinological, immunological, and behavioural stresses at an individual and/or sub-individual levels (Blaise et al., 2009).

Ecological indicators employ variations in the structure or function measured at population and community levels (Wernersson et al., 2014). In this approach, several numerical dimensional parameters are uttering the overall status of an ecosystem through the determination of various aspects of the structure and the sensitivity of population/community (e.g. abundance, diversity, and/or tolerance) are commonly used as ecological indices (Martinez-Haro et al., 2015). Overall, measurements at the community level are more suitable for evaluating the ecological quality of aquatic environments, while the biomarkers/bioassays are particularly useful as early warning systems and to establish the causes of ecological damage, permitting a better understanding of the cause-and-effect relationships (Martinez-Haro et al., 2015). In line with the objectives of this project, further discussions on effect-based methods will focus mainly on the bioassay approach. Water quality assessment using the bioassay approach generally involves sampling, sample pre-treatment and toxicity testing using a battery of in vitro and in vivo bio-tests. Both in vivo and in vitro bioassays commonly require representative environmental samples to be collected. Consequently, similar to chemical analysis, the frequency of sampling and sample pre-treatment are critical aspects that should be considered during sampling for bioassay tests. Even though the selection of sampling approaches is determined by the objective sought to be achieved, grab sampling (Jia et al., 2015; Leusch et al., 2014; Leusch et al., 2018; Polloni-Silva et al., 2017; Daniels et al., 2018; Neale et al., 2017) and composite sampling (Välitalo et al.,

2017; Deng et al., 2017; Lundqvist et al., 2019; Jálová et al., 2013; Gehrmann et al., 2018) and passive sampling (Jálová et al., 2013; Novák et al., 2018; De Baat et al., 2019; Toušová et al., 2019) are among the commonly reported sampling techniques in the literature.

Overall, it has been noted that the analysis of samples collected using the grab sampling approach provides only a snapshot of the concentrations of the pollutants at the time of sampling, not accounting variations of pollutant concentrations over time and missing episodic pollution occurrences. These limitations could be overcome by increasing the sampling frequency or to implement automated sampling techniques that can take large volume water samples over a specified period. However, such types of sampling are resource-intensive, laborious, and require a secure site as well as significant extraction of a large volume of water (Vrana et al., 2005). In the recent past, alternatives that can overcome these challenges have been sought. Among these, passive sampling methods have shown much promise as tools for measuring aqueous concentrations of a wide range of priority pollutants. Passive samplers avoid many of the problems outlined above since they collect the target analyte in situ and without affecting the bulk solution. Depending on sampler design, the mass of pollutants accumulated by a sampler should reflect either the concentration with which the device is at equilibrium or the time-weighted averaged (TWA) concentration to which the sampler was exposed (Jönsson and Mathiasson, 1999; Vrana et al., 2005).

Although a combined strategy of passive sampling followed by effect-based bioassay measurements has been proposed in the past (Wernersson, 2014; Hamers et al., 2013, 2010; Sabaliunas et al., 1998), the combination of both techniques has not been sufficiently scrutinized yet to serve as a serious alternative to the costly chemical monitoring. This work will explore prospects of combining toxicity profiling with time integrative passive sampling techniques [such as (1) Membrane Assisted Passive Sampler (MAPS), (2) Chemcatcher and (3) Polar Organic Chemical Integrative Sampler (POCIS)] and its applicability for water quality assessment. Extracts from passive sampling devices will be used for extensive chemical analyses and battery of in vitro bioassays covering a range of toxicological endpoints. The decision on the use of MAPS and POCIS devices will be to obtain a more representative sample of the entire range of organic contaminants than can be obtained with a single sampler (Petty et al., 2004). At the same time POCIS will be used for non-polar as well as for the more hydrophilic compounds, while MAPS will be for non-ionizable compounds at the sample pH but once in the acceptor are ionized and enriched.

Compounds that are ionized at the pH of the sample solution do not dissolve into the membrane since they are too polar. Similarly, larger molecules have slow diffusion in the membrane and will be excluded. During the deployment of passive samplers in the field, grab environmental water samples will be collected and extensively characterized using chemical analysis and bioassay methods. However, given the complex matrix and the trace level of contaminants in environmental waters, sample preparation prior to bioassay analysis is commonly required (Neale et al., 2018, Leusch et al., 2012). This could involve filtration to exclude suspended particles, clean-up, and enrichment. The filtration can be made during sampling, extraction step or separately by employing various kinds of filters having different physical forms and different diameters, glass fibre filters with the diameters in the range of 0.22 to 1.20 µm being the most reported (Locatelli et al., 2016).

The use of several clean-up and enrichment methods such as evaporation, solid-phase extraction (SPE), biological solid-phase micro-extraction (SPME), dispersive liquid-liquid microextraction (DLLME) and liquid-liquid extraction (LLE) has been mentioned in the literature (Kunz et al., 2017, Smital et al., 2013). The selection of sample clean-up and enrichment techniques is generally made in such a way that it meets three main demands. First, the method should be able to recover compounds with a broad range of physicochemical properties to make sure the inclusion of as many contaminants as possible as bioassays are often applied to water samples with no prior knowledge of contaminants composition (Houtman et al. 2007). Second, the method should provide adequately high recoveries to attain the desired sensitivity during

the bioassay and to get a good estimation of the total activity in the sample. In bioassays, usually, an enrichment factor of 2000-20,000 is necessary unlike the common enrichment factor of 10-1000 used in chemical analysis (Houtman et al. 2007, Kolkman et al., 2013). Third, the method should allow the use of mammalian/microbial cell non-toxic organic solvent compatible with both chemical analysis and bioassay (Kolkman et al., 2013). To this end, solid-phase extraction, DLLME and SPME will be used in this work since it has been preferred by researchers more often than the other methods (Neale et al., 2017, Liu et al., 2015, Di Paolo et al., 2016, Neale et al., 2018, Jia et al., 2015, Leusch et al., 2018).

Although effect-based methods can identify the effects of mixtures, coupling high sample enrichment and sensitive bioassays mean that toxic effects can be easily detected even in clean samples such as highly treated recycled water and drinking water (Jiang and Li, 2019). However, the detection of an effect does not necessarily mean that the water quality is unacceptable. For investigation and monitoring purposes, it becomes vital to establish thresholds, namely effect-based trigger values (EBT), that distinguish between poor quality and acceptable water quality pertaining to the organic pollutants, with an exceedance of EBT warranting further investigation (Escher et al., 2018). EBT should be sufficiently protective for the ecosystem and human health, while at the same time, avoiding unnecessary and expensive extra protection measures (Brand et al., 2013, Dingemans et al., 2019).

Several different approaches are reported in the literature to derive EBTs, based on either guideline values and human health thresholds or ecotoxicity data, and these are:

- The translation of concentrations of reference compounds that are considered nontoxic in vivo to the levels measurable in vitro. This approach is applied when an adverse effect as the point of departure (POD). For example, Brand et al. (2013) developed EBTs using this approach for hormonal activities in drinking water. This approach was limited to health based EBTs and needed data such as estimated bioavailability, protein binding in blood and acceptable daily intake (ADI) values (Brand et al., 2013). However, this approach does not consider the effect of mixtures.

- The derivation of EBTs based on available environmental quality standards (EQS) or guideline values (GV). GV or EQS values are derived from no observed adverse effect levels (NOAEL) in test animals and no observed effect concentrations (NOEC) for environmental organisms. The EQS or GV is then translated to bioanalytical equivalent concentrations (BEQ) and used as EBT. This approach has been applied by Kunz et al. (2015) for surface waters and Jarošová et al. (2014) for wastewaters to determine the threshold of estrogenic related activity (Jarošová et al., 2014, Kunz et al., 2015). The second approach is limited to assays in which one or a few compounds with known EQS are responsible for the effect.

- Escher et al. (2015) proposed the derivation of EBT using a read-across approach based on the available water quality guidelines. In this approach, bioassay effect concentrations are matched with relevant reference chemicals and guideline values. BEQs were computed from relative effect potencies (REP) and GVs and were used to construct a cumulative distribution per bioassay. The fifth percentile in the resulting distribution was then used as the EBT for that particular assay. Even though it accounted for the mixture effect, this approach was mainly applied to in vitro bioassays (Escher et al., 2015).

- Escher et al. (2015) proposed another approach to derive EBTs from European EQS for a large group of in vitro and in vivo bioassays by accounting mixture effects for the endpoints which can be activated by many chemicals. The calculated EBTs were compared with measured environmental effects for surface water and wastewater. Since European EQS are much lower than quality guidelines for drinking water, EBTs derived using this approach are believed to protect human health (Brion et al., 2019).

- EBTs were computed by van der Oost et al. (2016) for several in vitro bioassays in the Smart Integrated Monitoring (SIMONI) strategy, which is part of the conceptual framework of the Ecological Key Factors for the ecological assessment of water quality issues. SIMONI-EBTs for non-specific endpoints were derived from acute effect concentrations (ECs) supposing an acute-to-chronic ratio (ACR) of 10 (ten) and further safety factor of two for extraction recovery. Furthermore, ECs from in vivo data was used to evaluate the lowest observed chronic BEQ data (safe BEQ), BEQ level that negatively affects 5% of the water organisms as derived from species sensitivity data (SSD) (HC5-BEQ) and bioassay results from eight ecologically healthy sites (Background or benchmark BEQ). These three BEQ data were then used to compute for SIMONI-EBT values for the selected in vitro bioassays.

The different approaches use different parameters for the derivation of EBT. It can, therefore, be expected that the different methods will result in slightly different EBTs. Although toxic equivalency methods assume that compounds act via a well-known single mechanism such as activating a receptor, simultaneous antagonistic and agonistic activation can likely occur. Effects predicted from addition effect models can consequently diverge from the real effects observed in the water samples. It has been recommended, as a result, that EBTs be calibrated with real water samples with known compositions to ensure EBTs are exceeded only at the contaminated sites (Dingemans et al., 2019).

1.2 CONTEXTUALIZATION AND OBJECTIVE

The occurrence of emerging contaminants in treated municipal wastewater is of serious concern due to the associated potential health risks (Chen et al., 2019). The commonly used approach of water quality and risk assessment largely focuses on individual compounds listed as priority substances. However, chemical analysis reveals that the water systems contain a mixture several hundreds of potentially toxic chemical pollutants. The cocktail of chemicals in the water systems cause greater impacts on human health and the environment than the individual compounds. This implies that the use of chemical analysis alone is not sufficient to protect water systems from chemical pollution and a more comprehensive approach that accounts the effect of the mixture is necessary to provide a more realistic base for water quality protection, assessment, monitoring and management (Posthuma et al., 2019). Recently, increased attention has been put on the employment of in vitro or in vivo toxicity tests together with chemical analysis methods (i.e. EBM) to measure water quality and related potential risks. Several approaches have been developed for identifying chemical contaminants that majorly contribute to the toxicity so that appropriate measure can be implemented. Unlike in Europe, China, and America, the effect-based analysis of CECs is very limited in South Africa.

The objective of this study was evaluate the chemical removal efficiency of treatment plants, and assessment of the impact of wastewater discharges on the receiving water bodies such as surface water, will be conducted.

2 EXPERIMENTAL

2.1 INTRODUCTION

To achieve the aims of the project, samples were collected from different case studies / types of water treatment plants, including conventional drinking water treatment plant (DwTP), indirect potable water reuse plant (Ind-DwTP), direct potable water reuse plant (d-DwTP), a desalination plant (Des-P), as well wastewater treatment plants (Figure 2.1). The drinking water samples were collected from the four drinking water treatment technologies, i.e. conventional desalination, direct and indirect potable water reuse plants. As part of characterizing potential impacts of wastewater discharges to surface water, two wastewater treatment works were chosen as case studies. One facility, referred to as WwTW 1, treats both domestic and industrial waste, while the other facility, referred to as WwTW 2, exclusively treats domestic wastewater.

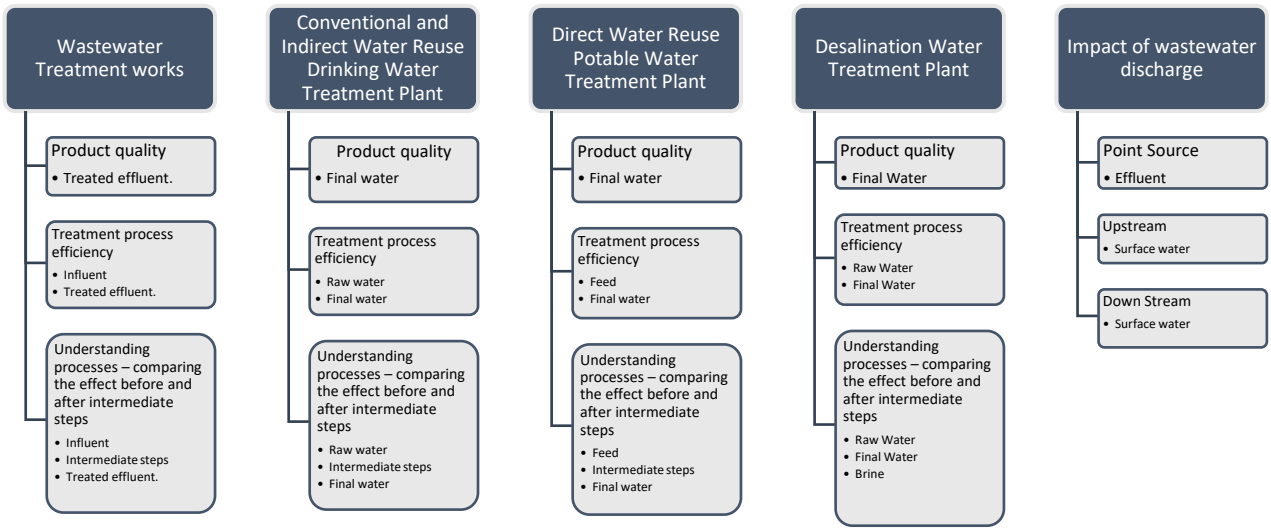


Figure 2-1: A summary of the sample types from different types of water treatment plants, including wastewater treatment works, a desalination plant, conventional drinking water treatment plant, as well as indirect and direct potable water reuse plants.

2.2 DESCRIPTION OF CASE STUDY SITES

2.2.1 Conventional Drinking Water treatment plant (DwTP)

The conventional drinking water treatment plant evaluated in this project, abstracts raw water from a wastewater discharge-free impoundment through canals and gravity pipelines. Before the water can be distributed to the consumer it undergoes several treatment steps such as screening, coagulation, flocculation, sedimentation, carbonation, and sand filtration followed by primary and secondary disinfection steps (Figure 2-2). Grab water samples were collected after every treatment process of the DwTP.

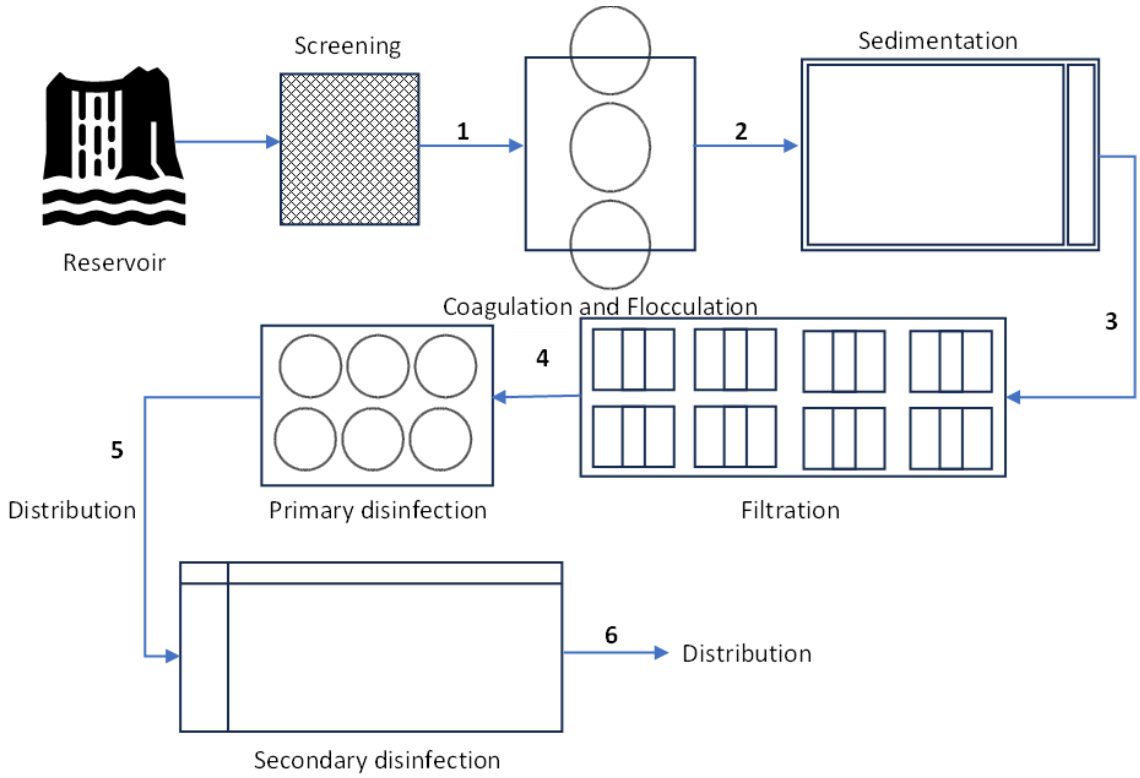


Figure 2-2: Conventional drinking water treatment plant (DwTP) layout showing the treatment train process and sampling points. (1) Raw water, (2 to 5) Intermediate steps and (6) final water.

2.2.2 Indirect potable water reuse plant (ind-DwTP)

The Indirect potable Water Treatment Plant (Ind-DwTP) abstracts raw water from an impoundment within the crocodile catchment area. Commercial farming practices nearby contribute to the presence of fertilizers and pesticides in the source water, potentially affecting its quality. Furthermore, the inflow of chemically enriched water through the channel from wastewater-receiving rivers further exacerbates poor water quality in the artificial lake.

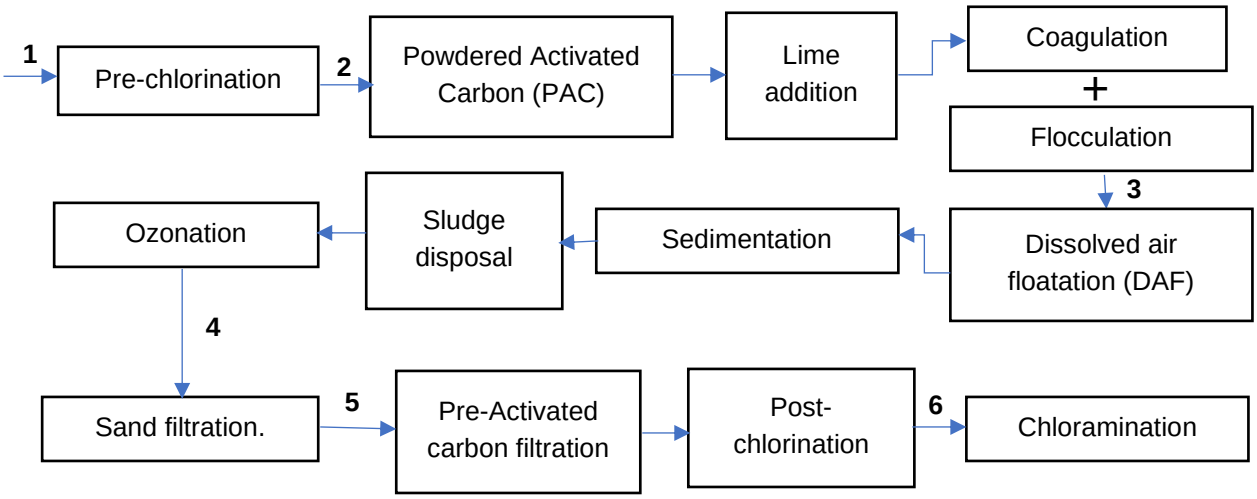


Figure 2-3: Indirect potable Water Treatment Plant (ind-DwTP) layout showing the treatment train process. (1) Raw water, (2 to 5) Intermediate steps and (6) final water.

The treatment process, illustrated in Figure 2-3, involves multiple stages which include pre-ozonation, flocculation, dissolved air floatation, inter-ozonation, sand filtration, granular activated carbon (GAC) filtration, disinfection, and chemical dosing. Grab water samples were collected after every treatment process of the ind-DwTP (1 to 6) with raw water (1) samples were collected from the intake tap before undergoing a series of treatment processes, Intermediate steps (2 to 5) and the product water samples (final water) were collected from a dedicated sampling tap after completion of the purification process.

2.2.3 Direct potable water reuse plant (d-DwTP)

A direct water reuse plant (d-DwTP) is a demonstration facility that receives treated effluent directly from wastewater treatment works and employs advanced technologies to treat it to potable drinking water standards. The treatment train processes include advanced oxidation, biologically activated filters, and ultrafiltration membranes, which collectively provide multiple barriers against contaminants of emerging concern, such as nanomaterials, pharmaceuticals, and endocrine disruptors (Figure 2-4). Plant staff assisted with the collection of grab water samples from both the treated effluent from wastewater treatment works (1) and (2) final water of the demonstration plant.

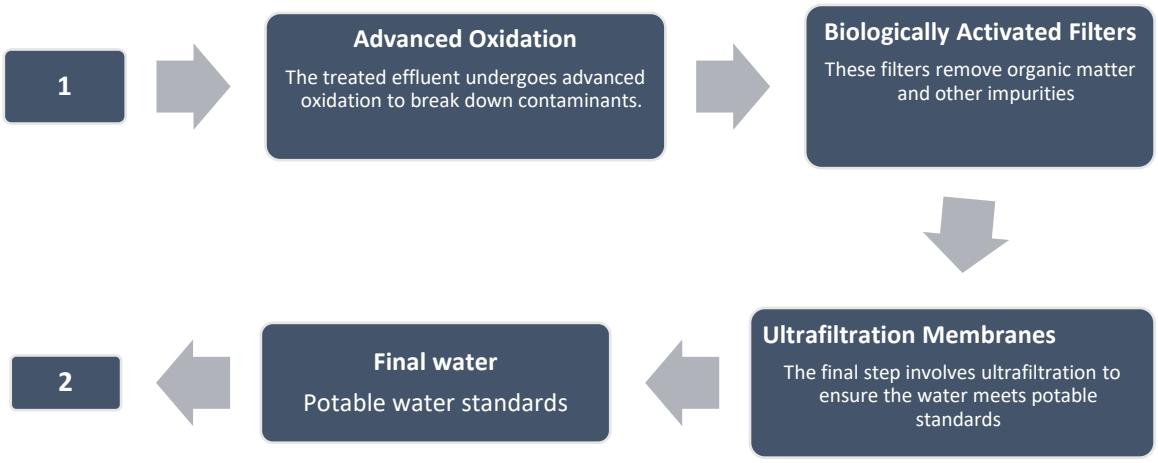


Figure 2-4: Direct potable Water Treatment Plant (d-DwTP) layout showing the process flow of the effluent reuse demonstration plant. Treated effluent from wastewater treatment works (1) and (2) final water.

2.2.4 Desalination plant (Des-P)

Sea water desalination plant takes water from the sea and passes it through a reverse osmosis processing plant to produce potable-quality water at a rate of 2 megalitres of water a day. The plant draws beach sand filtered borehole seawater through submersible pumps sinking, 12 m deep adjacent Beach (Figure 2-5). The waste product of the reverse osmosis process, brine is pumped through an outlet pipe to 250m out to sea, where the tides and wave action on the rocks ensures that the brine is mixed well with the seawater to reduce adverse effects of brine on the environment. The hydraulic retention time of the treatment process is 1 hour. Grab water samples were collected from the intake tap before undergoing a series of treatment processes Raw water (1) and the product water samples (final water) were collected from a dedicated sampling tap after completion of the purification process (2).

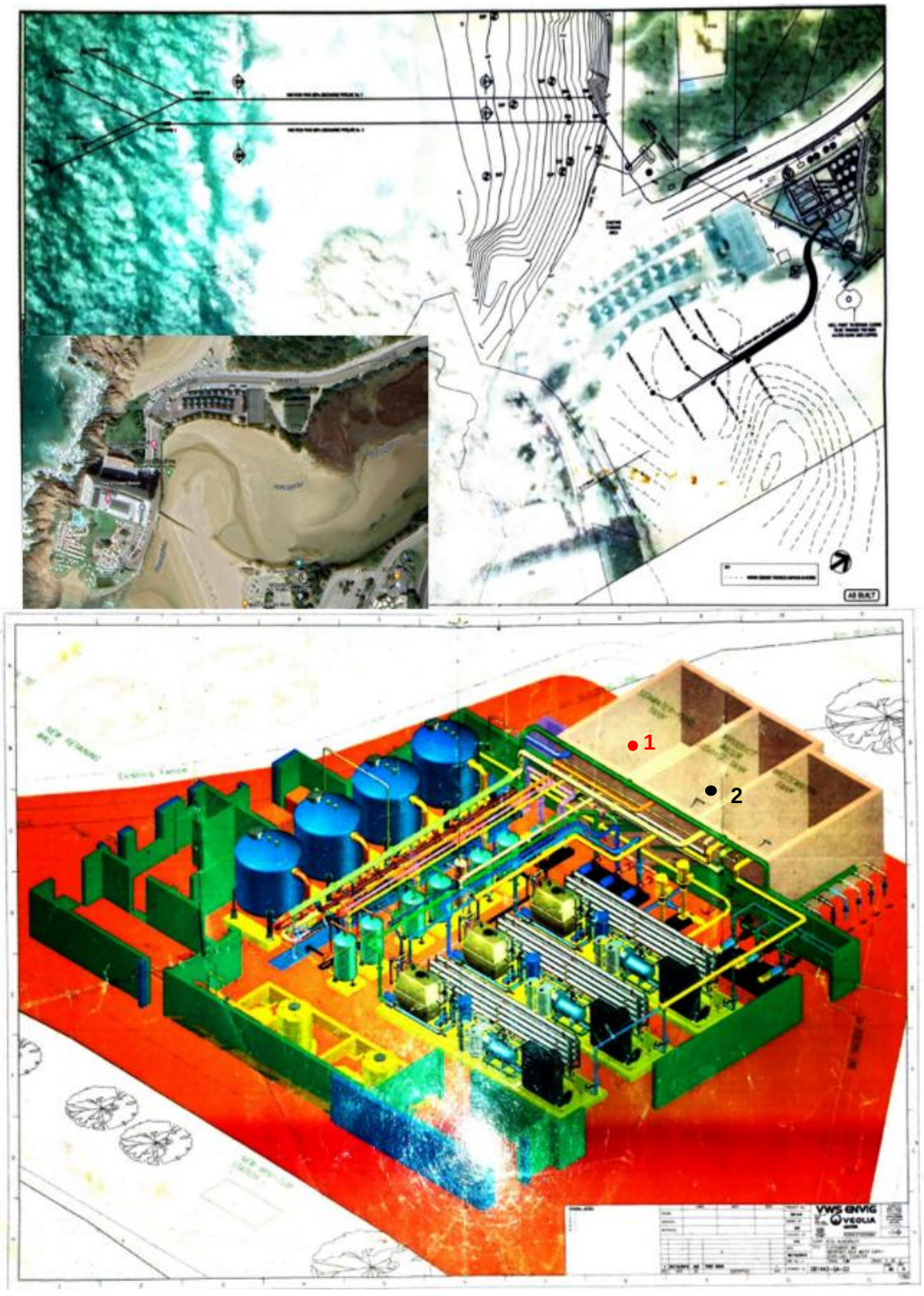


Figure 2-5: Desalination plant layout showing various stages of the treatment train. The seawater feed water tank (raw water) sampling point (1) and the product water (final water) storage tank sampling point (2).

2.2.5 Domestic Wastewater Treatment Works (WwTW)

Domestic Wastewater Treatment Works (WwTW1) draws influent wastewater from a main collector sewer and treats eight (8) megalitres of wastewater per day through various treatment processes shown in Figure 2-6. The influent undergoes pre-treatment, primary treatment, secondary treatment, and tertiary treatment. The preliminary treatment has three units, (1) a sand trap that traps the sand coming with raw wastewater (2) Manual and mechanical screens that remove large materials such as plastics, rags, papers, etc., and (3) a grit chamber (channel) that removes grit such as sand, silt, and corns. The primary treatment has four primary settling tanks which are Dortmund type of tanks each having a siphoning system to control the flow going to bio-filters. The secondary treatment consists of 16 bio-filters and two humus tanks. The tertiary treatment has a point where chlorine is added, and a chlorine contact channel for water to properly mix with chlorine thereby disinfecting it. The effluent from the biofilter plant and the activated plant get combined before the effluent goes to the river. Water takes one and a half (1.5) minutes to exit the grit section of the treatment train, four (4) minutes in the primary settling tanks, 240 minutes in the biological nutrient removal (BNR) activated sludge reactor, eight (8) minutes in the humas tank and 40 minutes in the chlorine contact tank (CCT).

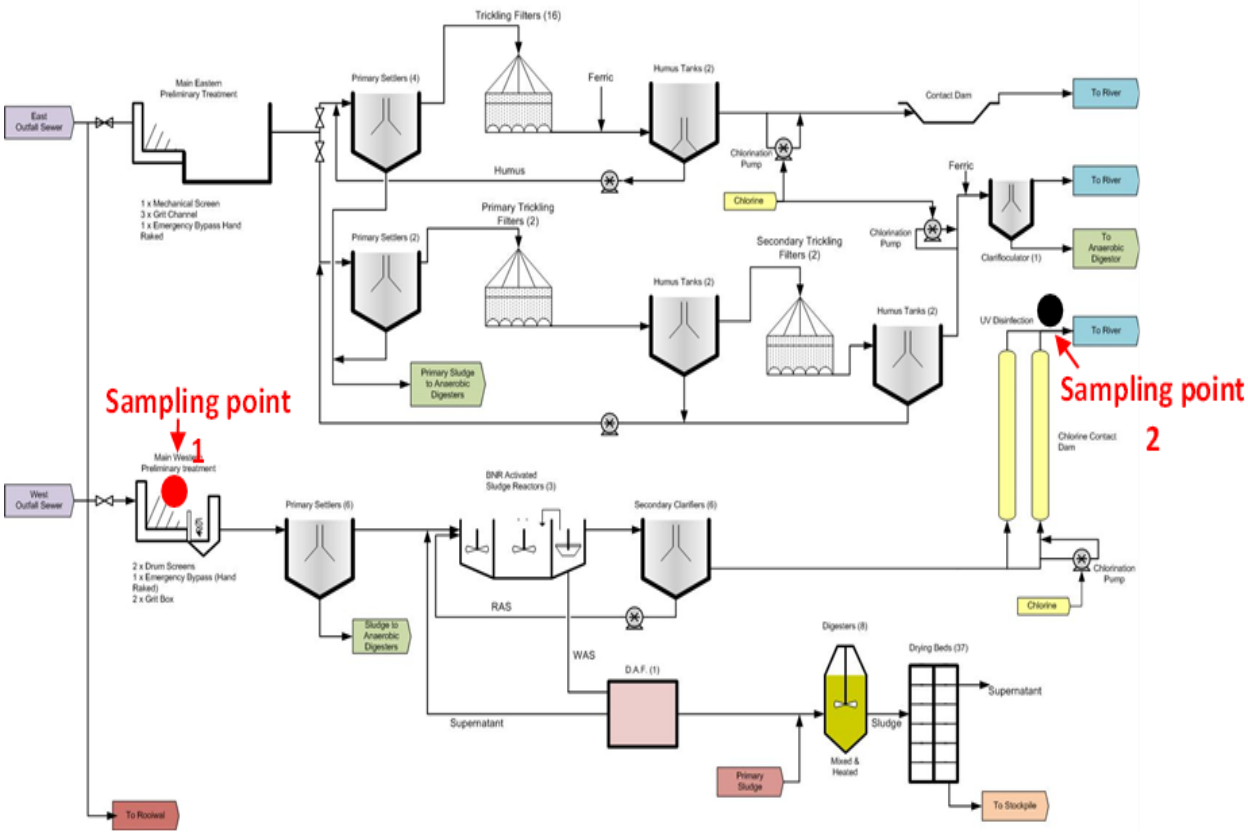


Figure 2-6: WwTW1 layout showing various stages of the treatment train. Influent sampling point 1 is indicated by a red mark (●) and effluent sampling point 2 is indicated by a black mark (●).

2.2.6 Combined Domestic and Industrial Wastewater Treatment Works (WwTW2)

The Wastewater Treatment Works (WwTW2) treats and discharges its final treated wastewater into a tributary of the Crocodile River. The facility is made up of five units, each with specific treatment processes and capacities, Unit 4 being the newest addition. It consists of screening, gritting, primary sedimentation, biological nutrient removal unit (comprising of Anaerobic, anoxic, and aerobic stages), secondary clarification, and chlorination before the effluent is discharged into the receiving river. Unit 4 incorporates additional treatment stages, such as sludge thickening, dewatering, solar drying, and composting. For this

facility, the water samples were collected from the influent, intermediary steps, and the effluent. Grab samples were also taken from upstream and downstream of the receiving river to assess the impacts of effluent discharge to the receiving water bodies.

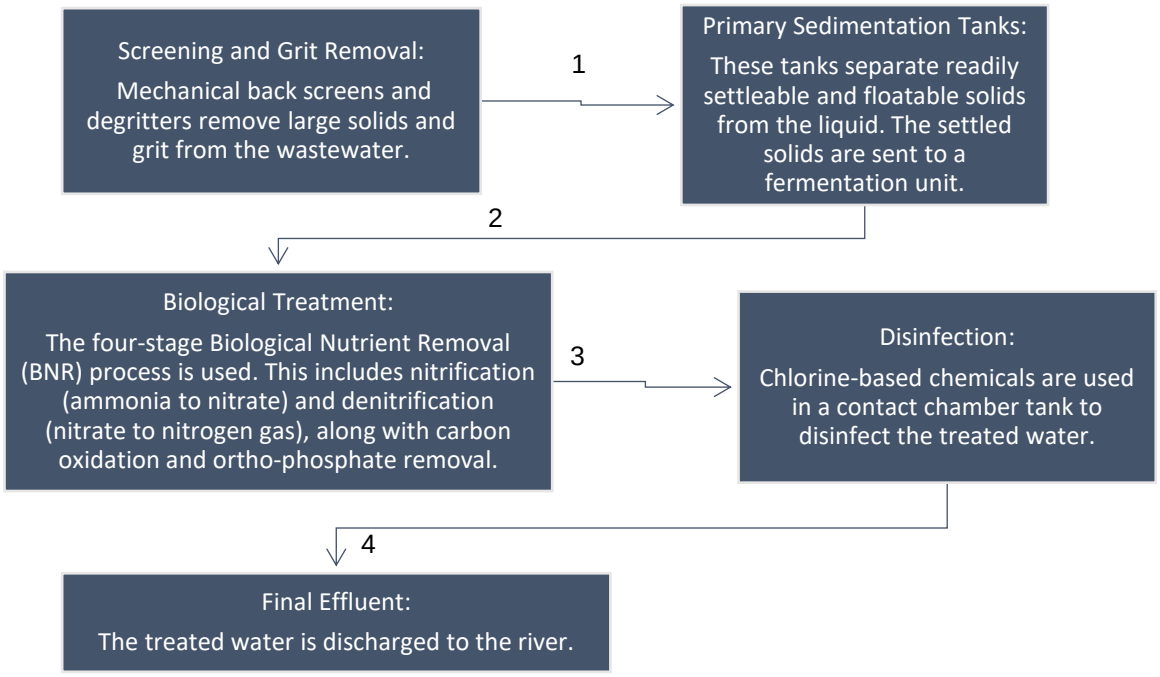


Figure 2-7: WwTP2 layout showing various stages of the treatment train and sampling points. (1) the influent, (2 and 3) intermediary steps, and (4) the effluent

2.3 PASSIVE SAMPLING METHODS

Passive samplers were exclusively deployed to assess the efficacy of treatment in a desalination plant, as well as to assess the impact of wastewater discharge in receiving water bodies. Three (3) types of passive samplers were used namely: Polar organic Integrative Passive Samplers (POCIS), Membrane Assisted Passive Sampler (MAPS) and Chemcatcher. The passive samples were fabricated as follows:

2.3.1 Membrane assisted passive sampler (MAPS)

Silicone membranes used for the fabricating MAPS were bought as long tubes and cut to appropriate lengths (48 cm x 0.1575 cm I.D x 0.2413 cm O.D giving a volume of approximately 1000 µL). Silicone membranes, previously soaked in deionised water, were filled with a pH 2.2 acceptor buffer of the LC MS grade water acidified with 0.1% formic acid. The membranes were tightened together and made in the form of a loop about 3 cm in diameter (Nyoni et al., 2011). The outside was rinsed with deionized water thoroughly to remove any buffer spills. After exposure, the samplers were taken out of the water, the outside briefly flushed with deionised water to remove debris and contents transferred into a 1.5 mL vials.

2.3.2 Polar organic chemical integrative sampler (POCIS)

Two types of in house-made POCIS samplers (pharmaceutical configuration) were constructed using (1) polyethersulphone membranes and sorbent Oasis HLB as described previously and (2) polyethersulphone membranes and Empore Styrene Divinyl Benzene (SDB-XC) membrane disks as receiving phase (Mills et al., 2007). The PES membranes were kept in the stainless-steel holder by stainless steel bolts and nut (30.0

mm ID 40.4 mm OD). This design ensured the ideal stretch of the membrane, uniform distribution of the sorbent material and provided a very good seal. The dimensions of the holder allowed applications of commercially available 47 mm or 90 mm membranes. Total exchanging surface area of the membrane (both sides counted) was 14.1 cm^2. Laboratory and field blanks were exposed to the air during calibration and field deployment as part of quality assurance. Handling and elution of POCIS followed procedures described previously (Alvarez 2004; Jones-Lepp et al. 2004). After the exposure period, each individual POCIS device was removed from its deployment canister, briefly rinsed with water if needed to remove debris and opened. The contents of the POCIS were transferred using approximately 10 mL of high-purity methanol acidified with 0.1% formic acid directly into 40 mL ember glass vials and extracted two times for 15 min in an ultrasonic bath. After centrifugation (10 min at 7500 rpm); supernatants were pooled, evaporated to dryness at 40˚C under a stream of nitrogen and reconstituted with 1 mL of 50% LC MS grade methanol-water solution. The extracts were quantitatively transferred to autosampler vials for analysis by ultra-high resolution quadrupole time-of-flight mass spectrometry (LC-Q-TOF/MS). Standards were prepared from stock solutions (10 µg/mL) in methanol. Calibration solutions (0.50, 0.10, 0.50 and 1 µg/mL) were prepared in 50:50 methanol and water. All standards and extracts were stored in amber vials at -20˚C.

2.3.3 Chemcatcher

Chemcatcher sampling device were constructed from a polycarbonate body, a 40-µm thick polyethersulphone (PES) diffusion-limiting membrane and (3) a C18 Empore® disk. Before use, the PES membranes and receiving phase disks were pre-cleaned for by soaking in ultrapure methanol for 24 h and then rinsed with deionized water. The conditioned disks were placed on the Chemcatcher body first and a PES membrane put on top of the receiving disk. Air bubbles were removed from the space between the disk and the PES membrane by gently pressing the top surface of the membrane using a lint-free paper towel. The assembled samplers were covered by a transport lid and placed in transport bottles filled with deionized water. Laboratory and field blanks were fabricated as part of quality assurance. Laboratory blanks remained in the laboratory and were used to account for any contamination during the processing and analysis of the samplers. The field blanks were used to account for contamination during transport to and from study sites, exposure to airborne contaminants during the deployment and retrieval periods, and contamination from storage, processing, and analysis. Field blanks were stored in airtight containers and transported to the field sites in insulated containers filled with blue ice. At the study sites and during the deployment and retrieval operations, the lids of field blank airtight containers were opened to allow for exposure to the surrounding air. All samplers were deployed in a stainless-steel canister for a period of 14 days. The three samplers were positioned at three key locations: the effluent point, upstream, and downstream of the two wastewater sampling sites. Additionally, passive samplers used to evaluate the desalination treatment technology were placed on both the raw water and the final water tanks.

2.4 CHEMICALS AND REAGENTS

Solvents and reagents used in this work were of high purity (Analytical grade and LC MS grade, > 99%) were purchased from Sigma-Aldrich South Africa and some from Honeywell (North Carolina, USA) supplied by Anatech Instruments (Pty) Ltd (Johannesburg, SA) Merck (SA). Standard were purchased from Industrial Analytical (Pty) Ltd. a subsidiary of LGC Standards, Ltd. (Teddington, UK). PALL polyethersulphone membranes disks and Empore Styrene Divinyl Benzene (SDB-XC), 90 mm and 47 mm in diameter respectively, were purchased from Sigma-Aldrich South Africa. Silicone membranes were obtained from Technical Products Inc. (Georgia, USA). The stainless-steel protective cages and POCIS holder washers were purchased from ExposMeter Sampling Technologies (Tavelsjo, Sweden).

2.5 SOLID PHASE EXTRACTION

To thoroughly evaluate water quality, we collected water samples from several treatment technologies. These included a conventional drinking water treatment plant, a desalination plant, direct and indirect potable water reuse facilities, domestic and industrial wastewater treatment plants, as well as upstream and downstream sites of effluent-receiving rivers and dams that serve as sources for drinking water treatment. At each designated sampling site grab sampling techniques was employed. We accounted for the hydraulic retention time of each treatment plant during the collection of influents, intermediate, and effluent water samples. To preserve sample integrity, all collected samples were immediately placed in ice-filled coolers for transport to the laboratory, where they were processed within 48 hours.

2.5.1 Oasis^{TM} HLB

Extraction was performed using preconditioned Oasis^{TM} HLB SPE cartridges. Cartridges used for extraction were sequentially conditioned with 5 mL of methanol and 5 mL of ultrapure water at a flow rate of 5 mLmin-1. Thereafter, 500 mL of water sample was loaded to the cartridge at a flow rate of 5 mLmin-1. The cartridge was then washed with 5 mL of 5% methanol in water followed by vacuum drying with the help of vacuum suction for 5 min. Elution was performed with 2 x 5 mL of methanol at 2.5 mLmin^{-1}. Methanol extracts were concentrated to dryness under a stream of nitrogen and reconstituted to a final volume of 1 mL in 50% methanol: ultra-pure water and stored at -20°C until analysis.

2.5.2 Dual stack of MCX and MAX

The extraction process utilized a tandem cartridge configuration with Waters Oasis MAX and MCX SPE cartridges (Figure 6). This configuration facilitated a 3-tiered extraction mechanism that employed reversed-phase, anion exchange, and cation exchange methods. The extraction protocol was designed to ensure the retention of acidic, basic, and neutral compounds. The Oasis MCX cartridge was connected below the MAX cartridge, and both cartridges were conditioned by passing 5 mL of methanol and 5 mL of water. A vacuum was used to load a 1L water sample at 10 mL/min onto the dual stack using bottle to SPE adapter. After the loading step was complete, the cartridge stack was disassembled, and each cartridge underwent specific wash and elution steps as shown in the Figure 2-8.

The Oasis MAX cartridge was washed with 5 mL of ammonium hydroxide in water. The elution was performed in two steps: first with 5 mL of methanol (neutral) and second with 5 mL of methanol containing 5% formic acid (acidic compounds). Both elution fractions were collected in a 20 mL glass tube. The Oasis MCX cartridge was washed with 5% formic acid and eluted with 5 mL of methanol containing 5% ammonium hydroxide (basic). The MCX and MAX elution fractions were pooled and evaporated to dryness at 60°C under a gentle stream of nitrogen. The dried eluate was reconstituted with 1000 µL of 10 mM ammonium formate.

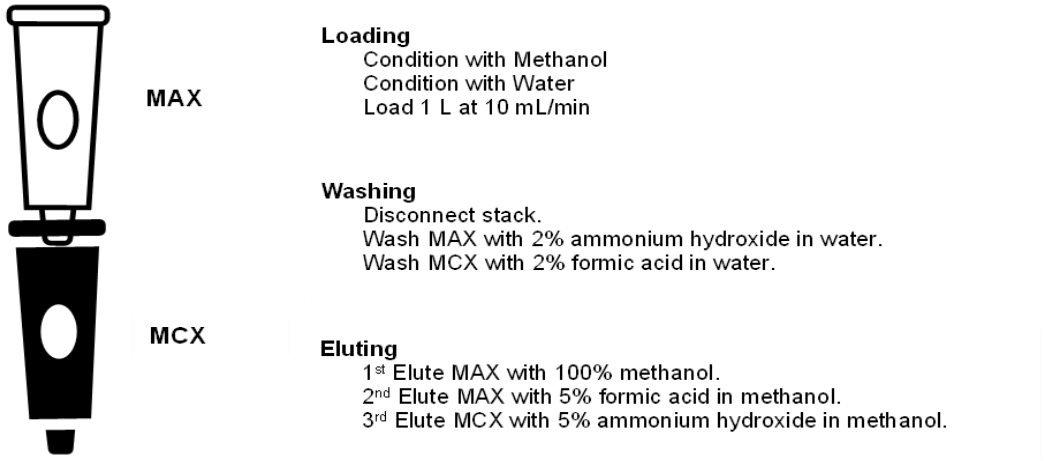


Figure 2-8: Schematic of a dual stack of MCX cartridge connected below a MAX cartridge employed for the 2-tiered extraction of acidic, basic, and neutral compounds from a single water sample.

2.6 ANALYTICAL EQUIPMENT

2.6.1 Optimised UPLC/Q-TOF-MS

The separation of the analytes was carried out using a Dionex Ultimate 3000 UHPLC system (Dionex Softron GmbH, Dornierstr. 4, Germany) equipped with a reversed-phase C18 analytical column of 100 mm × 2.1 mm and 1.7 µm particle size (Acquity UPLC® BEH, Waters, Ireland). Column temperature was maintained at 35 ºC. The injected sample volume was 5 µL. Mobile phases A and B were water and methanol with 0.1% formic acid, respectively. The optimized chromatographic method was programmed as follows: the initial mobile phase composition (2% B) constant for 1 min, followed by a linear gradient from 2% B to 100% B for 9 mins, kept 100% B for 2 mins and then dropped back to 2% B 12.1mins and kept constant at 2% B for 2 mins. The flow rate used was 0.3 mL/min and the total run time was 14 mins. This UHPLC system was connected to an ultrahigh resolution quadrupole time-of-flight mass spectrometer Impact II Bruker (Bruker Daltonics GmbH Fahrenheitstr. 4, Bremen, Germany) equipped with electrospray ionisation, operating in positive ion mode. LC/MS accurate mass spectra were recorded across the range 50-1600 m/z. The data recorded was processed with Bruker Compass DataAnalysis 4.3 software. Accurate mass measurements of each peak from the extracted ion chromatograms were obtained by means of a sodium formate calibrant solution delivered by a KdScientific external pump. The instrument was operated in full-scan mode, except in those cases where automated MS-MS was necessary to discriminate isobars/isomers, as well as for identification of selected compounds and degradation products as explained in the results.

2.6.2 Optimised LC-HRAMS Q Exactive system

The Q Exactive mass spectrometer was run in both positive and negative ionization mode. The electrospray ionization was set at 2.5 kV (for negative) and 3.5 kV (for positive) with an auxiliary gas set at 5 arbitrary units, the sheath gas set at 36 arbitrary units, and the capillary temperature was set at 320°C. The scan parameters for the mass spectrometer included a run time of 13 min duration time and 6 s chromatogram peak width in DDA mode. MS1 used the Orbitrap mass analyser with a resolution of 70,000, a maximum injection time (MIT) of 300 ms, one, scan, an RF lens (%) of 50, and a scan range from 65 to 750 m/z. The Automatic Gain Control (AGC) target was set to 3e6. MS2 data were acquired using a resolution of 17,500,

MIT of 80 ms, AGC target of 1e5 and a scan range from 65 to 750 m/z. The top 1 abundant precursor within an isolation window of 1.0 m/z was chosen for MS/MS analysis. A minimum intensity threshold of 1.0e5 and dynamic exclusion of 6 s were used during the data-dependent scanning. For precursor fragmentation, high energy collision dissociation (HCD) normalized three-step collision energy was set to 10, 30, and 60. For the PRM method, the scan parameters for the mass spectrometer included a run time of 13 min duration time and 6 s chromatogram peak width in PRM mode. MS2 data were acquired using a resolution of 17,500, MIT of 160 ms, AGC target of 2e5 and an inclusion list of all the precursor ions of our target compounds. The loop and maximum number of precursors to be multiplexed in a scan event were set at 1 within an isolation window of 4.0 m/z. For precursor fragmentation, high energy collision dissociation (HCD) normalized collision energy for specific precursor was listed in the inclusion list and ranged from 10 to 40eV.

2.6.3 GC TOF MS

DLLME n-hexane extracts as well as methanol extracts of Chemcatcher, were analysed by gas chromatography (Agilent Technologies, Inc., Wilmington, Delaware, USA) coupled with a LECO HT time of flight mass spectrometer (LECO Corporation, St. Joseph, MI, USA) and a Gerstel Multi-Purpose Sampler MPS 2 from Gerstel GmbH (Mülheim an der Ruhr, Germany).) on-column injection system in a splitless injection mode. The GC oven was equipped with a Restek Rxi®-5Sil MS, 30 m, 0.25 mm ID, 0.25 µm and the helium carrier gas was maintained at a constant flow of 1 mL per minute. The injection temperature was set at 300ºC, and the oven temperature was programmed as follows: 40ºC held for 2 minutes; ramped from 40-240ºC at 30ºCmin-1, then 240-320ºC at 10ºC per minute. The mass spectrometry conditions were set as follows: Transfer line temperature: 300°C; Ionization: Electron ionization at -70 eV; source temperature: 280°C; stored mass range: 50-500 um; solvent delay: 240 seconds; acquisition rate: 8 spectra/second; detector voltage: -1654 V. Also, the system was equipped with ChromaTOF data acquisition software and the NIST library for performing the integration of chromatograms and compound quantification. External calibration standards were used for quantification.

2.6.4 NexION 350D ICP MS

The elemental analysis of water samples was performed by Perkin Elmer NexION 350 ICP-MS system. The typical instrumental parameters were set as follows: cell gas: argon; nebulizer: glass concentric; spray chamber: glass cyclonic, sample uptake rate: 0.3 mLmin-1; RF power:1600 W, Triple cone interface: nickel/aluminium, sweeps per reading: 10, replicates: 3-10, dwell time: 50-150 ms, lens: Quadrupole Ion Deflector, scanning mode: STD or KED (He) or DRC (NH3).

2.7 SAMPLE ANALYSIS

2.7.1 Non target qualitative analysis of compounds

Non-target qualitative analysis was used for assessing the efficiency of the drinking water treatment in the following plants: conventional drinking treatment plant (DwTP), Indirect potable water reuse plant (In-DwTP), direct potable water reuse plant (d-DwTP) and seawater desalination plant (Des-P). Compound Discoverer (version 3.3.1.111 ThermoFisher Scientific, Waltham, MA) was used to perform non-targeted environmental research identification workflow without statistics (Figure 2-8 to 2-11).

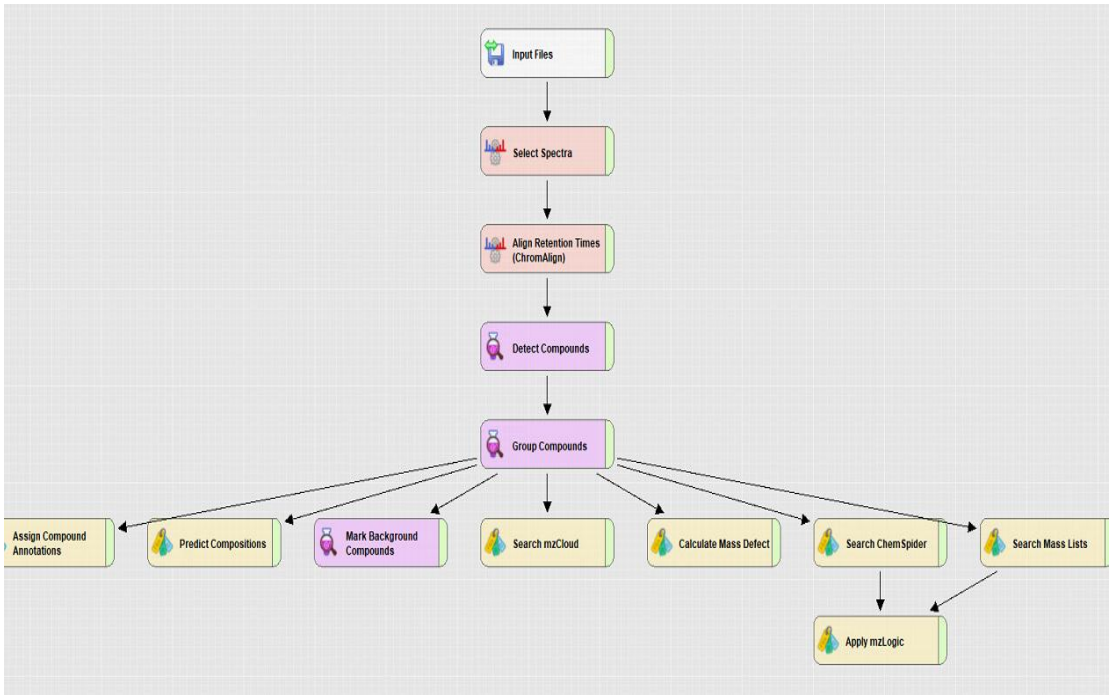
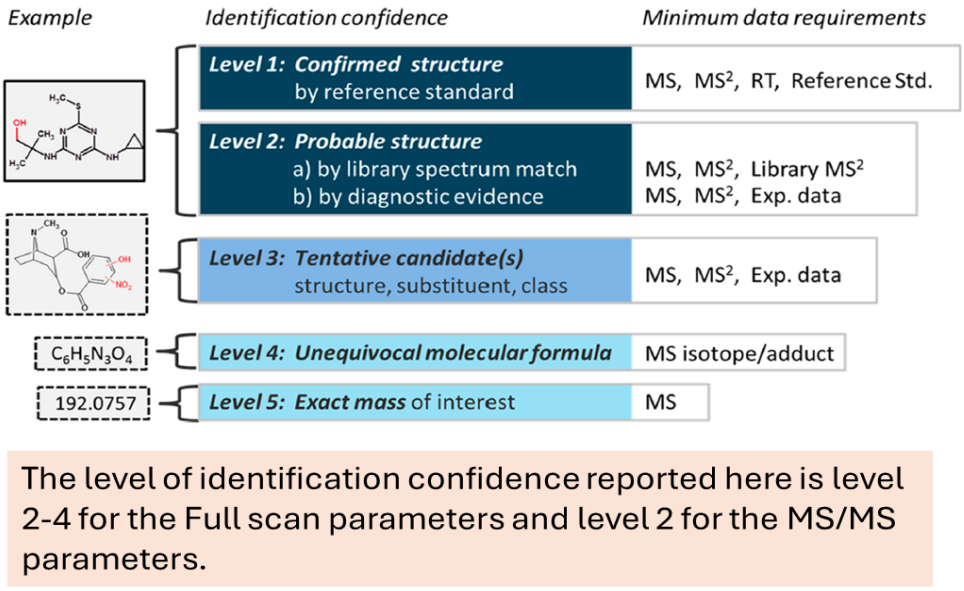


Figure 2-8: Workflow tree from Compound Discoverer 3.3 SP1 software displaying data processing nodes and the associated workflow connections.



The level of identification confidence reported here is level 2-4 for the Full scan parameters and level 2 for the MS/MS parameters.

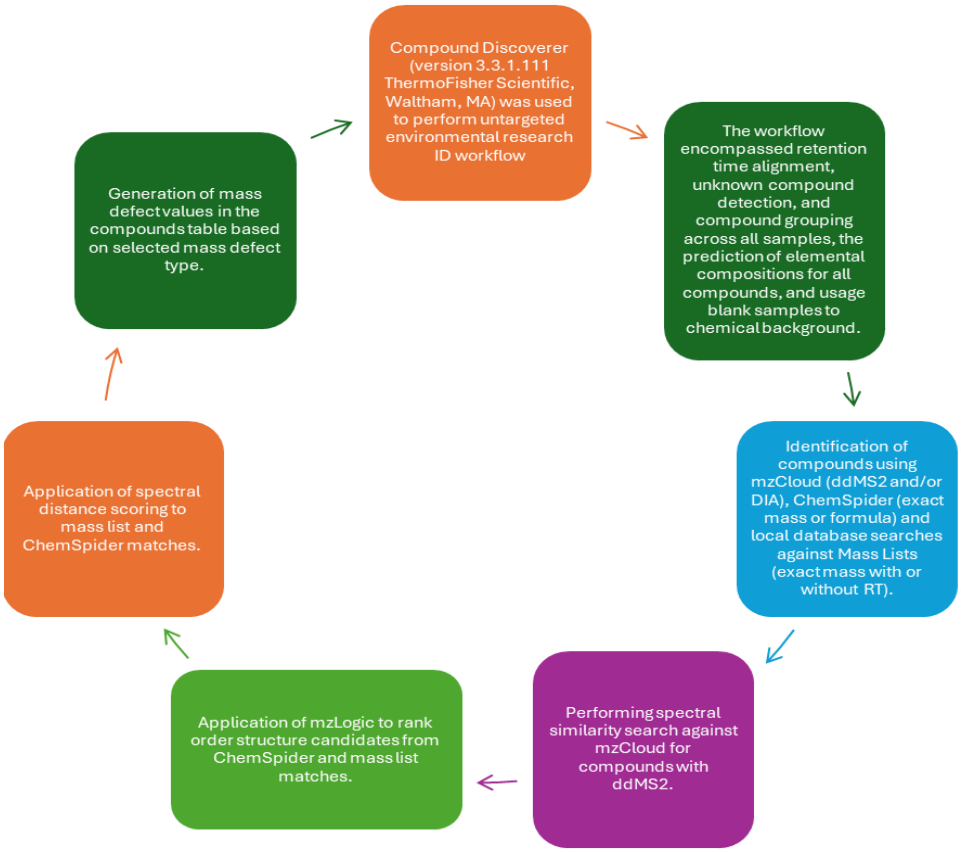


Figure 2-9: Non-targeted HRAM data Analysis Workflow using Compound Discoverer Software (Identification confidence taken from Schymanski et al., 2014. Environ. Sci. Technol., 48, 2097−2098.

The workflow encompassed retention time alignment, unknown compound detection, compound grouping across all samples, the prediction of elemental compositions for all compounds, and the usage of blank samples to the chemical background. Identification of compounds using mzCloud (ddMS2 and/or DIA), ChemSpider (exact mass or formula), and local database searches against Mass Lists (exact mass with or without RT). Performing spectral similarity search against mzCloud for compounds with ddMS2. Application of mzLogic to rank order structure candidates from ChemSpider and mass list matches. Application of spectral distance scoring to mass list and ChemSpider matches. Generation of mass defect values in the compounds table based on selected mass defect type. Figure 2-10 shows an example of a chromatogram and Figure 2-11 shows an example of a mass spectrum from wastewater treatment plant samples and reference spectrum from mzCloud (bottom) with m/z 254.0589 compound identified as sulfamethoxazole. The level of identification reported here is level 2-4 for the Full scan parameters and level 2 for the MS/MS parameters. The FullMS data was used for peak selection and the ddMS/MS data for identification only. The characterization of the influence of each FullMS parameter entailed an examination of the total number of features and annotations. Also, the evaluation of MS/MS parameters included factors such as the MS/MS counts, the number of annotated compounds with MS/MS information and the spectral quality. Following these general filters were applied to exclude features. These filters were background removal, mass accuracy (± 0.5 ppm), and MS/MS for specific ions. To assess spectral quality, a matching process was performed, aligning experimental spectra with the MS/MS spectral library. The mzCloud best match score greater than or equal to 70% was used as cut-off for spectral similarity. Optimal values for the MS/MS

parameters were identified as the values that gave the greatest number of annotated compounds with an MS/MS spectral quality within a mass accuracy of 5ppm.

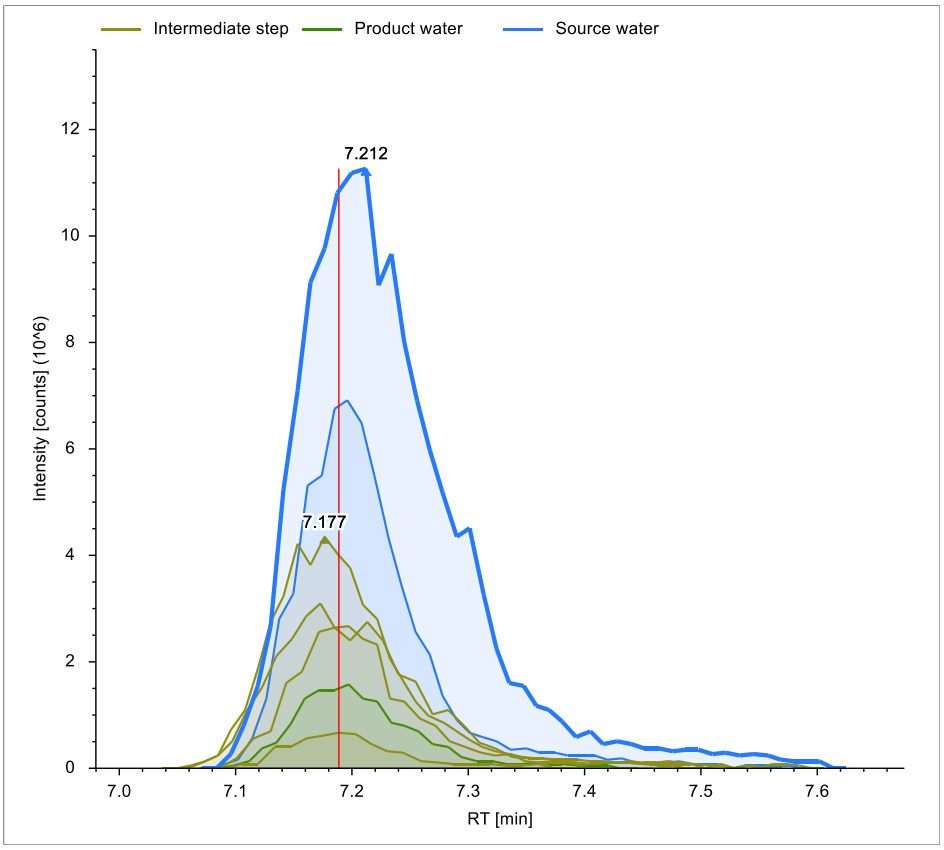


Figure 2-10: An example of a chromatogram from wastewater treatment plant samples and reference spectrum from mzCloud (bottom) with m/z 254.0589 compound identified as sulfamethoxazole.

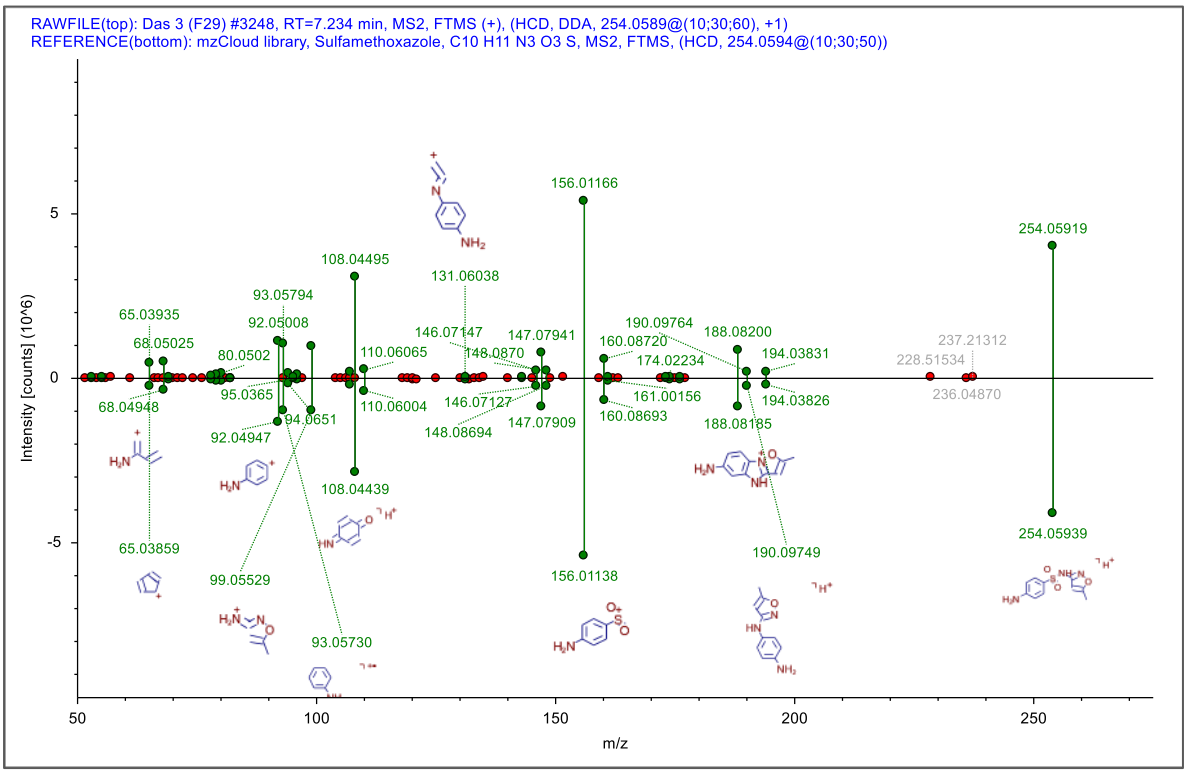


Figure 2-11: An example of a mass spectrum from wastewater treatment plant samples and reference spectrum from mzCloud (bottom) with m/z 254.0589 compound identified as sulfamethoxazole.

2.7.2 Targeted screening of compounds

The Trace Finder software was used to conduct targeted screening for organic micropollutants. The search was focused on the retention time, fragment ions, and isotopic pattern of the compounds. To increase confidence in the screening results, a customizable EFS HRAM compound database with 1729 registered compounds was used together with a spectral library integrated with high-resolution accurate mass data. This provided an unmatched level of confidence in the targeted screening workflow. A screenshot of compound m/z 216.1011 with mass list search hit atrazine is shown in Figure 2-12. The adducts [M+Na]+,[2M+H]+ and [2M+Na]+ were detected along with [M+H]+. The compound was only found in the raw water samples for the indirect water reuse plant. The library search gave a library score of 93%.

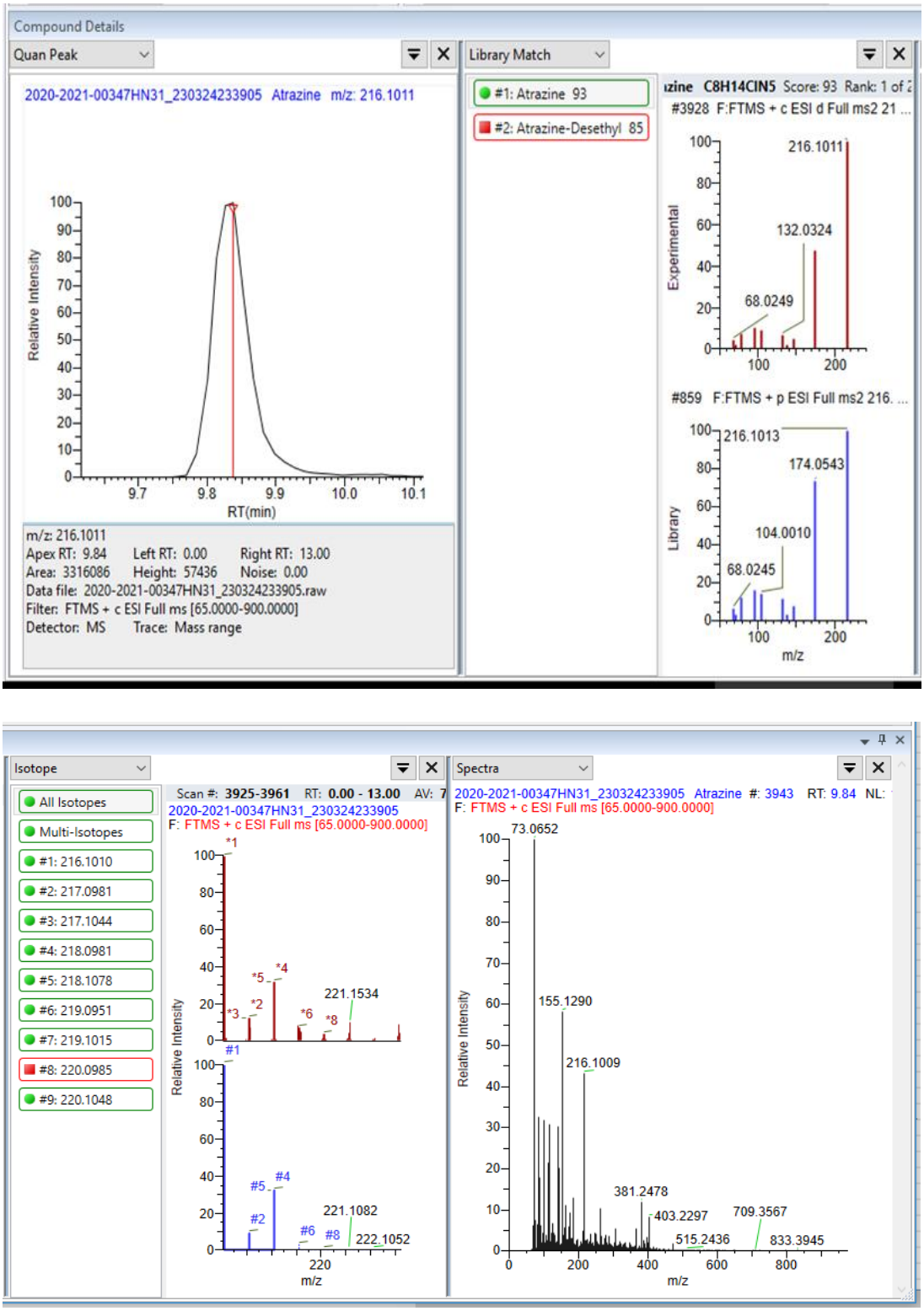


Figure 2-12: Illustrative examples for the tentative identification of atrazine compounds using Q-Exactive plus orbitrap mass spectrometry.

2.7.3 Targeted quantitative analysis of CECs

2.7.3.1 Target list of compounds

The target list of compounds analysed is provided in Table 2-1. These compounds have been detected in similar water samples and were readily available to be used for method development and validation. None of the target list compounds were detected above the reporting limits

Table 2-1: Target list of compounds analysed in water samples.

Compound name	Retention time (mins)	Formula
(R) (+) Atenalol	4.09	$(CH_3)_2CHNHCH_2CH(OH)CH_2OC_6H_4CH_2CONH_2$
± Metoprolol tartrate Salt	5.42	$C_{15}H_{25}NO_3$
± Sotalol	4.08	$C_{12}H_{20}N_2O_3S$
1,7 Dimethylxanthine	4.35	$C_7H_8N_4O_2$
17-α-Ethinyl estradiol	8.39	$C_{20}H_{24}O_2$
4-Aminobiphenyl	6.19	C12H11N
Acetaminophen	3.43	C8H9NO2
Acetylpyrazine	4.53	$C_6H_6N_2O$
Albendazole	6.83	$C_{12}H_{15}N_3O_2S$
Ampicillin #108	4.52	$C_{16}H_{19}N_3O_4S$
Aspirin	12.53	$2\text{-}(CH_3CO_2)C_6H_4CO_2H$
Atenolol	3.59	C14H22N2O3
Atrazine	7.75	C8H14ClN5
Azithromycin	5.56	$C_{38}H_{72}N_2O_{12} \cdot 2H_2O$
Benzophenone	8.46	C13H10O
Bisphenol A	9.34	C15H16O2
Bufexamac	7.63	C12H17NO3
Buspidone hydrochloride	6.07	$C_{21}H_{31}N_5O_2 \cdot HCl$
Caffeine	4.59	C8H10N4O2
Carbamazepine	7.36	C15H12N2O
Cefotaxime sodium salt	5.14	$C_{16}H_{16}N_5NaO_7S_2$
Ciprofloxacin	5.00	$C_{17}H_{18}FN_3O_3$
Cloxacillin sodium salt	8.10	$C_{19}H_{18}ClN_3O_5S$
D (-) Norgestrel	8.91	$C_{21}H_{28}O_2$
Danofloxacin	4.92	C19H20FN3O3
Diclofenac	9.32	$C_{14}H_{11}Cl_2NO_2$
Difloxicin	5.50	$C_{21}H_{19}F_2N_3O_3$
Digoxin	6.78	$C_{41}H_{64}O_{14}$
Digoxin	7.84	C41H64O14
Efavirenz	9.17	C14H9ClF3NO2
Enrofloxacin	4.9	C19H22FN3O3
Erythromycin	6.48	$C_{37}H_{67}NO_{13}$
Estriol	6.38	$C_{18}H_{24}O_3$

Compound name	Retention time (mins)	Formula
Estrone	8.55	$C_{18}H_{22}O_2$
Famciclovir	4.83	$C_{14}H_{19}N_5O_4$
Fenbendazole	7.66	$C_{15}H_{13}N_3O_2S$
Fenoprofen	8.95	$C_{15}H_{14}O_3$
Flumequine	7.17	C14H12FNO3
Fluoxetine hydrochloride	7.25	$C_{17}H_{18}F_3NO \cdot HCl$
Ibuprofen	9.50	$C_{13}H_{18}O_2$
Imidacloprid	5.2	C9H10ClN5O2
Isoniazid	0.82	C6H7N3O
Ketoprofen	8.12	C16H14O3
Lamivudine	2.24	$C_8H_{11}N_3O_3S$
Levoflaxacin	7.32	C18H20FN3O4
Lidocaine	4.91	C14H22N2O
Lincomycin hydrochloride	4.58	$C_{18}H_{34}N_2O_6S \cdot HCl \cdot H_2O$
Lomefloxacin hydrochloride	5.09	$C_{17}H_{19}F_2N_3O_3 \cdot HCl$
Lopinavir	9.61	C37H48N4O5
Mebendazole	6.91	$C_{16}H_{13}N_3O_3$
Medroxyprogesterone	9.01	C22H32O3
Mestranol	10.35	$C_{21}H_{26}O_2$
Metoprolol Tartrate	5.5	C34H56N2O12
Miconazole nitrate salt	8.21	$C_{18}H_{14}Cl_4N_2O \cdot HN$
Naproxen	8.31	$C_{14}H_{14}O_3$
Nevirapine	5.99	$C_{15}H_{14}N_4O$
Norfloxacin	4.71	$C_{16}H_{18}FN_3O_3$
Ofloxacin	4.50	$C_{18}H_{20}FN_3O_4$
Oxacillin sodium salt	7.79	$C_{19}H_{18}N_3NaO_5S$
Oxibendazole	6.00	$C_{12}H_{15}N_3O_3$
Oxytetracyclic hydrochloride	4.74	$C_{22}H_{24}N_2O_9 \cdot HCl$
Paracetamol	3.43	C8H9NO2
Penciclovir	0.97	$C_{10}H_{15}N_5O_3$
Penicillin G/ Benzylpenicillin	5.19	$C_{16}H_{17}KN_2O_4S$
Phenacetin	6.31	C10H13NO2
Pindolol	4.31	C14H20N2O2
Primidone	5.17	C12H14N2O2
Progesterone	9.78	$C_{21}H_{30}O_2$
Propanolol hydrochloride	6.29	$C_{16}H_{22}ClNO_2$
Ribavirin	2.06	$C_8H_{12}N_4O_5$
Roxithromycin	8.11	C41H76N2O15

Compound name	Retention time (mins)	Formula
Sarafloxacin hydrochliride	5.45	C20H18ClF2N3O3
Spiramycin from streptomyces	5.53	$C_{43}H_{74}N_2O_{14}$
Sulfabenzamide	6.71	$C_{13}H_{12}N_2O_3S$
Sulfacetamide	4.10	$C_8H_{10}N_2O_3S$
Sulfachloropyridazine	5.98	$C_{10}H_9ClN_4O_2S$
Sulfadiazine	4.52	$C_{10}H_{10}N_4O_2S$
Sulfadimethoxine	5.21	C12H14N4O4S
Sulfadoxine	5.15	C12H14N4O4S
Sulfaguanidine	1.29	$C_7H_{10}N_4O_2S$
Sulfamerazine	5.00	$C_{11}H_{12}N_4O_2S$
Sulfameter	5.49	$C_{11}H_{12}N_4O_3S$
Sulfamethazine	5.34	$C_{12}H_{14}N_4O_2S$
Sulfamethizole	5.47	$C_9H_{10}N_4O_2S_2$
Sulfamethoxazole	5.03	C10H11N3O3S
Sulfamethoxypyridazine	5.82	$C_{11}H_{12}N_4O_3S$
Sulfamoxol	6.42	$C_{11}H_{13}N_3O_3S$
Sulfanilamide	1.68	$C_6H_8N_2O_2S$
Sulfanitran	7.53	$C_{14}H_{13}N_3O_5S$
Sulfapyridine	4.86	$C_{11}H_{11}N_3O_2S$
Sulfaquinoxaline	6.80	$C_{14}H_{12}N_4O_2S$
Sulfasalazine	7.53	$C_{18}H_{14}N_4O_5S$
Sulfathiazole	4.82	$C_9H_9N_3O_2S_2$
Sulfisoxazole	5.25	C11H13N3O3S
Terbuthylazine	8.45	C9H16ClN5
Terbutryn	7.3	C10H19N5S
Testosterone	8.20	$C_{19}H_{28}O_2$
Thiabendazole	4.59	C10H7N3S
Thiacloprid	6	C10H9ClN4S
Tramadol	5.41	C16H25NO2
Triclabendazole	9.73	$C_{14}H_9Cl_3N_2OS$
Trimethoprim	4.53	C14H18N4O3
Tylosin tartrate	6.66	C49H81NO23
Valacyclovir hydrochloride	3.85	C13H20N6O4 · HCl
Valsartan	8.54	C24H29N5O3
α-Estradiol	8.29	$C_{18}H_{24}O_2$

2.7.3.2 Preparation of standards

Calibration solutions, with concentrations of 0.02-20 ng/mL, were prepared by serial dilutions of the stock solution in 50:50 (v/v) methanol/water as shown in Table 2-2.

Table 2-2: Volumes used to prepare standard calibration solutions containing target list of analytes.

#	Target CEC Conc. (ng/mL)	Stock Solution Conc. (ng/mL)	Stock Solution Volume (µL)	Volume MeOH (µL)	Volume H2O (µL)	Total Solution Volume (µL)
1	0.02	0.2	100	400	500	1000
2	0.04	0.2	200	300	500	1000
3	0.1	2	50	450	500	1000
4	0.2	2	100	400	500	1000
5	0.4	2	200	300	500	1000
6	1	20	50	450	500	1000
7	2	20	100	400	500	1000
8	4	20	200	300	500	1000
9	10	200	50	450	500	1000
10	20	200	100	400	500	1000

2.8 METHODS DEVELOPMENT AND VALIDATION

To obtain optimized retention times (Rt), percent recoveries (%), method detection limits (MDLs), and method reporting limits (MRLs), solid phase extraction experiments were conducted, using EPA Method 1694 as a guideline for procedure validation and optimization.

2.8.1 Method detection limit

In particular, the method detection limit (MDL) was determined by fortifying, extracting, and analysing seven replicate laboratory fortified blanks (LFBs) at a concentration near the estimated detection limit. Each replicate was processed identically, and the standard deviation (s) of the measured concentrations was calculated. The MDL was then calculated by multiplying the standard deviation by the t-value corresponding to a 99% confidence level for seven replicates, as follows:

$$MDL = t_{(n-1,0.99)} \times s$$, where $t_{(n-1,0.99)}$ = 3.143 for seven replicates.

2.8.2 Method reporting limit

The method reporting limit (MRL) was determined by fortifying, extracting, and analysing seven replicate LFBs at the proposed reporting limit (RL) concentration. The mean measured concentration and standard deviation(s) of these replicates were calculated. The Half Range for the Prediction Interval of Results (HRPIR) was then determined using the equation:

$$HRPIR = 3.963s$$

where s represents the standard deviation and 3.963 denotes a constant for seven replicates. The MRL was established as the concentration at which the HRPIR did not exceed the difference between the mean measured concentration and the fortification level.

2.8.3 Retention times

Retention times (Rt) were optimized by varying the mobile phase composition, flow rate, and column temperature. Systematic experiments were conducted to identify the conditions that provided the best separation of analytes with minimal retention time and peak broadening. The selected conditions were those that provided sharp, well-resolved peaks within a reasonable analysis time.

2.8.4 Percent recovery

Percent recovery was assessed by fortifying samples at different concentrations and volumes, then subjecting them to the extraction and analysis procedures. Recoveries were optimized by adjusting extraction conditions, including solvent type, extraction time, and sample matrix considerations. The goal was to achieve recoveries within the acceptable range of 70-130%, as specified by EPA Method 1694. These rigorous experimental procedures ensured that the optimized retention times, % recoveries, MDLs, and MRLs were robust, reliable, and compliant with the regulatory standards set forth by EPA Method 1694. Figures 2-13 and 2-14 present the results of the assessment of sample concentration and volume on the percent (%) recovery of selected representative compound classes, including stimulants, herbicides, insecticides, and nonsteroidal anti-inflammatory drugs (NSAIDs). The observed recoveries for caffeine, thiamethoxam and ketoprofen raged from 70% to 140%, with an average recovery of 77.6% which is within the acceptable range reported by USA EPA Method 1694. Atrazine on the other hand exhibited lower recoveries. Given our objective of accounting for diverse chemical mixtures, the generic solid-phase extraction (SPE) conditions were good enough to be utilised for this study.

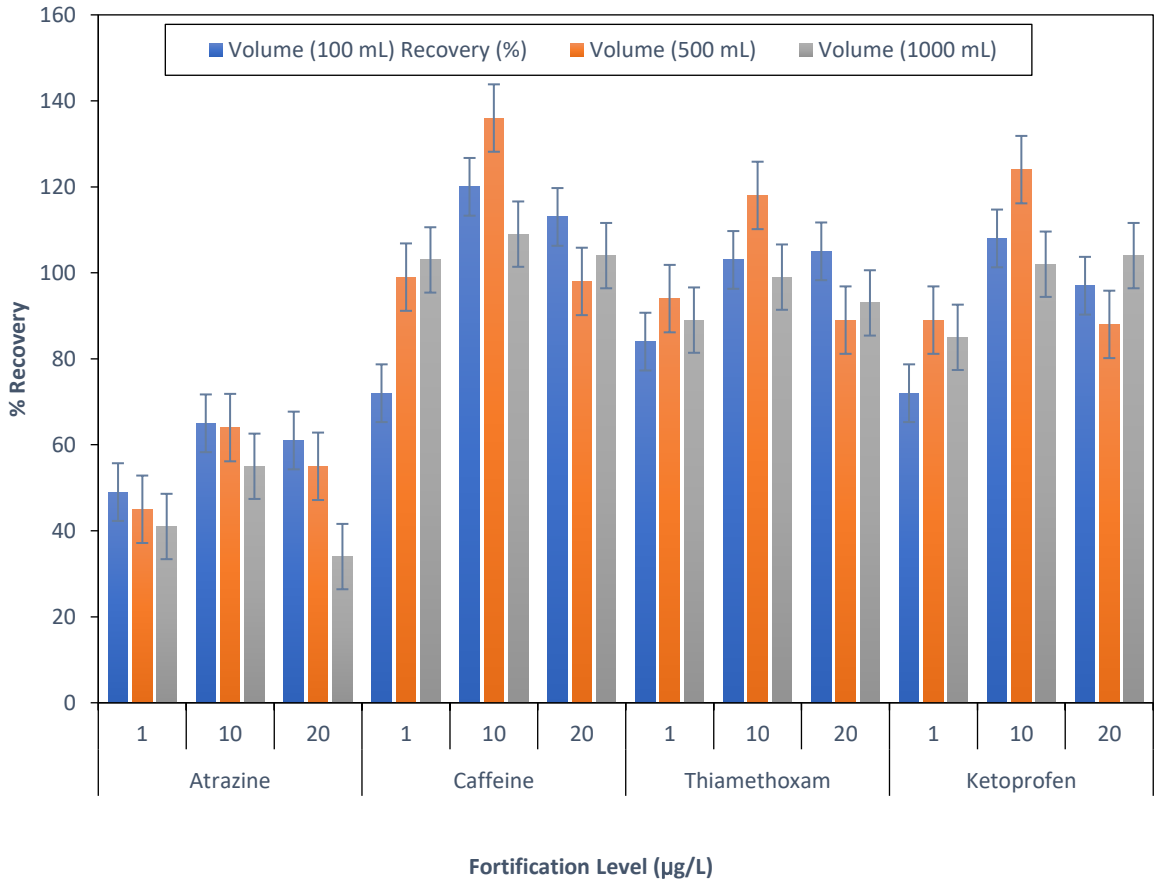


Figure 2-13: Effect of sample concentration and volume on percent (%) recovery. Error bars set at 10% margin of error.

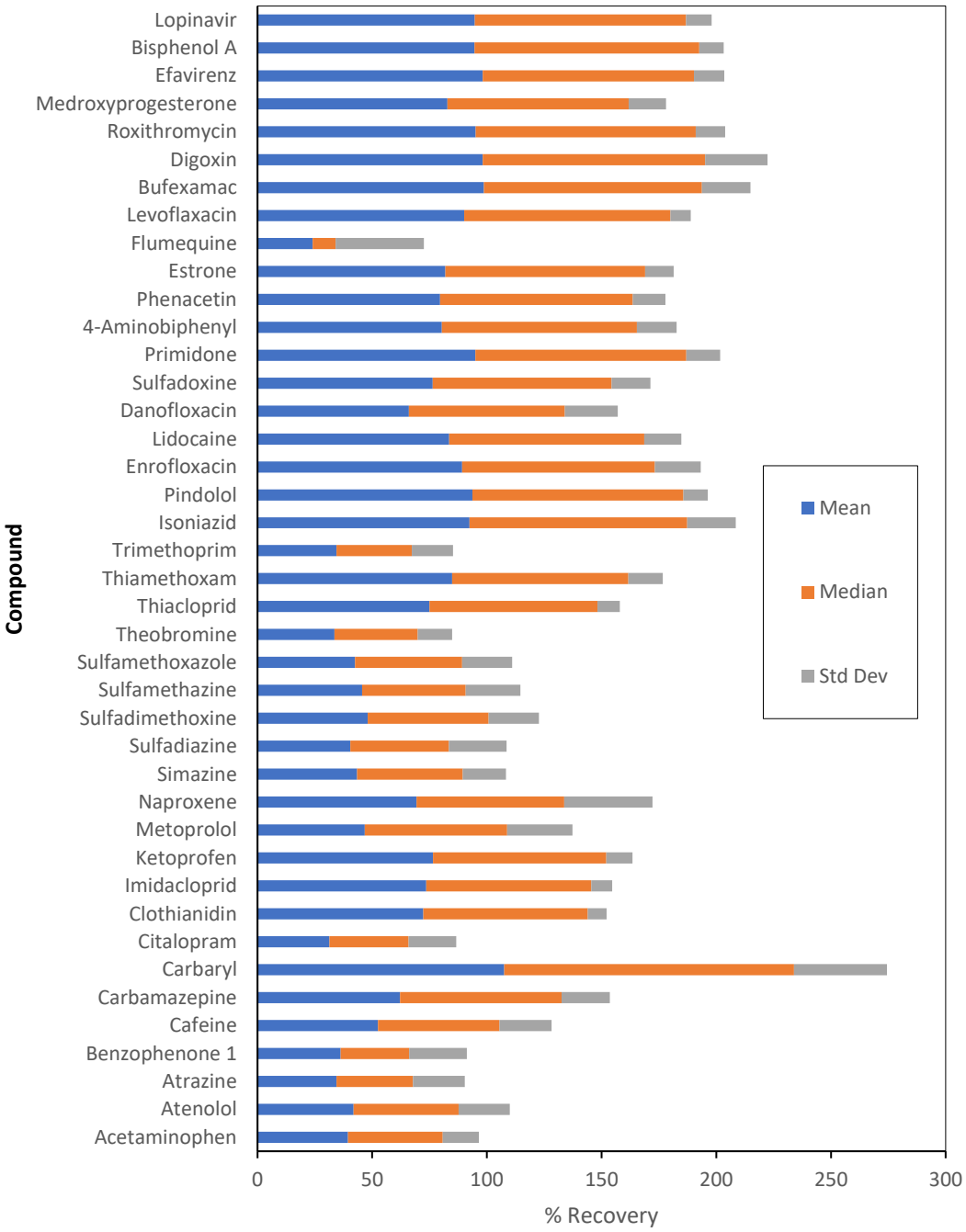


Figure 2-14: Percent (%) recovery for the target list of compounds used to assesses the overall performance of the SPE LC MS/MS quantification workflow.

3 RESULTS AND DISCUSSION

3.1 INTRODUCTION

Chemical data analysis strategy employed in this study incorporated both non-target and target approaches. Non-target analysis provided a holistic view of the presence of contaminants of emerging concern (CECs) throughout treatment processes. In contrast, targeted analysis focused on the detection and quantification of specific, pre-identified contaminants using established methodologies and standards. The combined insights from these two data analytical approaches enabled a thorough evaluation of the treatment technologies' effectiveness across the different sites. Results from targeted screening showed the presence of a variety of chemicals some used for the treatment of hypertension, others used as a corrosion inhibitor, vulcanization accelerator (metabolite), lipid-lowering agent, beta-blocker, anticonvulsant, NSAID, a metabolite of carbamazepine, fungicide, antipsychotic, antibiotic, insect repellents, analgesic, benzodiazepine, and anticonvulsant. The screening was also conducted for other toxicants and contaminants.

3.2 ASSESSMENT OF THE TREATMENT EFFICIENCY OF DIFFERENT DRINKING WATER TREATMENT TECHNOLOGIES

3.2.1 Baseline profile of contaminants of emerging concern in untreated drinking water

To establish the baseline profile of CECs, water samples were analysed to establish the range of CECs in the source water using non target qualitative analysis. The obtained results reveal the presence of a diverse array of chemicals, including leachable, therapeutic/prescription drugs, endogenous metabolites, pesticides/herbicides, personal care products, and industrial chemicals in the untreated (source) water for drinking water production (Figure 3-1).

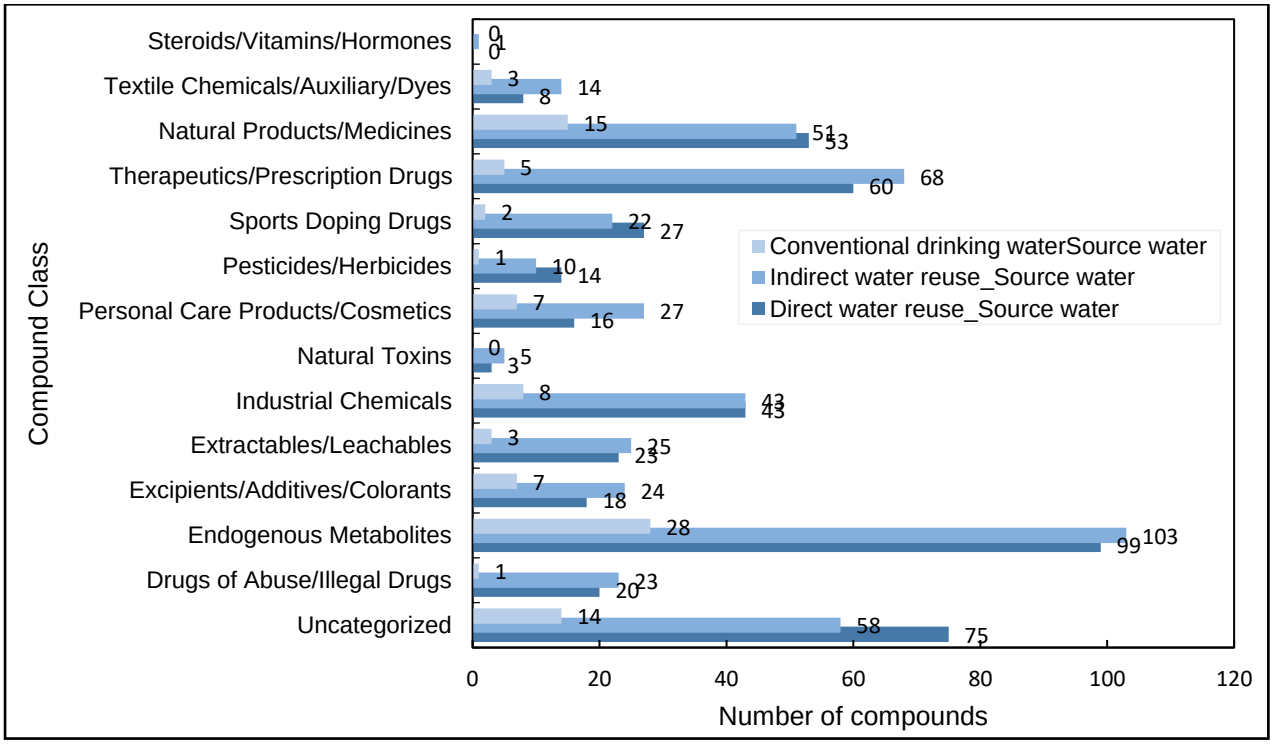


Figure 3-1: Results showing the presence of a diverse array of chemicals, including leachable, therapeutic/prescription drugs, endogenous metabolites, pesticides/herbicides, personal care products, and industrial chemicals.

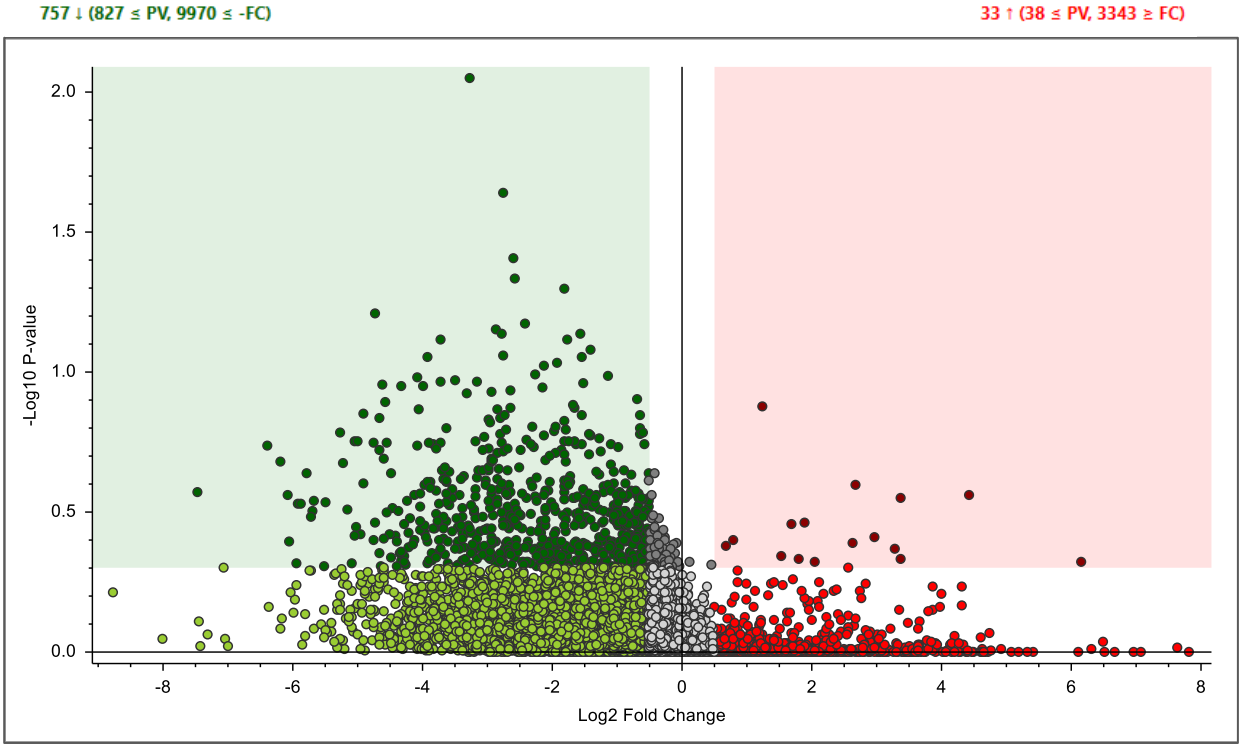
Analysis of compound classification indicates that all classes of compounds detected in these waters are more abundant in the direct potable water reuse, followed by indirect water reuse, than in conventional treatment technology source waters. Notably, endogenous metabolites, therapeutic/prescription drugs, natural medicines, and industrial chemicals are particularly prominent in direct and indirect water sources compared to conventional drinking water treatment technology.

3.2.2 Analysis of CECs in a conventional drinking water treatment plant

Differential analysis in Compound Discoverer was used to assess the effectiveness of the conventional treatment technology in removing chemical compounds across raw (source water) and final (product water). Table A3-1 (Appendices) shows the diverse range of classes detected. These compounds include naturally occurring compounds within organisms, compounds derived from natural sources or used in medicinal applications, chemicals used in various industrial processes, medications prescribed for therapeutic purposes, compounds that can be extracted or leached from materials (often found in packaging or manufacturing), ingredients used in personal care and cosmetic products, chemicals used in textile manufacturing and dyeing processes, substances used illicitly, compounds used to enhance athletic performance, chemicals used for pest and weed control, substances added to products to aid in manufacturing or to enhance properties, and toxic compounds produced by living organisms. The presence of 33 upregulated compounds, however, raises important considerations. Understanding the specific compounds that are not effectively removed or are introduced during treatment can inform targeted improvements in treatment protocols. This could involve integrating advanced treatment methods, such as advanced oxidation processes or membrane filtration, to enhance the removal efficiency for these persistent or emerging contaminants. Overall, the differential analysis and the resulting volcano plot provide a comprehensive overview of the treatment technology's performance, guiding future efforts in water quality management and ensuring the provision of safe and clean water.

Figure 3-2 presents a volcano plot illustrating the variation in chemical compounds between the raw and final water samples, along with statistical analyses to determine the significance of the observed differences. This includes p-values, fold changes, and other statistical metrics to validate the findings. The differential analysis revealed significant changes in the abundance of various compounds when comparing raw water to final treated water. The volcano plot (Figure 3-2) highlights these changes, with compounds found to be downregulated (green segment on the left) and compounds upregulated (red segment on the right). A total of 757 compounds showed a significant decrease in abundance post-treatment, while 33 compounds exhibited a significant increase in abundance after treatment. This analysis was conducted with a stringent threshold, considering compounds with a p-value less than or equal to 0.5 and a Log2 fold change greater than or equal to 0.5. The p-value, ranging from 0 to 1, indicates the probability of observing the data assuming the null hypothesis is true. A low p-value (≤ 0.5) suggests that we can reject the null hypothesis with a low probability of error, supporting the alternate hypothesis that there is a significant difference between the sample groups. The significant reduction in 757 compounds post-treatment underscores the efficacy of the conventional treatment technology in removing a wide array of contaminants. These downregulated

compounds include various industrial chemicals, pharmaceuticals, and personal care products, effectively



mitigated through the treatment processes employed.

Figure 3-2: Volcano Plot of Differential Analysis illustrating the variation in compounds between raw (source water) and final (product water) samples of a conventional treatment technology. The volcano plot highlights significant changes in compound abundance, with downregulated compounds shown in green (left) and upregulated compounds in red (right) with a p-value threshold of ≤ 0.5 and a log2 fold change threshold of ≥ 0.5.

3.2.3 Analysis of CECs in an indirect potable water reuse plant

A list of compounds contributing to the observed differences in these types of water is provided in Table A3-2 (Appendix section). Principal Component Analysis (PCA) was performed to distinguish the chemical characteristics of water samples at different stages of treatment: Source water, Intermediate steps, and Product water. The PCA plot in Figure 3-3 displays the first two principal components (PCs), which together account for 66.9% of the total variability in the dataset (PC1: 46.0%, PC2: 20.9%). The source water (represented by blue circles) shows clustering on the left side of the plot, primarily associated with negative values along PC1. In contrast, the intermediate step samples (represented by light green circles) cluster in the upper-right quadrant with positive values on both PC1 and PC2. Product water (represented by dark green circles) also appears on the right side, though it is distinctly separated from the intermediate step samples, reflecting a tighter grouping with lower PC2 values.

The PCA results highlight clear differentiation between the three water treatment stages based on their chemical profiles. The distinct clustering of the source water indicates that it is compositionally different from the intermediate and product waters. The negative PC1 values for the source water suggest that it has a specific set of chemical characteristics that diminish through the treatment process. The intermediate step samples show higher variability along PC2, which might be attributed to ongoing treatment processes affecting certain chemical parameters. The close clustering of product water, particularly along PC1, demonstrates the efficiency of the treatment process in the final water characteristics, likely resulting from

the removal of contaminants or the adjustment of key chemical factors. The small separation between intermediate and product water along PC1 suggests that the final treatment stages involve fine-tuning or polishing processes rather than dramatic chemical alterations. The successful reduction in variability and the clear separation between stages indicate the effectiveness of the treatment process in transforming the chemical properties of source water into a more uniform product, adhering to quality standards.

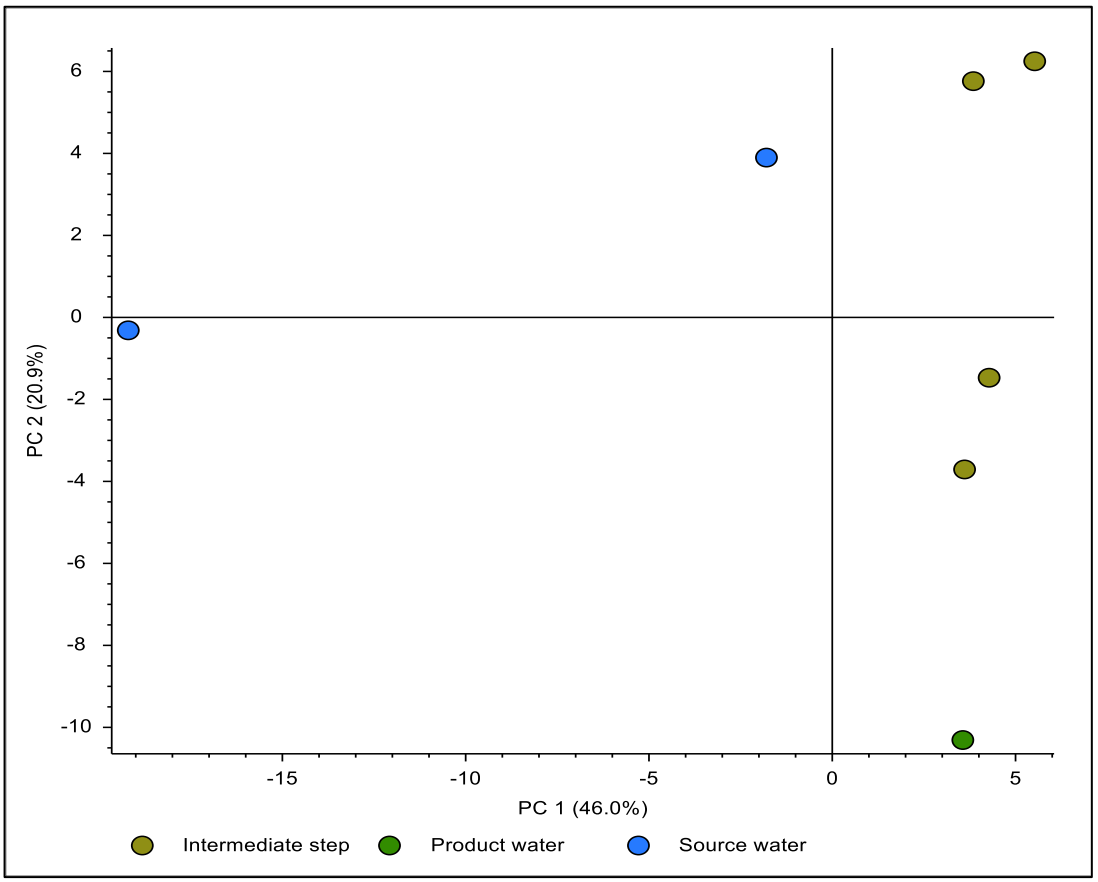


Figure 3-3: Principal Component Analysis (PCA) plot displaying the clustering of water samples from three stages of treatment of an indirect potable water reuse plant: Source water (blue), Intermediate steps (light green), and Product water (dark green).

3.2.4 Analysis of CECs in a direct potable water reuse plant

Table A3-3 provides a list of compounds identified in water samples collected from d-DwTP and used in this cluster analysis. The hierarchical clustering heatmap (Figure 3-4) represents the compounds identified in water samples collected from d-DwTP. The water samples are divided into two primary categories based on treatment process efficiency: source water (treated effluent) and product water (final water). The colour gradient, ranging from green to red, visualizes the compound abundance across the different sample groups. The source water samples show significant contamination, with high concentrations of various compounds, as evidenced by the prevalent red areas in the untreated water samples (left-hand clusters). Conversely, the product water (right-hand clusters) displays a predominantly green coloration, indicating the successful removal or reduction of the contaminants after treatment. The clear separation in clustering between source and product water further confirms that the treatment process leads to distinct chemical profiles. The variation observed within the source water cluster could be due to differences in contaminant loads in various samples,

possibly originating from diverse sources or fluctuating factors. The product water's uniform clustering suggests a consistent and robust treatment efficacy, which is a critical finding for ensuring the reliability of the water treatment process. Moreover, the treatment process appears particularly effective in removing compounds that exhibit higher concentrations in the source water. This is especially evident for compounds in the central and right-hand clusters, where drastic reductions in concentrations are observed post-treatment. The minor presence of residual compounds in the product water, as indicated by the occasional black regions in the heatmap, warrants further investigation to optimize the treatment process for complete elimination of these trace compounds. In summary, the hierarchical clustering analysis shows valuable insights into the composition of the water samples pre- and post-treatment. The marked difference in chemical profiles between source and product water strongly supports the efficacy of the treatment process in significantly reducing contaminants.

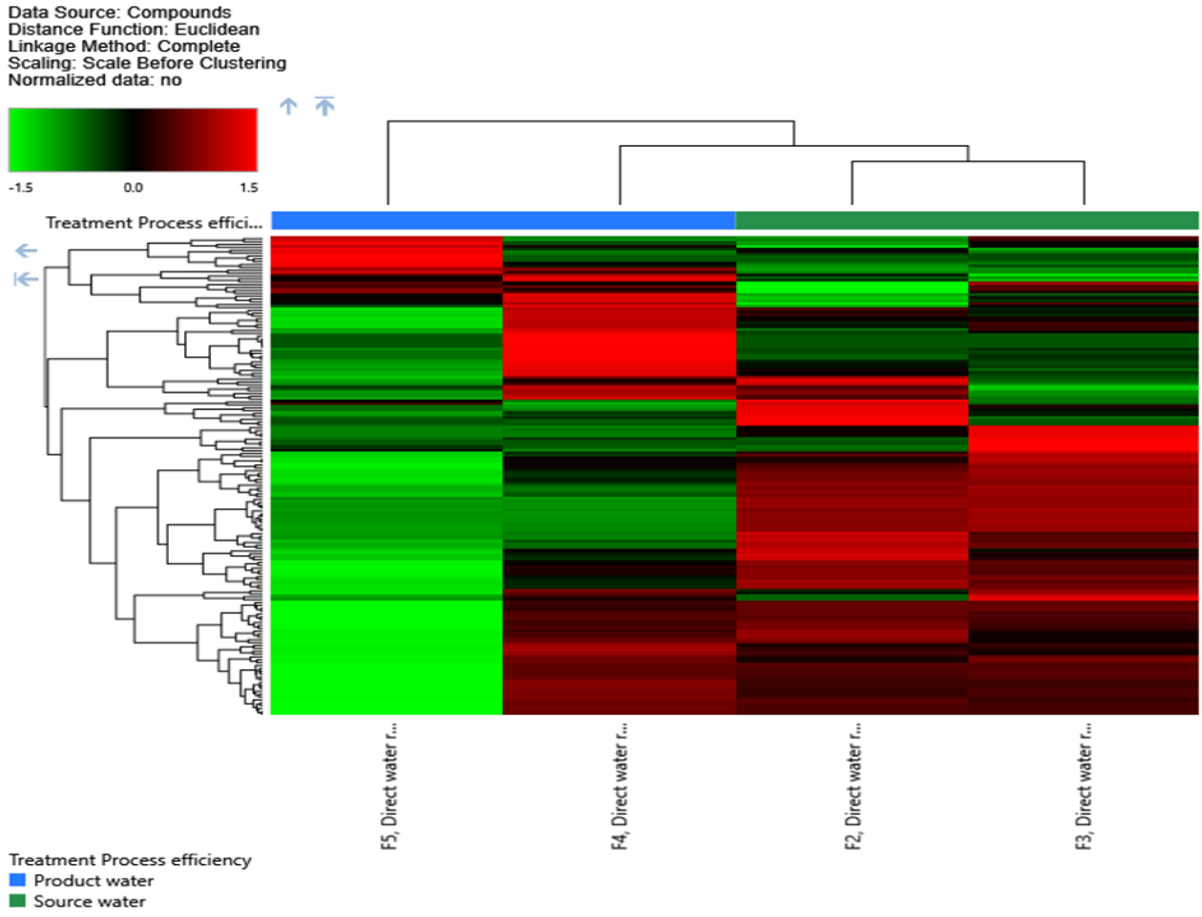


Figure 3-4: Hierarchical clustering heatmap of compounds identified in water samples from d-DwTP.

3.2.5 Quantification of CECs in a desalination plant

Figure 3-5 summaries the number of compounds identified in the desalination plant samples, extracted by MAPS, POCIS and SPE and analysed using an LC QTOF MS system. Accurate masses were obtained from base peak chromatogram (BPC) through the average spectrum function of Compass Data Analysis 4.3 software (Bruker Daltonics, Germany). Extracted ion chromatogram (EIC±0.005 mDa) of accurate masses was added to analysis list using add extracted ion chromatogram function of the data analysis software.

Online databases of KEGG, CHEBI, HMBD, and FOR-IDENT were used to annotate the proposed formulas through the Metfrag function in the compound crawler.

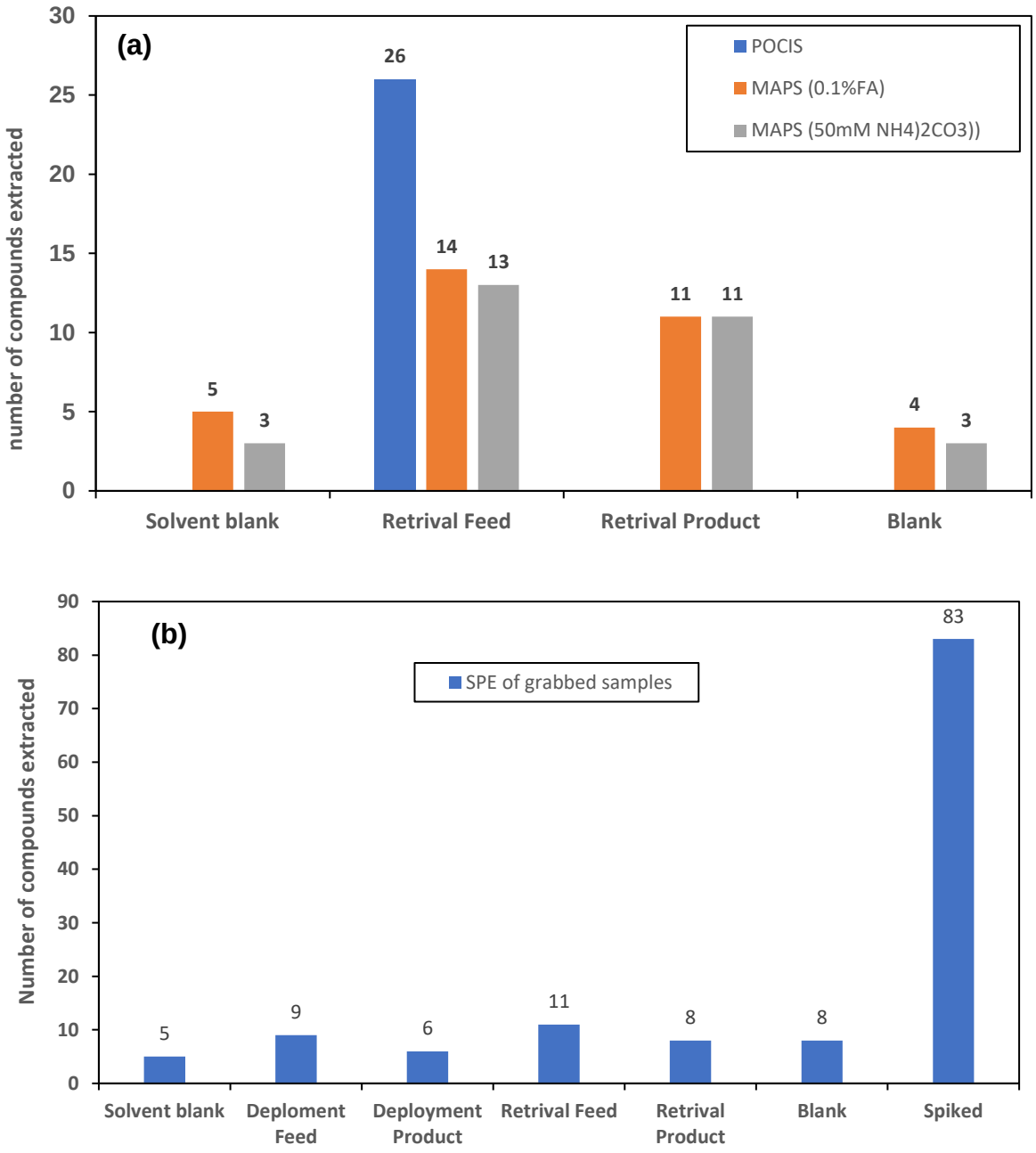


Figure 3-5: Bar graphs summarizing the number of compounds extracted from (a) POCIS and MAPS devices and (b) SPE of grab samples.

Twenty-six (26) compounds, all with very low mass errors (< 2 ppm) were detected in POCIS extract which was by far the highest number compared to eleven detected from SPE and fourteen from MAPS extracts (Figure 3-6). In general, the feed and product water samples collected from the desalination plant showed the presence of fumigants, industrial surfactants and plasticisers.

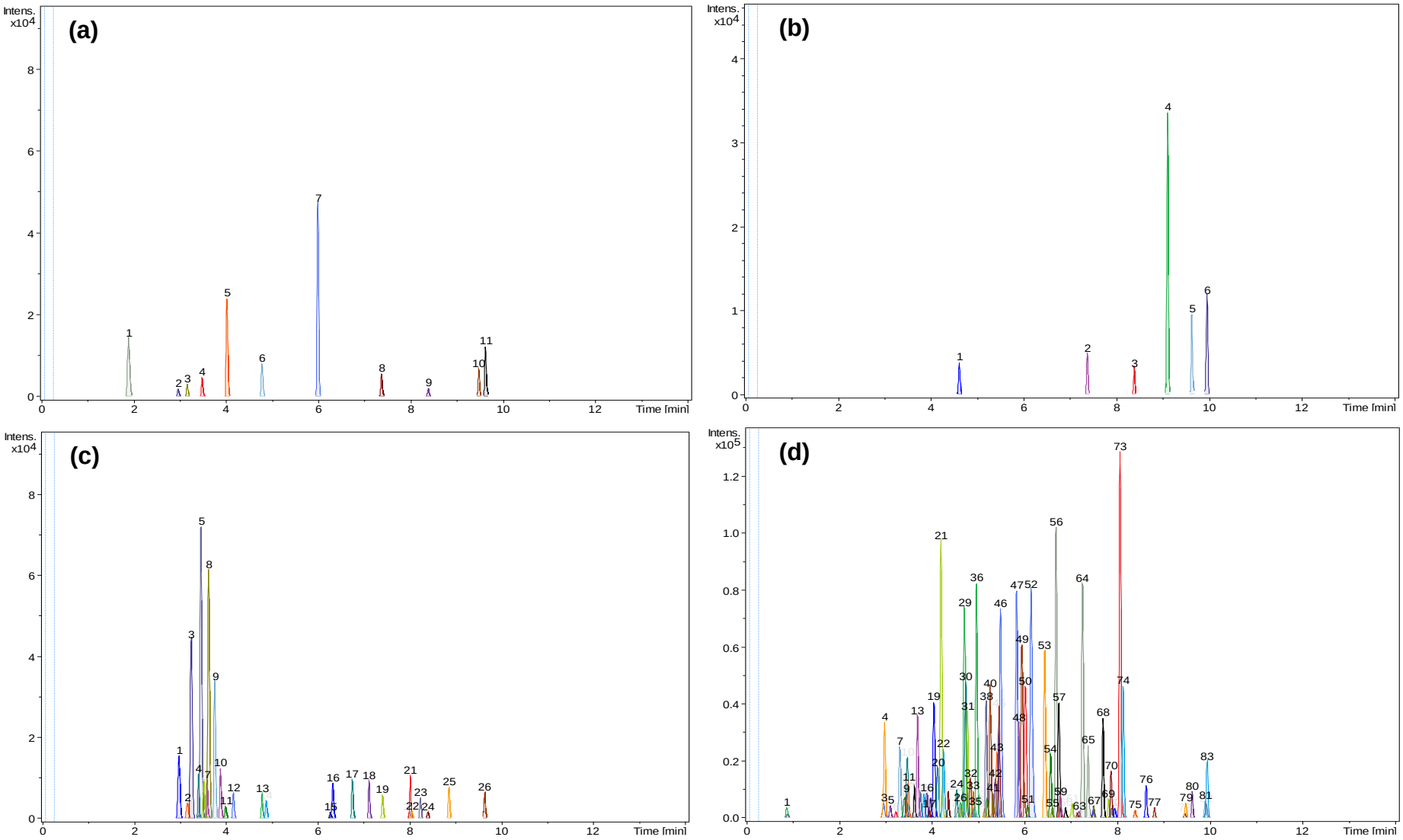


Figure 3-6: Example LC-MS chromatograms showing the number of peaks detected from (a) MAPS extracts obtained from the product water samples – 11 peaks; (b) grab water samples collected from the seawater feed water tank at deployment and preconcentrated using HLB.

Table 3-1 shows the metals identified by NexION 350 D ICP MS. The element removal efficiency of the desalination process was high, with elements like arsenic, calcium, copper, iron, lithium, magnesium, strontium, and vanadium concentrations being reduced significantly to acceptable levels for potable water. It is worth mentioning that the chemical analysis conducted by the UNISA laboratory specifically focused on assessing organic contaminants of emerging concerns. However, the micro-determinants reported in Table 3-3 become more relevant to be shown in this report especially in seawater desalination, where they could influence the levels of CECs. Other parameters stipulated in SANS 241 were closely monitored by the water treatment plants.

Table 3-1: Metal concentrations in desalination plant.

		Desalination Treatment Technology			
		Grab water samples at deployment		**Grab water samples at retrieval**	
		Sea water feed tank	Product water storage tank	Sea water feed tank	Product water storage tank
	pH	7.26	9.19	7.26	9.19
	Conductivity	53	222	32	217
Determinant	**Units**				
As (10)	μgL^{-1}	32.4	2.43	39.9	6.21
Be(4)	μgL^{-1}	0.00	0.02	0.05	0.03
Ca	μgL^{-1}	96344	3116	107882	3503
Cd(5)	μgL^{-1}	0.02	0.01	0.04	0.02
Co	μgL^{-1}	1.13	0.03	1.24	0.03
Cr(50)	μgL^{-1}	0.30	13.7	2.25	0.28
Cu(2000)	μgL^{-1}	223	16.4	236	26.8
Fe(200)	μgL^{-1}	1168	50.7	1328	51.4
Li	μgL^{-1}	59.2	0.52	63.8	0.92
Mg	μgL^{-1}	S	639	S	696
Mn(50)	μgL^{-1}	0.34	0.10	0.23	0.13
Mo	μgL^{-1}	3.00	0.22	6.67	0.45
Ni(20)	μgL^{-1}	7.15	0.92	7.25	0.92
Pb(10)	μgL^{-1}	0.01	0.00	0.04	0.02
Sb(5)	μgL^{-1}	0.16	0.06	0.18	0.14
Se(40)	μgL^{-1}	ND	ND	ND	ND
Sr	μgL^{-1}	2769	6.90	2961	6.95
Ti	μgL^{-1}	2.59	ND	3.86	0.64
Tl	μgL^{-1}	0.01	0.00	0.05	0.00
V	μgL^{-1}	38.9	2.43	43.7	5.32
Zn(5000)	μgL^{-1}	2.61	ND	2.69	ND

ND = Not detected S = Saturated

Principal component analysis (PCA) separated the sampling approaches into distinct groupings. The scores and loading plots of the sampling approaches (Figure 3-7) showed a vast significant difference in classes of compounds accumulated by the three sampling techniques. The overall spatial variation in the substances detected in the water samples from the feed and product water samples could be attributed to the sampling technique rather than the performance of the treatment technology. Extracts from the membrane-assisted passive sampling devices were mainly characterised by fumigates while POCIS samplers and SPE extracts had mainly industrial chemicals like Amino-PEG3-C2-acid. Furthermore, substances accumulated by the MAPS were mainly compounds that are non-ionizable at the sample pH which gets ionized at the pH of the acceptor phase. At the same time POCIS-HLB samplers accumulated polar organic compounds that are traditionally known to be extracted by a hydrophilic lipophilic balanced sorbent. More compounds were accumulated by the passive sampling devices than were with the grab sampling approach. Similar groupings were observed with PCA of classes of compounds detected by the GC TOF MS (Figure 3-8).

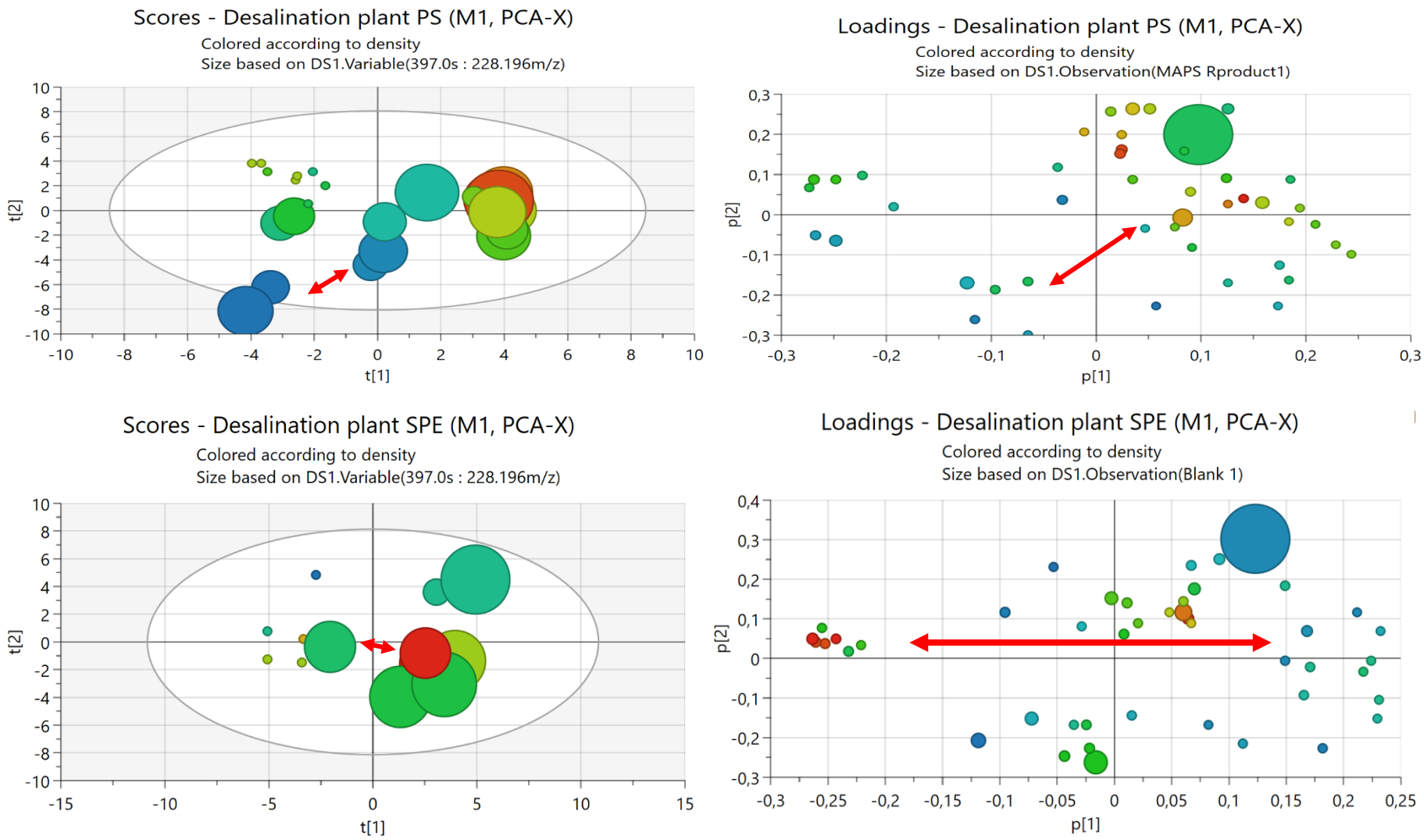


Figure 3-7: Principal component analysis (PCA) showing the loadings, and scores plots of desalination plant samples preconcentrated by various approaches versus substances detected by the LC Q TOF MS measurement technique

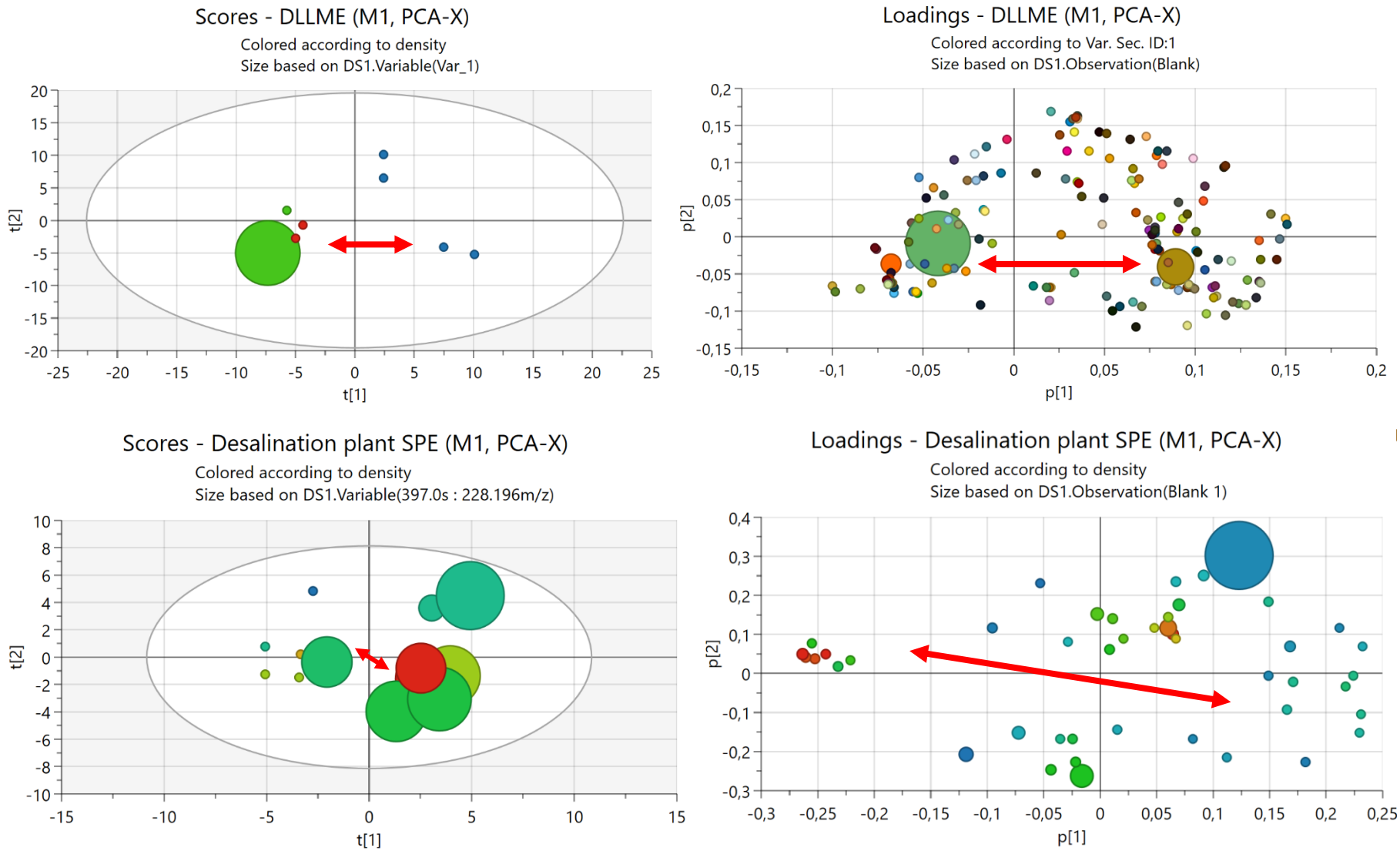


Figure 3-8: Principal component analysis (PCA) showing the loadings and scores plots of desalination plant samples preconcentrated by various sampling approaches versus substances detected by the GC TOF MS measurement technique.

3.3 ASSESSMENT OF THE PERFORMANCE OF WASTEWATER TREATMENT TECHNOLOGIES

3.3.1 Treatment efficacy of wastewater technologies

Water samples were collected from various key points to thoroughly assess water quality. Grab samples were taken from domestic and industrial wastewater treatment facilities, as well as from upstream and downstream locations of the respective effluent-receiving rivers. The hydraulic retention time of each treatment plant was considered during the collection of influents, intermediate treatment steps, and effluent water samples. To ensure sample integrity, the collected samples were promptly placed in ice-filled coolers for transportation to the laboratory, where they were processed and subjected to chemical analysis and effect-based assays within 48 hours. In addition to traditional sampling methods, passive sampling techniques such as Membrane Assisted Passive Sampler (MAPS), Chemcatcher, and Polar Organic Chemical Integrative Sampler (POCIS) were employed for monitoring emerging contaminants in WwTW2. Specifically, passive samplers were deployed in the effluent, upstream, and downstream locations of WwTP2. Extracts from these passive sampling devices were used for extensive chemical analyses.

3.3.2 Detection of CECs in wastewater effluent and receiving waters

The characterization of chemical pollutants in wastewater treatment technologies and receiving waters was performed using LC-MS/MS system, followed by comprehensive non-target and target data analysis strategy. To assess the impact of wastewater effluent discharge on the receiving river, water samples were collected from the domestic and industrial wastewater treatment plant, and the upstream and downstream of the receiving rivers. The distribution of the detected compounds within the selected study area is shown in Figure 3-9. A total of 1560 compounds were detected and identified in samples from the treatment effluents and influents from the treatment plants (Table A3-4).

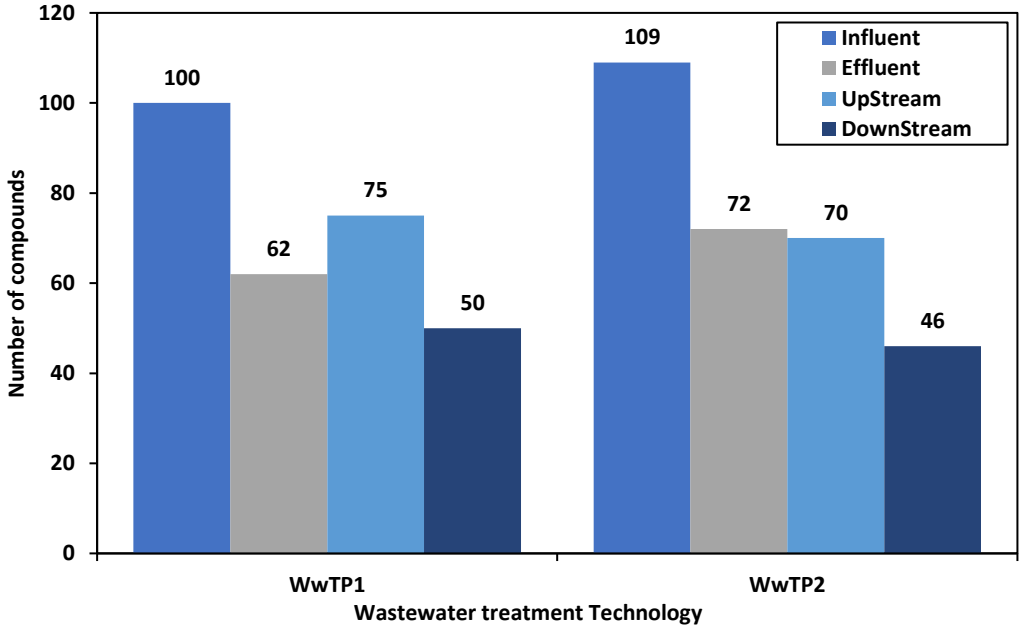


Figure 3-9: Distribution of the detected compounds in the sampling sites.

Among 1560 identified compounds, approximately 54% were exclusively detected in samples from domestic WwTP, while 46% were detected in samples from industrial WwTP. Approximately 56% of the identified compounds were exclusively detected in untreated wastewater samples, while 44% were detected in treated wastewater samples (see Figure 3-9). Water samples downstream (500 m) of the WwTPs were also collected and analysed to assess the impact of the WwTP effluents on receiving rivers. As shown in Figure 3-9, there was a decrease in the number of detected compounds when moving from the influent to the downstream of the WwTPs. The decrease in the number of detected compounds could be attributed to the wastewater treatment processes of the treatment plant. Furthermore, a high contamination load was observed upstream of the domestic WwTP, also suggesting possible contamination due to the non-formal settlements through which the river passes. In urban areas, such as those used in this study, the contaminants in surface waters can be attributed to stormwater drains, septic systems, and damaged sewer pipes. The identified compounds belong to a wide range of classes including pharmaceuticals, Personal care products pesticides, herbicides, and industrial chemicals as well as natural toxins and some uncategorized compounds (Figure 3-10). It is observed that the Endogenous metabolites were the most detected groups in both treated wastewater and surface water samples followed by the uncategorized group of compounds. Some examples of the active metabolites detected include O-desmethyl-tramadol and N-desmethyl-tramadol which are metabolites of tramadol (an opioid analgesic), as well as mebendazole-amine and Carbamazepine-epoxide, which are metabolites of mebendazole, and carbamazepine (anticonvulsant and analgesic drug), respectively. Some of the Pharmaceutical compounds identified included antiretroviral drugs (ARVs), non-steroidal anti-inflammatory drugs (NSAIDs), and antibiotics. As previously reported, ARVs are frequently detected at high concentrations in African countries due to the high HIV burden (Ncube et al., 2018).

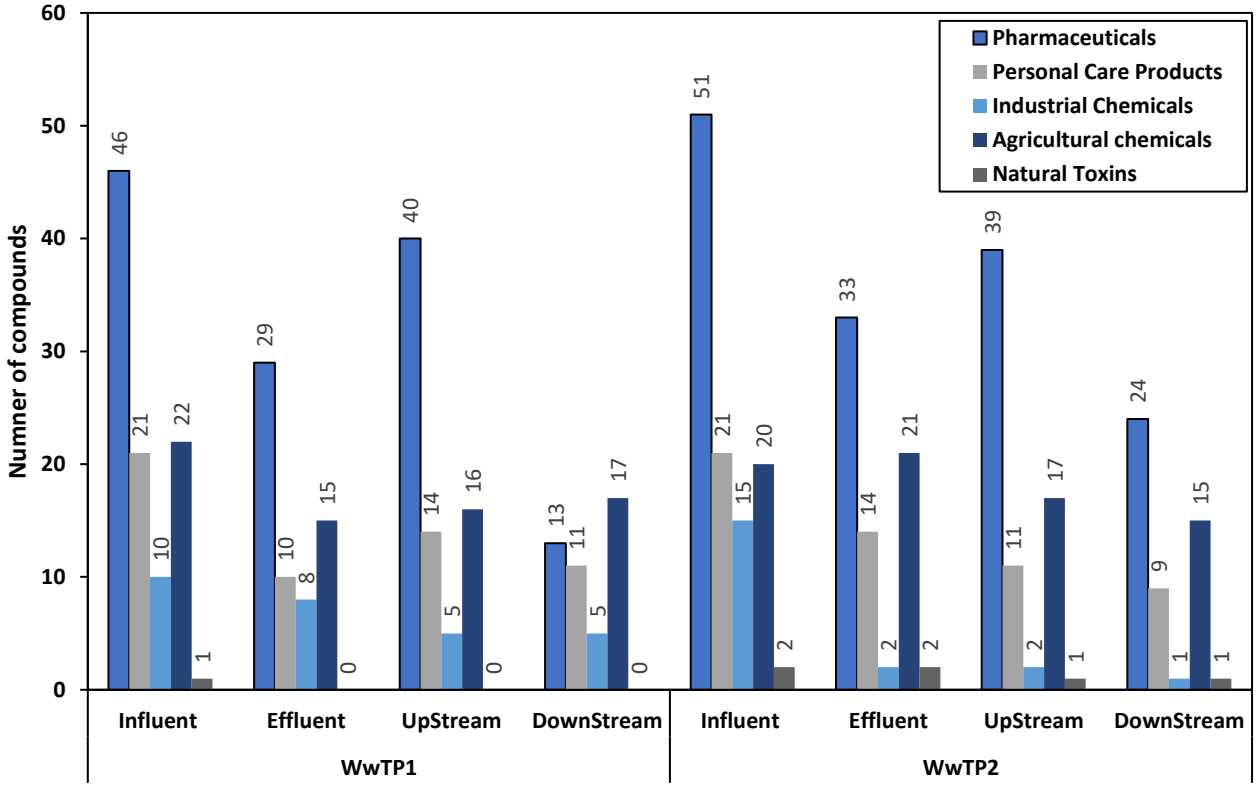


Figure 3-10: Distribution of the different classes across the sampling sites.

In addition, the detected ARVs included lamivudine and Abacavir. Among the compounds identified, NSAIDs of interest include codeine, which has been rated as one of the most abused over-the-counter drugs in South Africa (Carney et al., 2018). Other identified compounds of interest include dextrorphan. Although used primarily as an antitussive used to treat cough, it can also be abused as it has psychoactive and dissociative hallucinogenic effects. Some of the identified antibiotics included Sulfadimethoxine, sulfamethoxazole, and trimethoprim. Large quantities of antibiotics are administered to humans and animals to treat diseases and infections every year, and these detected antibiotics are among the most consumed antibiotics. The detected antibiotics are among the most consumed antibiotics. Furthermore, Glycol dimethyl ether, 3,3'-Dimethoxybenzidine, 2-Aminophenol and Triethyl phosphate were among the identified industrial contaminants detected in the samples. Figure 3-10 also reveals that the same classes of compounds found in surface waters are also present in WwTP effluents. This suggests that effluents from both industrial and domestic WwTPs are the main source of downstream surface water contamination by these compounds. All compounds that were detected upstream of the wastewater treatment plant were also detected downstream while fewer compounds, especially sporting doping compounds, prescribed drugs, and textile chemicals, were detected upstream compared to downstream.

3.3.3 Characterisation of CECs in wastewater using passive sampling

Figure 3-11 shows the extracted ion chromatogram for the selected pharmaceuticals accumulated by MAPS and POCIS respectively. The identity of the analytes was established by analyzing the masses obtained from the base peak chromatogram (BPC) using the average spectrum function of Compass Data Analysis 4.3 software (Bruker Daltonics, Germany). Accurate masses of compounds that were not present in the procedural blank were extracted using the add extracted ion chromatogram function of the software, with a tolerance of ±0.005 mDa. The selection of masses for further analysis was based on their intensity and the presence of MS/MS information (Figure 3-12). The possible molecular formulas were generated using the compound crawler function in Compass Data Analysis 4.3, which included C, H, O, P, S, Cl, and F elements. To annotate the proposed formulas, online databases of KEGG, CHEBI, HMBD, and FOR-IDENT were used through the Metfrag and Metfusion functions in the compound crawler.

The screening parameters used in this study included a mass accuracy of 5 ppm, an isotopic fit (mSigma) of less than or equal to 100, a signal to noise ratio of 3, a minimum intensity threshold of 500, and the presence of at least one product ion. The MS/MS spectra of the suspect compounds found in the afore mentioned online databases were verified with spectral libraries such as MassBank (https://massbank.eu/MassBank/), METLIN (http://METLIN.scripps.edu), Drug Bank (https://www.drugbank.ca/), and In Silico fragmentation platforms (CFM-ID) (cfmid.wishartlab.com/). Available reference standards were then used for unequivocal identification.

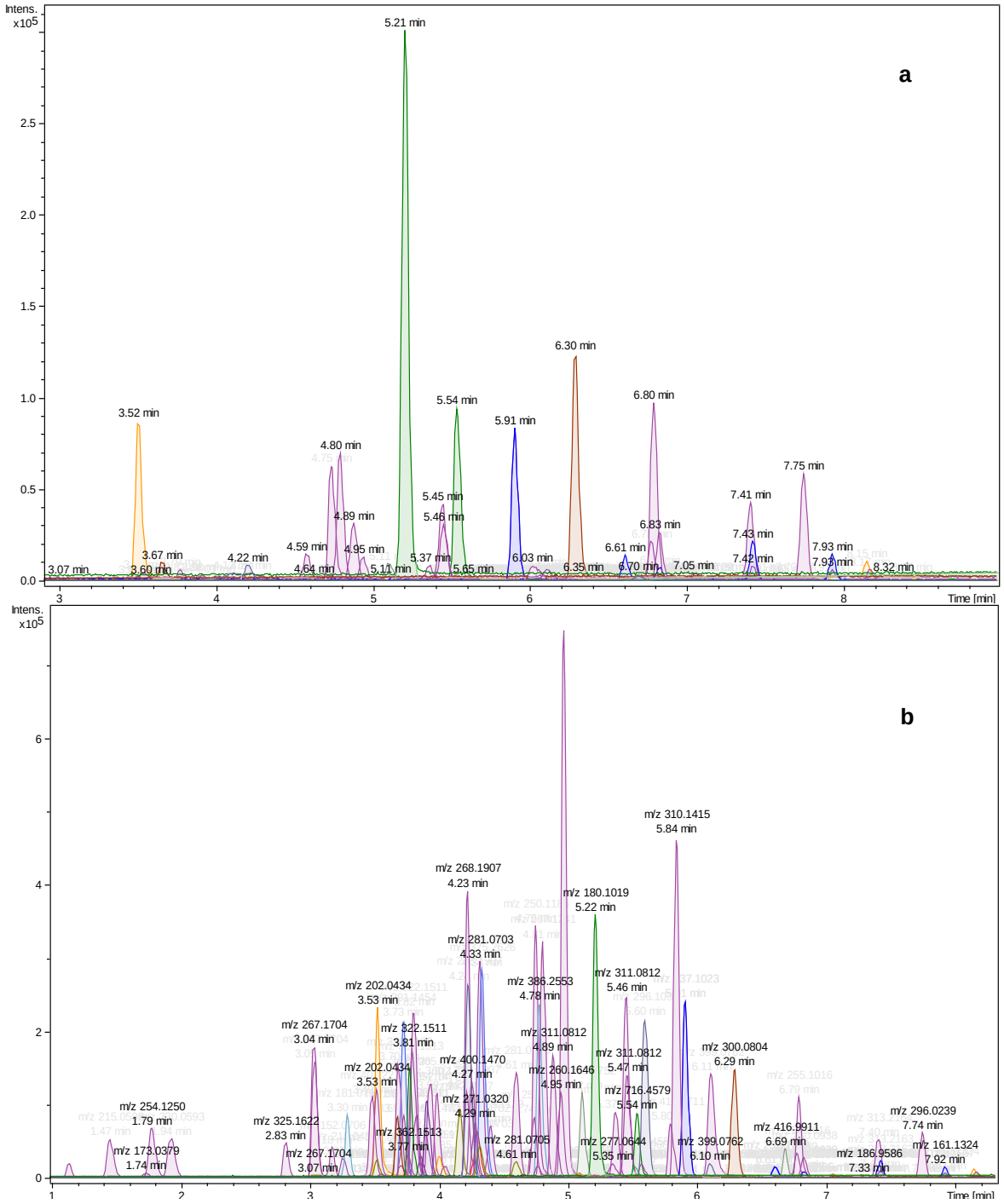


Figure 3-11: Extracted ion chromatograms corresponding to the organic micropollutants accumulated by the MAPS (a) and POCIS (b) after 14 days exposure.

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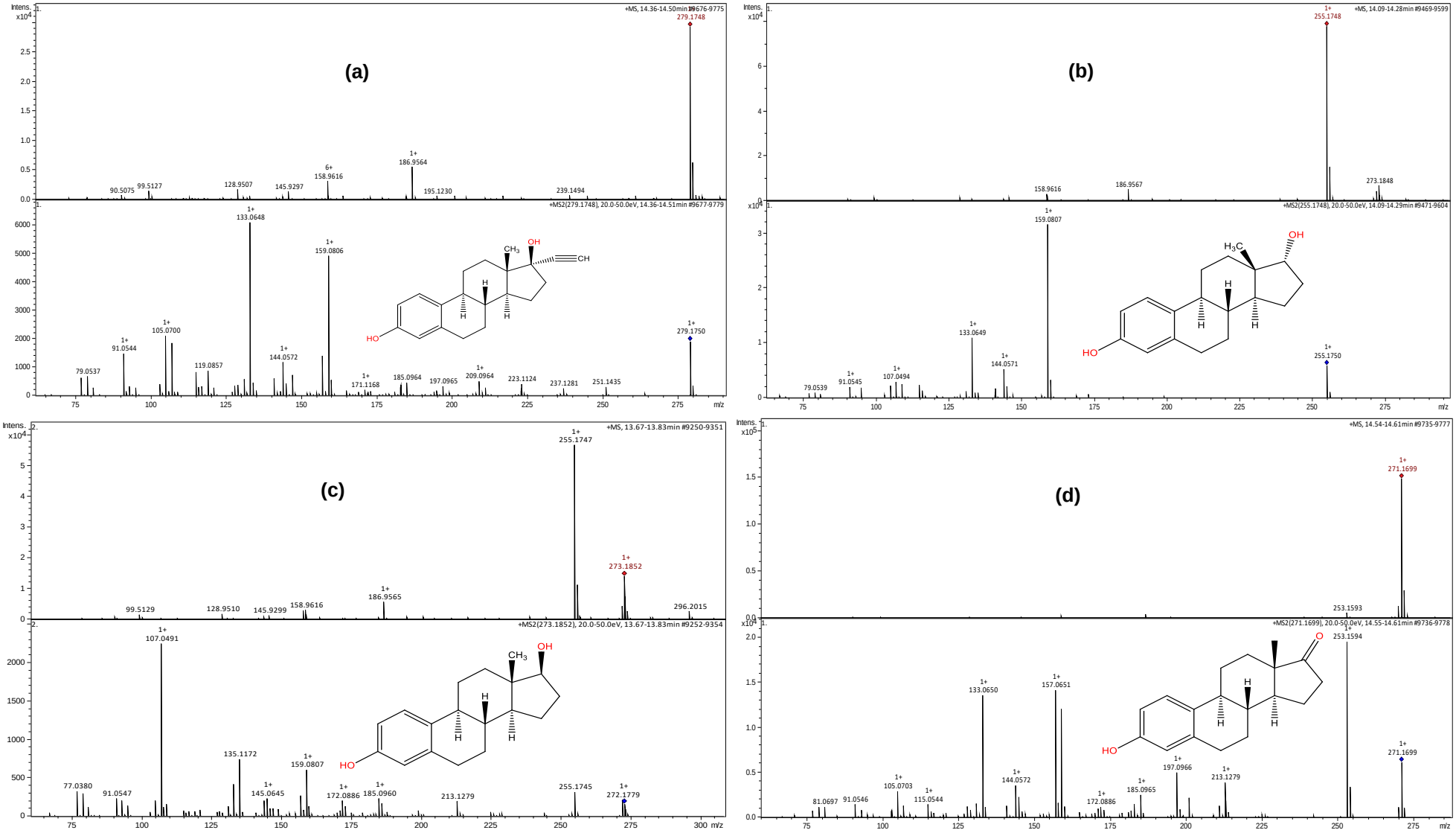

Figure 3-12: Typical MS-MS product ion spectra of four steroids (a) 17-α-Ethynyl estradiol (b) α-Estradiol (c) β-Estradione and (d) Estrone.

Table 3-2 shows the metal concentrations in wastewater effluent identified by NexION 350 D ICP MS. The element removal efficiency of the wastewater treatment plant was low.

Table 3-2: Metal concentration in wastewater influent and effluent.

		Domestic Wastewater Treatment Technology			
		Grab water Samples at deployment		Grab water Samples at retrieval	
		Influent	Effluent	Influent	Effluent
	pH	7.41	7.30	6.89	7.41
	Conductivity	673	569	394	545
Determinant					
As (10)	μgL^{-1}	2.523	5.20	1.08	1.17
Be(4)	μgL^{-1}	0.034	0.043	0.034	0.025
Ca	μgL^{-1}	25105	26442	20299	27152
Cd(5)	μgL^{-1}	0.006	0.020	ND	0.003
Co	μgL^{-1}	0.806	0.685	1.27	0.694
Cr(50)	μgL^{-1}	7.61	2.86	3.31	2.62
Cu(2000)	μgL^{-1}	10.4	13.5	1.43	2.79
Fe(200)	μgL^{-1}	561	427	741	446
Li	μgL^{-1}	8.34	5.67	3.52	4.57
Mg	μgL^{-1}	21045	20853	14273	22356
Mn(50)	μgL^{-1}	144	1.49	216	52.7
Mo	μgL^{-1}	0.613	1.20	0.309	1.85
Ni(20)	μgL^{-1}	5.02	4.31	3.74	4.23
Pb(10)	μgL^{-1}	0.208	0.100	0.137	0.053
Sb(5)	μgL^{-1}	0.167	0.553	0.210	0.430
Se(40)	μgL^{-1}	18.9	ND	6.99	2.35
Sr	μgL^{-1}	144	153	114	146
Ti	μgL^{-1}	ND	ND	ND	ND
Tl	μgL^{-1}	14.8	4.93	3.82	9.17
V	μgL^{-1}	2.72	6.95	1.37	2.11
Zn(5000)	μgL^{-1}	11.7	25.6	8.42	13.2

ND = Not detected S = Saturated

The chemical characterization of wastewater discharges into surface waters revealed key insights:

- pH Levels: Ranged from 6.38 to 7.95, within acceptable health risk limits (6.50 to 8.50). WwTP1 (domestic and industrial waste) had a lower influent pH (6.38) but secondary treatment raised it to 7.35. WwTP2 (domestic waste) had higher influent pH values.
- Electrical Conductivity (EC): Ranged from 220 to 1268 µS/cm, with high levels in WwTP2 effluent and WwTP1 anoxic samples. Secondary treatment reduced EC concentrations.
- Total Dissolved Solids (TDS): Ranged from 120 to 634 ppm, within regulatory guidelines.
- Turbidity: Ranged from 0.1 to 51 NTU, with higher levels in influent samples but effluent meeting discharge standards.

A total of 1560 organic compounds were identified, with 54% found in domestic WwTP2 samples and 46% in industrial WwTP1 samples. The most detected were endogenous metabolites, pharmaceuticals (ARVs, NSAIDs), and industrial contaminants (glycol dimethyl ether, 3,3'-dimethoxybenzidine). Effluents from both WwTPs were the main sources of downstream contamination, though treatment processes reduced compound levels downstream. Non-formal settlements and overflows contributed to upstream contamination.

4 CONCLUSIONS AND RECOMMENDATIONS

4.1 CONCLUSIONS

The assessment of drinking water treatment technologies, including conventional, desalination, direct, and indirect potable water plants, demonstrated compliance with regulated levels for various parameters, affirming their efficacy in ensuring safe drinking water. Analysis of chemical contaminants revealed a consistent reduction from source water through treatment stages to the final product, with conventional treatment showing the lowest contaminant load. However, direct water reuse technology exhibited a comparatively higher chemical burden, underscoring the heightened risk associated with direct wastewater reuse. This highlights the imperative for advanced treatment methods, particularly in direct reuse scenarios, to effectively manage complex water matrices. Furthermore, the overflow of holding dams at wastewater treatment plants resulted in the discharge of raw sewage into the receiving river, exacerbating contamination upstream. This underscores the pressing need for improved infrastructure management and capacity planning in wastewater treatment facilities.

Chemical analysis of desalination plant samples unveiled a distinct chemical profile primarily originating from biocides and other treatment chemicals, suggesting a unique contamination pattern associated with desalination processes, distinct from typical marine environments. Discharges of wastewater into receiving surface waters exhibited significant variations in parameters between domestic and industrial sources. Despite downstream contamination, the efficacy of wastewater treatment processes was evident through reductions in detected compounds downstream. However, the discharge of raw sewage due to dam overflows poses a notable challenge to wastewater management and infrastructure capacity.

Passive sampling devices proved more effective than grab sampling, providing comprehensive insights into contaminant accumulation. Different passive samplers displayed varying capabilities in capturing specific compound types, enhancing our understanding of contaminant profiles. In conclusion, robust non-target analysis employing advanced chemical analysis techniques facilitated a comprehensive assessment of organic chemicals across various treatment technologies and wastewater discharges. These findings underscore the importance of continuous monitoring and the adoption of advanced treatment approaches to safeguard water quality and environmental health.

4.2 RECOMMENDATIONS

Based on the limitations encountered in the current study, it is recommended that future research undertakings focus on addressing key gaps and enhancing the robustness of the findings. We recommend allocating resources and time to conduct fully-fledged quantitation experiments of the lists of contaminants identified in this work, adhering to established standards and protocols such as EPA Method 1694 and 1699. This includes the incorporation of isotopically labelled compounds as surrogates and internal standards to ensure accurate quantitation, as well as the implementation of rigorous quality control and assurance workflows to validate analytical measurements and ensure data reliability. Additionally, we recommend prioritizing the evaluation of passive sampling approaches and utilizing extracts from the sampler to evaluate a battery of bioassays targeting various toxicological pathways. We believe these future studies can contribute significantly to our understanding of the environmental implications of wastewater treatment processes and facilitate the development of sustainable water management strategies.

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APPENDIX

Table A3-1: A list of compounds identified in water samples collected from DwTP and used in this volcano plot differential analysis

Name	Compound Class	Final water	Raw water
(2E,4E)-N-(2-methylpropyl)dodeca-2,4-dienamide	Endogenous Metabolites; Natural Products/Medicines	5.1E+05	9.2E+05
(2S,5aS,8aR)-2-{3-[(2R)-2-(Methoxymethyl)-1-pyrrolidinyl]-3-oxopropyl}-1,6-dimethyloctahydropyrrolo[3,2-E][1,4]diazepin-5(2H)-one		3.7E+06	3.1E+06
1-(3,4-dichlorophenyl)ethan-1-one 1-(1H-1,2,4-triazol-3-yl)hydrazone		1.0E+06	5.6E+05
1,10-Diamino-4,7-dioxadecane		1.4E+05	3.8E+05
1,2,3-Benzotriazole	Industrial Chemicals	1.1E+07	2.0E+08
1,2-bis(2-methylphenyl)guanidine	Industrial Chemicals; Therapeutics/Prescription Drugs	2.4E+05	3.5E+05
1,3-Diphenylguanidine	Extractables/Leachables; Industrial Chemicals	2.0E+06	4.6E+07
12-Aminododecanoic acid		7.1E+05	3.0E+05
1-Dodecyl-2-pyrrolidinone	Extractables/Leachables; Personal Care Products/Cosmetics; Textile Chemicals/Auxiliary/Dyes	4.3E+07	1.5E+08
1-Methylxanthine	Endogenous Metabolites	1.7E+05	3.1E+05
1-phenyl-2-[(2-{[4-(trifluoromethyl)pyrimidin-2-yl]amino}ethyl)amino]ethan-1-ol		7.4E+06	6.7E+06
1-PHENYL-2-BUTANONE		6.0E+06	1.9E+07
2-(2H-benzotriazol-2-yl)-4-tert-butylphenol	Extractables/Leachables	2.5E+05	3.5E+05
2-(3-chloro-2-methylanilino)benzoic acid		6.9E+06	4.1E+06
2,2,6,6-Tetramethyl-4-piperidinol	Extractables/Leachables; Industrial Chemicals	3.3E+07	3.2E+07
2-[(14E,16S,17S)-2-Oxo-8-(1-piperazinyl)-12-oxa-1,4-diazatricyclo[14.3.1.06,11]icosa-6,8,10,14-tetraen-17-yl]-N-(3-pyridinylmethyl)acetamide		1.0E+06	1.1E+07

Name	Compound Class	Final water	Raw water
2-[(3R,4S)-3-{[5-(Cyclohexylmethyl)-1,2-oxazol-3-yl]methyl}-4-piperidinyl]-1-(4-morpholinyl)ethanone		1.9E+05	1.7E+05
2-aminoquinoline-3-carbonitrile		1.6E+05	2.7E+05
2-Isopropyl-6-methyl-4-pyrimidinol		8.9E+05	3.6E+05
2-methyl-1,2-dihydrophthalazin-1-one		3.4E+06	2.8E+06
2-sec-Butyl-3-methoxypyrazin	Excipients/Additives/Colorants	1.9E+07	8.5E+06
3,3'-Dimethoxybiphenyl-4,4'-diamine	Industrial Chemicals	7.7E+06	3.4E+05
3,6,9,12,15,18-Hexaoxaicosane-1,20-diol	Industrial Chemicals	5.1E+07	2.4E+08
3-Aminopyrrolidine		6.1E+06	2.1E+06
3-Hydroxypyridine	Endogenous Metabolites	1.2E+06	2.1E+06
4-(4,5-dihydro-1H-imidazol-2-yl)-2,6-dimethylmorpholine hydrobromide		5.1E+06	9.7E+06
4,6-dimethyl-2,7-diphenyl-3,7-dihydro-2H-pyrazolo[3,4-b]pyridin-3-one		2.4E+05	2.3E+05
4-Acetamidoantipyrine	Therapeutics/Prescription Drugs	4.6E+05	2.3E+06
4-Oxo-4-[(3-oxo-2-decanyl)amino]butanoic acid		2.0E+05	2.9E+06
4-Oxo-4-[(3-oxo-2-decanyl)amino]butanoic acid		1.6E+05	7.0E+05
5,6-Dimethylbenzimidazole	Endogenous Metabolites	4.7E+06	1.2E+07
5-[4-(2,5-dimethyl-1H-pyrrol-1-yl)phenyl]-4-(4-methylphenyl)-4H-1,2,4-triazole-3-thiol		7.1E+05	2.4E+05
5-Fluorocytosine	Therapeutics/Prescription Drugs	1.7E+05	1.7E+06
5-Methoxyindole		1.0E+06	8.3E+06
6beta-Naltrexol-d3	Drugs of Abuse/Illegal Drugs; Sports Doping Drugs	7.7E+05	1.2E+06
6-Chloro-5-methyl-1H-1,2,3-benzotriazole		1.3E+06	4.1E+05
8-Hydroxyquinoline	Therapeutics/Prescription Drugs; Endogenous Metabolites; Industrial Chemicals; Personal Care Products/Cosmetics; Pesticides/Herbicides	7.6E+06	3.1E+07
Abacavir	Therapeutics/Prescription Drugs	4.8E+05	1.0E+06

Name	Compound Class	Final water	Raw water
acenaphtho[1,2-b]quinoxaline		1.1E+06	7.0E+05
Acetylcholine	Endogenous Metabolites	1.7E+06	1.0E+07
Acridine	Industrial Chemicals	7.8E+06	1.1E+07
Atazanavir	Therapeutics/Prescription Drugs	4.0E+06	9.0E+06
AUDA		2.8E+06	1.3E+07
Azoxystrobin acid	Pesticides/Herbicides	3.8E+05	3.3E+05
Berberine	Endogenous Metabolites; Natural Products/Medicines	1.6E+06	5.0E+06
Betaine	Endogenous Metabolites	2.4E+07	2.3E+07
Bezafibrate	Therapeutics/Prescription Drugs	7.0E+05	2.2E+05
Caffeine	Endogenous Metabolites; Natural Products/Medicines	2.3E+06	3.9E+06
Carbamazepine	Therapeutics/Prescription Drugs	7.6E+07	1.1E+08
Chlorpheniramine	Therapeutics/Prescription Drugs	4.3E+06	1.1E+07
Choline	Endogenous Metabolites	5.2E+07	8.7E+07
Cinchonine		1.5E+05	3.9E+05
Citalopram	Sports Doping Drugs	1.9E+06	1.7E+07
Climbazole	Therapeutics/Prescription Drugs	4.4E+06	6.4E+06
Cotinine	Endogenous Metabolites	3.7E+06	1.8E+07
Cyclohexylamine	Extractables/Leachables	9.0E+06	5.0E+07
Cyproheptadine	Therapeutics/Prescription Drugs	6.9E+05	4.1E+06
Cytosine	Endogenous Metabolites	1.1E+06	2.5E+06
Decanamide		2.5E+06	1.6E+06
Desmethylcitalopram	Therapeutics/Prescription Drugs; Sports Doping Drugs	2.3E+06	5.2E+06
Dextromethorphan	Sports Doping Drugs	2.2E+06	3.4E+06
Didecyldimethylammonium	Therapeutics/Prescription Drugs; Personal Care Products/Cosmetics; Textile Chemicals/Auxiliary/Dyes	3.0E+07	8.1E+07
Diethanolamine	Industrial Chemicals	1.5E+07	1.1E+07

Name	Compound Class	Final water	Raw water
Diethyl phosphate	Pesticides/Herbicides	3.9E+05	1.5E+06
Diisodecyl phthalate	Extractables/Leachables; Textile Chemicals/Auxiliary/Dyes; Industrial Chemicals	6.7E+07	1.5E+07
diisopropylethylamine	Industrial Chemicals	1.1E+07	1.4E+08
Diltiazem	Therapeutics/Prescription Drugs; Drugs of Abuse/Illegal Drugs; Sports Doping Drugs	6.1E+05	1.8E+06
Dimethyl phosphate	Industrial Chemicals	2.8E+06	1.8E+06
Dimetridazole	Therapeutics/Prescription Drugs; Excipients/Additives/Colorants	2.7E+06	4.4E+06
Diuron	Pesticides/Herbicides; Industrial Chemicals	9.9E+05	2.7E+06
DL-Homoserine	Endogenous Metabolites	1.6E+06	1.0E+07
DL-Lysine	Endogenous Metabolites	2.9E+07	3.0E+07
DL-Serine	Endogenous Metabolites	5.2E+07	4.8E+07
DQH	Endogenous Metabolites	2.1E+07	1.2E+06
D-Serine	Endogenous Metabolites	1.3E+08	6.0E+07
Efavirenz	Therapeutics/Prescription Drugs; Drugs of Abuse/Illegal Drugs	1.1E+07	2.4E+07
Epinephrine	Therapeutics/Prescription Drugs; Endogenous Metabolites	3.2E+06	1.2E+07
ethyl 4-[2-(2-chlorophenyl)ethanehydrazonoyl]-5-methylisoxazole-3-carboxylate		1.4E+06	2.4E+06
Fluocinolone Acetonide	Therapeutics/Prescription Drugs; Sports Doping Drugs	8.3E+07	2.6E+08
GNH	Endogenous Metabolites	1.5E+08	1.3E+08
Guanine	Endogenous Metabolites	5.7E+05	3.2E+06
hexadecandioic acid	Endogenous Metabolites; Natural Products/Medicines	7.6E+07	4.9E+07
Lamotrigine	Therapeutics/Prescription Drugs	6.1E+07	4.2E+07
L-Aspartic acid	Endogenous Metabolites	7.0E+07	6.3E+07
Lidocaine	Therapeutics/Prescription Drugs	3.5E+05	1.3E+06

Name	Compound Class	Final water	Raw water
Macrosphelide D	Endogenous Metabolites; Natural Products/Medicines	2.5E+05	4.7E+05
Memantine	Therapeutics/Prescription Drugs; Sports Doping Drugs	8.3E+05	1.7E+06
Meprobamate	Therapeutics/Prescription Drugs; Sports Doping Drugs; Drugs of Abuse/Illegal Drugs	5.2E+06	8.9E+06
mesityl (4-methylphenyl) sulfone		4.1E+06	1.3E+07
Metformin	Therapeutics/Prescription Drugs	5.1E+05	4.7E+06
Methaqualone	Therapeutics/Prescription Drugs; Drugs of Abuse/Illegal Drugs; Sports Doping Drugs	4.0E+07	7.3E+07
Metronidazole	Therapeutics/Prescription Drugs	4.2E+05	5.0E+05
MPBP	Drugs of Abuse/Illegal Drugs	2.1E+06	5.2E+06
N-(1-Benzothiophen-3-yl)-N'-(3-cyclopropyl-1-methyl-1H-pyrazol-5-yl)urea		3.4E+06	9.3E+05
N-(2-Acetamidoethyl)-2-{(3R,4S)-3-[(5-butyl-1,2-oxazol-3-yl)methyl]-4-piperidinyl}acetamide		6.4E+05	7.5E+05
N-(3-Chlorophenyl)-6,7-dimethoxyquinazolin-4-amine		1.3E+07	5.2E+06
N,N,N',N',N'',N''-Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine	Extractables/Leachables; Industrial Chemicals; Textile Chemicals/Auxiliary/Dyes	4.2E+06	1.0E+07
N,N-Diethyl-3-methylbenzamide	Pesticides/Herbicides	1.1E+07	3.2E+07
N,N-dimethyl-9H-purin-6-amine		1.8E+06	5.1E+05
N-{6-[(7-Chloro-4-quinazolinyl)oxy]-3-pyridinyl}-2-thiophenesulfonamide		1.8E+07	5.2E+07
N2-(2,4-dimethylphenyl)-1,3-benzothiazol-2-amine		1.8E+06	7.5E+05
N-Amino(4-chloroanilino)methylideneguanidine		5.5E+05	8.5E+05
N-Arachidonoyl-L-serine	Endogenous Metabolites	5.0E+05	1.4E+06
N-Cyanoimido-S,S-dimethyl-dithiocarbonate		2.3E+06	1.9E+05
N'-Cyclohexylidenaminomethanehydrazonamide		9.9E+05	5.1E+06
N-Methyl-2-AI	Drugs of Abuse/Illegal Drugs	1.2E+06	3.5E+07
NP-016582	Endogenous Metabolites; Natural Products/Medicines	1.1E+05	2.2E+05

Name	Compound Class	Final water	Raw water
NP-021844	Endogenous Metabolites; Natural Products/Medicines	9.3E+06	1.4E+07
Ornithine	Endogenous Metabolites	7.0E+07	6.6E+07
Panthenol	Personal Care Products/Cosmetics	2.3E+05	8.9E+05
PEG Monolaurate n5	Extractables/Leachables; Industrial Chemicals	2.2E+06	7.1E+06
PEG Monolaurate n6	Extractables/Leachables; Industrial Chemicals	3.2E+06	1.1E+07
PEG n5	Industrial Chemicals	3.7E+07	1.0E+08
PEG n8	Industrial Chemicals	2.6E+08	5.7E+08
Piperine	Endogenous Metabolites; Natural Products/Medicines	1.5E+06	2.1E+06
PPG n5	Extractables/Leachables; Industrial Chemicals	2.0E+07	2.2E+07
PPG n6	Extractables/Leachables; Industrial Chemicals	1.5E+07	1.4E+07
PPG n7	Extractables/Leachables; Industrial Chemicals	7.5E+05	7.7E+05
PPG n8	Extractables/Leachables; Industrial Chemicals	1.1E+06	9.6E+05
Quinine	Endogenous Metabolites; Natural Products/Medicines	1.7E+05	2.3E+06
Rhodamine 6G		4.4E+05	1.1E+07
Ricinine	Endogenous Metabolites; Natural Toxins	2.3E+06	3.1E+06
Sodium [dodecanoyl(methyl)amino]acetate	Extractables/Leachables; Personal Care Products/Cosmetics; Textile Chemicals/Auxiliary/Dyes; Industrial Chemicals	3.4E+05	4.9E+05
Solanidine	Natural Toxins; Endogenous Metabolites	1.9E+05	2.8E+05
Sorbic acid	Extractables/Leachables; Excipients/Additives/Colorants; Industrial	2.3E+07	2.4E+07

Name	Compound Class	Final water	Raw water
	Chemicals; Endogenous Metabolites; Personal Care Products/Cosmetics		
Sulfadimethoxine	Therapeutics/Prescription Drugs	2.0E+05	3.3E+05
Sulfamethoxazole	Therapeutics/Prescription Drugs; Endogenous Metabolites	5.1E+06	9.7E+07
Sulfapyridine	Therapeutics/Prescription Drugs; Pesticides/Herbicides	3.6E+06	3.5E+07
Tebuthiuron	Pesticides/Herbicides	2.0E+06	3.7E+06
TMK	Endogenous Metabolites	1.6E+05	1.9E+05
tolytriazole	Textile Chemicals/Auxiliary/Dyes; Endogenous Metabolites	6.4E+07	1.1E+09
Tributyl phosphate	Industrial Chemicals	3.8E+06	4.8E+06
Triethyl citrate	Extractables/Leachables; Excipients/Additives/Colorants; Personal Care Products/Cosmetics; Industrial Chemicals	2.0E+07	1.7E+07
Triethylene glycol monobutyl ether	Industrial Chemicals	6.9E+06	8.6E+06
Triethylphosphate	Industrial Chemicals	5.2E+06	8.9E+06
Triisopropanolamine	Extractables/Leachables; Industrial Chemicals; Textile Chemicals/Auxiliary/Dyes; Personal Care Products/Cosmetics; Pesticides/Herbicides	6.2E+06	1.4E+07
Trimethoprim	Therapeutics/Prescription Drugs	9.7E+04	3.8E+06
Triphenylphosphine oxide		1.8E+07	2.8E+07
Tris(2-butoxyethyl) phosphate	Extractables/Leachables; Textile Chemicals/Auxiliary/Dyes; Industrial Chemicals	1.3E+08	1.3E+08
Tyroscherin		3.4E+06	2.7E+06
Valsartan	Therapeutics/Prescription Drugs	1.7E+06	1.3E+06
Vatalanib dihydrochloride		1.6E+05	1.9E+05

Table A3-2: Compounds identified in drinking water samples using a non-targeted analysis approach with the Compound Discoverer software

Name	Formula	m/z	RT [min]
Tris(2-butoxyethyl) phosphate	C18 H39 O7 P	399.249	12.314
3-methyl-5-(4-methyl-1,2,3-thiadiazol-5-yl)-4-isoxazolecarboxamide	C8 H8 N4 O2 S	225.0433	10.353
N-Acetyltyramine	C10 H13 N O2	180.1018	6.093
1-Ethyl-3-[(1S,2S,3S,4R,5R)-3-hydroxy-4-(4-phenyl-1-piperazinyl)-6,8-dioxabicyclo[3.2.1]oct-2-yl]urea	C19 H28 N4 O4	377.2184	11.155
Fluocinolone acetonide	C24 H30 F2 O6	453.2082	7.356
6-Pentyl-2H-pyran-2-one	C10 H14 O2	167.1067	7.154
Arecoline	C8 H13 N O2	156.102	7.173
3,4-Dimethoxy-α-pyrrolidinopentiophenone	C17 H25 N O3	292.1902	6.443
NP-018660	C13 H22 O3	209.1534	9.581
Cytidine	C9 H13 N3 O5	244.0938	7.69
BMPEA	C9 H13 N	136.1122	1.311
7-Hydroxycoumarine	C9 H6 O3	163.039	7.669
1-(4-methoxyphenyl)propane-1,2-diol	C10 H14 O3	205.0831	9.383
Venlafaxine	C17 H27 N O2	278.2108	6.95
2-Amino-6-methylmercaptopurine	C6 H7 N5 S	182.0494	4.835
Quinine	C20 H24 N2 O2	325.19	6.875
D-Panthenol	C9 H19 N O4	206.1383	1.157
NP-016516	C16 H24 O4	281.1732	10.651
N-(9-oxodecyl)acetamide	C12 H23 N O2	214.1798	10.194
Methyl isonicotinate	C7 H7 N O2	138.0551	6.373
Clarithromycin	C38 H69 N O13	748.4815	9.859
NP-012972	C14 H24 O3	263.1611	11.909
Oxazepam	C15 H11 Cl N2 O2	287.0574	10.36
NP-006862	C20 H32 O4	359.2183	10.963
NP-018661	C8 H16 O3	143.1067	6.685
L-Histidine	C6 H9 N3 O2	156.0765	0.414
2,6-Dimethyl-γ-pyrone	C7 H8 O2	125.06	6.64
D-(+)-Pyroglutamic Acid	C5 H7 N O3	130.0501	1.095

Name	Formula	m/z	RT [min]
NP-016668	C10 H12 N2 O	215.0588	8.792
2-(1,3-benzodioxol-5-yl)-7-ethylimidazo[1,2-a]pyridine	C16 H14 N2 O2	267.1123	9.041
N-{4-[(2R,3R)-3-(Hydroxymethyl)-4-methyl-5-oxo-2-morpholinyl]phenyl}-2,2-dimethylpropanamide	C17 H24 N2 O4	321.1822	12.771
DL-Serine	C3 H7 N O3	106.0502	0.405
5α-Androstan-3,6,17-trione	C19 H26 O3	303.1947	10
4-(1H-imidazol-1-yl)benzoic acid	C10 H8 N2 O2	189.0658	6.177
1,5-Isoquinolinediol	C9 H7 N O2	162.055	5.449
4-(Diethylamino)salicylaldehyde	C11 H15 N O2	194.1173	11.041
NP-006656	C12 H22 O4	213.1484	11.037
NP-021030	C9 H8 O4	163.039	10.316
6-Methyl-2-pyridinemethanol	C7 H9 N O	124.0761	6.082
Apocynin	C9 H10 O3	167.0705	7.337
Doxylamine	C17 H22 N2 O	271.1799	5.614
NP-007065	C8 H10 O3	155.0705	6.738
2-{[(4,5-dimethoxy-2-nitrophenethyl)imino]methyl}phenol	C17 H18 N2 O5	331.1296	11.345
1-Methylbenzotriazole	C7 H7 N3	134.0716	7.215
Triamterene	C12 H11 N7	254.1161	8.905
trans,trans-2,4-Heptadienal	C7 H10 O	111.0809	6.786
6-Methyl-2-pyridinemethanol	C7 H9 N O	124.0761	6.68
3-[3-(1,3-dimethyl-1H-pyrazol-4-yl)-1H-1,2,4-triazol-1-yl]-5-methylisoxazole	C11 H12 N6 O	245.1145	10.641
5-Ethylcyclohexane-1,3-dione	C8 H12 O2	141.0912	10.206
NP-021018	C12 H18 O4	249.1092	9.439
NP-007909	C13 H20 O3	247.1298	9.382
(3S,4aR,5R,6R)-3,6-dihydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-one	C15 H22 O3	251.1633	11.668
Metronidazole	C6 H9 N3 O3	172.0717	1.453
2-Methylcyclohexan-1,3-dione	C7 H10 O2	127.0756	6.963
NP-019374	C10 H18 O4	203.1276	9.406
1-adamantyl(piperidino)methanone	C16 H25 N O	248.2006	8.975

Name	Formula	m/z	RT [min]
Propranolol	C16 H21 N O2	260.1641	8.488
NP-001130	C8 H12 O4	205.1067	8.966
N,N-Diethyldodecanamide	C16 H33 N O	256.263	13.34
NP-011223	C10 H18 O3	169.1224	7.334
Citral	C10 H16 O	153.1274	9.81
2-Aminophenol	C6 H7 N O	110.0604	5.829
NP-006656	C12 H22 O4	253.1404	10.345
2-Phenylbenzimidazole-5-sulfonic acid	C13 H10 N2 O3 S	275.0479	6.446
19-Norandrostenedione	C18 H24 O2	273.184	11.224
Ricinine	C8 H8 N2 O2	165.0659	1.178
Eucalyptol	C10 H18 O	137.1326	9.981
8-Hydroxyquinoline	C9 H7 N O	146.0601	5.349
NP-018660	C13 H22 O3	227.1639	11.67
NP-019491	C15 H22 O4	289.1401	10.342
2-Hydroxyatrazine	C8 H15 N5 O	198.1348	1.194
Isophorone	C9 H14 O	139.1119	9.345
Desnitro-imidacloprid	C9 H11 Cl N4	211.0751	10.379
NP-018661	C8 H16 O3	183.0988	10.243
5-Hydroxyindole	C8 H7 N O	134.0604	6.8
Benzophenone	C13 H10 O	183.0803	10.913
5-Fluorocytosine	C4 H4 F N3 O	130.0414	1.15
Phenethyl isothiocyanate	C9 H9 N S	164.0529	0.981
Dehydroepiandrosterone (DHEA)	C19 H28 O2	289.2153	10.752
NP-012972	C14 H24 O3	241.1793	11.278
Sedanolide	C12 H18 O2	195.138	9.749
Ethyl-2-amino-1-cyclohexene-1-carboxylate	C9 H15 N O2	170.1175	8.769
α-Pinene-2-oxide	C10 H16 O	153.1274	6.073
NP-006888	C13 H24 O4	227.1638	10.802
2-(3,5-dichlorophenyl)-6-methyl-2,3,4,5-tetrahydropyridazin-3-one	C11 H10 Cl2 N2 O	257.0239	7.594
Jasmonic acid	C12 H18 O3	211.1328	9.158

Name	Formula	m/z	RT [min]
NP-020156	C9 H17 N O4	226.1045	9.399
Diazinon	C12 H21 N2 O3 P S	305.1075	11.773
(2S,8R)-8-hydroxy-2-[(1S)-1-hydroxyheptyl]-3,4,5,6,7,8-hexahydro-2H-1-benzopyran-5-one	C16 H26 O4	305.1716	10.396
1,2,3,4-Tetramethyl-1,3-cyclopentadiene	C9 H14	123.1171	8.575
Tetraglyme	C10 H22 O5	223.1534	6.653
NP-007909	C13 H20 O3	225.1483	8.693
Scoparone	C11 H10 O4	207.065	9.872
NP-001846	C11 H20 O4	217.143	10.867
YM218	C35 H38 F2 N4 O4	617.291	12.58
Creatine	C4 H9 N3 O2	132.0771	12.324
6-Pentyl-2H-pyran-2-one	C10 H14 O2	167.1067	9.991
Tributyl phosphate	C12 H27 O4 P	267.1712	12.156
(3S,4aR,5R,6R)-3,6-dihydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-one	C15 H22 O3	251.164	12.506
AUDA	C23 H40 N2 O3	393.3098	11.227
NP-015145	C14 H13 N O2	228.1008	7.894
Cinchonidine	C19 H22 N2 O	295.1799	8.577
Tetrahydrocortisone	C21 H32 O5	365.231	10.797
5-Ethylcyclohexane-1,3-dione	C8 H12 O2	141.0913	9.476
Olomoucine	C15 H18 N6 O	299.1609	11.392
9-hydroxy-2,10,10-trimethyltricyclo[6.3.0.0Âa,â• µ]undec-6-ene-6-carboxylic acid	C15 H22 O3	251.1637	11.103
NP-003800	C10 H15 N O3	198.1123	8.084
NP-018661	C8 H16 O3	183.099	8.448
1-[(1S,2S,3S,4R,5R)-4-(Diethylamino)-3-hydroxy-6,8-dioxabicyclo[3.2.1]oct-2-yl]-3-(4-methoxyphenyl)urea	C18 H27 N3 O5	366.2032	11.754
2-{[(cyanoimino)(methylthio)methyl]amino}propane	C6 H11 N3 S	158.0747	7.284
N'-(2-Chlorophenyl)-N-(2-cyanoethyl)-N-isopropylurea	C13 H16 Cl N3 O	266.1063	9.016
Acetanilide	C8 H9 N O	136.0759	8.305
1-ethyl-6-imino-5-[(1E)-2-(4-methylphenyl)diazen-1-yl]-1,3-diazinane-2,4-dione	C13 H15 N5 O2	274.1292	8.565
N-Acetyl-L-leucine	C8 H15 N O3	174.1125	7.822

Name	Formula	m/z	RT [min]
[(3R,4S)-3-[(6-Methoxy-3,4-dihydro-1-isoquinolinyl)methyl]-1-(4-morpholinylcarbonyl)-4-piperidinyl]acetic acid	C23 H31 N3 O5	430.232	7.58
Trimethoprim	C14 H18 N4 O3	291.1443	1.295
Desnitro-imidacloprid	C9 H11 Cl N4	211.7016	10.1
NP-020014	C15 H26 O3	277.1766	11.811
Urocanic acid	C6 H6 N2 O2	121.0398	0.425
3,4-Dimethoxy-α-pyrrolidinopentiophenone	C17 H25 N O3	292.1897	10.211
N-Acetyl-L-leucine	C8 H15 N O3	174.1124	7.66
Dimidium	C20 H17 N3	300.1503	8.305
NP-020400	C12 H18 O5	265.1041	9.994
4-styrylpyridine	C13 H11 N	182.0964	1.123
Arecoline	C8 H13 N O2	156.1021	1.219
2-(5-tert-Butyl-2-hydroxyphenyl)benzotriazole	C16 H17 N3 O	268.1437	8.184
Palmitoleic acid	C16 H30 O2	255.231	12.583
Ethyl 3-acetyl-4-oxopentanoate	C9 H14 O4	187.0964	9.114
Climbazole	C15 H17 Cl N2 O2	293.1045	9.817
5-Methoxyindole	C9 H9 N O	148.0759	7.875
Dodecyltrimethylammonium	C15 H33 N	228.2681	13.362
N-Cyanoimido-S,S-dimethyl-dithiocarbonate	C4 H6 N2 S2	147.0047	7.091
NP-003459	C9 H14 O4	169.0861	8.27
Meptazinol	C15 H23 N O	234.1849	8.263
Decarbamoyloxysaxitoxin	C9 H16 N6 O2	241.1404	10.165
Megestrol acetate	C24 H32 O4	385.2356	11.196
Tropine	C8 H15 N O	142.123	8.938
NP-020632	C16 H20 O4	299.1247	10.513
PEG Monolaurate n6	C24 H48 O8	465.3405	11.761
NP-008563	C16 H28 O4	285.2051	11.432
2-Hydroxyquinoline	C9 H7 N O	146.0602	7.879
NP-008095	C15 H24 O3	235.1687	9.92
NP-008993	C18 H34 O4	315.2519	12.084

Name	Formula	m/z	RT [min]
Cyproheptadine	C21 H21 N	288.1742	9.551
Cocaine	C17 H21 N O4	304.1535	6.975
N-Methyloctan-1-amine	C9 H21 N	144.1749	1.299
L-Histidine	C6 H9 N3 O2	156.0768	1.087
2-[(2R,4aR,8R,8aR)-8-hydroxy-4a,8-dimethyl-decahydronaphthalen-2-yl]prop-2-enoic acid	C15 H24 O3	235.1689	11.196
NP-019374	C10 H18 O4	203.1275	9.209
Diethyleneglycol diacetate	C8 H14 O5	191.0911	8.437
2,6-Diaminotoluene	C7 H10 N2	123.0918	0.386
Azobenzene	C12 H10 N2	183.0916	6.713
Apocynin	C9 H10 O3	167.0706	7.431
Normeperidine	C14 H19 N O2	234.1486	7.85
N-Butylbenzenesulfonamide	C10 H15 N O2 S	214.0892	9.96
N-Arachidonoyl-L-serine	C23 H37 N O4	392.2776	11.512
Nalorphine	C19 H21 N O3	312.1583	11.735
Methyprylon	C10 H17 N O2	167.1067	8.822
Tapentadol	C14 H23 N O	222.1849	8.989
DL-Arginine	C6 H14 N4 O2	175.1188	1.059
4-[(6E)-3-Hydroxy-8,10-dimethyl-2-(methylamino)-6-dodecen-1-yl]phenol	C21 H35 N O2	334.2728	11.926
Melamine	C3 H6 N6	127.0729	1.085
Phenazone	C11 H12 N2 O	189.1023	7.092
4-heptyl-3-methyl-1H-pyrazol-5-ol	C11 H20 N2 O	197.1647	7.548
(±)15-HETE	C20 H32 O3	321.2413	11.722
4-(4,5-dihydro-1H-imidazol-2-yl)-2,6-dimethylmorpholine hydrobromide	C9 H17 N3 O	184.1444	6.461
NP-020014	C15 H26 O3	277.1766	11.984
Meperidine	C15 H21 N O2	248.1641	7.528
NP-006888	C13 H24 O4	267.1558	10.926
Ethyl-2-amino-1-cyclohexene-1-carboxylate	C9 H15 N O2	170.1176	7.089
Carbamazepine 10,11-epoxide	C15 H12 N2 O2	253.0967	9.101
L-Tyrosine	C9 H11 N O3	182.0812	8.797

Name	Formula	m/z	RT [min]
3,5-Dimethyl-1-phenylpyrazole	C11 H12 N2	173.1074	1.033
6-hydroxy-4a-(hydroxymethyl)-5-methyl-3-(prop-1-en-2-yl)-2,3,4,4a,5,6,7,8-octahydronaphthalen-2-one	C15 H22 O3	273.1453	9.563
Decanamide	C10 H21 N O	172.1696	10.18
(2S,8R)-8-hydroxy-2-[(1S)-1-hydroxyheptyl]-3,4,5,6,7,8-hexahydro-2H-1-benzopyran-5-one	C16 H26 O4	283.1896	10.503
1,3-di-o-Tolylguanidine	C15 H17 N3	240.1492	7.562
2,6-Di-tert-butyl-1,4-benzoquinone	C14 H20 O2	221.1533	10.487
Methamphetamine	C10 H15 N	150.1279	1.226
2,4-Dimethylbenzaldehyde	C9 H10 O	135.0807	7.576
Gabapentin	C9 H17 N O2	172.1331	9.245
Lidocaine	C14 H22 N2 O	235.1802	5.904
(8aR,12S,12aR)-12-Hydroxy-4-methyl-4,5,6,7,8,8a,12,12a-octahydro-2H-3-benzoxecine-2,9(1H)-dione	C14 H20 O4	275.1247	10.316
NP-012972	C14 H24 O3	241.1793	11.541
(2R,3R,4S,5S,6R)-2-[(3Z)-hex-3-en-1-yloxy]-6-(hydroxymethyl)oxane-3,4,5-triol	C12 H22 O6	285.13	8.594
1-Phenyl-2-butanone	C10 H12 O	149.0962	7.887
3-Amino-2-naphthoic acid	C11 H9 N O2	188.0705	9.305
2-(3-chloro-2-methylanilino)benzoic acid	C14 H12 Cl N O2	262.0623	9.858
6-Methylindole	C9 H9 N	132.081	0.982
Tropine	C8 H15 N O	142.1228	8.682
Tropine	C8 H15 N O	142.1229	8.225
Pramocaine	C17 H27 N O3	294.2057	10.014
L-Methionine sulfoxide	C5 H11 N O3 S	166.0532	0.921
Mebendazole amine	C14 H11 N3 O	238.097	8.15
NP-018131	C15 H28 O7	343.1717	9.014
2-[(1S)-1-Hydroxyethyl]-4(1H)-quinazolinone	C10 H10 N2 O2	191.0814	7.416
(6S)-6-[(1S,2R)-1,2-dihydroxypentyl]-4-methoxy-5,6-dihydro-2H-pyran-2-one	C11 H18 O5	231.1222	8.309
2-methyl-1,2-dihydrophthalazin-1-one	C9 H8 N2 O	161.071	1.19
Jasmone	C11 H16 O	165.1274	10.592
N1-[4-(acetylamino)phenyl]-2,2-dimethylcyclopropane-1-carboxamide	C14 H18 N2 O2	247.1436	1.004

Name	Formula	m/z	RT [min]
1,8-Diazabicyclo [5.4.0]undec-7-ene	C9 H16 N2	153.1388	6.291
3-Hydroxy-5-(hydroxymethyl)-2-methylisonicotinaldehyde oxime	C8 H10 N2 O3	200.1027	0.988
Cuminaldehyde	C10 H12 O	149.0963	11.693
NP-019360	C8 H12 O4	155.0706	9.118
4-Methoxycinnamaldehyde	C10 H10 O2	163.0756	9.276
Vanillin	C8 H8 O3	153.0548	8.57
4-Ethylbenzaldehyde	C9 H10 O	135.0807	7.212
5-(tert-butyl)-2-methyl-N-(5-methyl-3-isoxazolyl)-3-furamide	C14 H18 N2 O3	301.0951	8.831
Desnitro-imidacloprid	C9 H11 Cl N4	211.0754	10.387
4-Phenylbutyric acid	C10 H12 O2	165.0912	7.591
1-(5H-dibenzo[b,f]azepin-5-yl)ethan-1-one	C16 H13 N O	236.1063	1.01
4-Methoxychalcone	C16 H14 O2	239.1076	8.963
4,4'-Dihydroxybenzophenone	C13 H10 O3	215.0701	8.568
NP-022473	C18 H26 O5	323.1832	8.895
(4S,5S,8S,10R)-4,5,8-trihydroxy-10-methyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	C10 H16 O5	217.1067	8.968
NP-016668	C10 H12 N2 O	215.0586	9.5
Creatine	C4 H9 N3 O2	132.077	9.003
PEG n6	C12 H26 O7	283.1749	7.19
4-tert-Butylcyclohexyl acetate	C12 H22 O2	199.169	10.286
NP-001130	C8 H12 O4	155.0704	8.46
4'-Methoxyacetophenone	C9 H10 O2	151.0754	8.305
trans-Cinnamaldehyde	C9 H8 O	133.065	10.89
9-acridinecarboxylic acid hydrate	C14 H9 N O2	224.0705	1.095
NP-019374	C10 H18 O4	203.1277	8.865
(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-(propan-2-yloxy)oxane-3,4,5-triol	C9 H18 O6	223.1173	1.264
Acetyl norfentanyl	C13 H18 N2 O	219.1488	10.49
N-Methyl-2-pyrrolidone	C5 H9 N O	100.0761	5.486
(-)-Caryophyllene oxide	C15 H24 O	221.1896	11.579
6-(3-hydroxybutan-2-yl)-5-(hydroxymethyl)-4-methoxy-2H-pyran-2-one	C11 H16 O5	251.0886	7.48

Name	Formula	m/z	RT [min]
N,N-Dimethylaniline	C8 H11 N	122.0968	5.277
N,N-Dimethylpentylone	C14 H19 N O3	251.9617	0.954
Kynurenic acid	C10 H7 N O3	190.0497	7.128
4-Methyl-5-thiazoleethanol	C6 H9 N O S	144.048	1.281
trans-Cinnamaldehyde	C9 H8 O	133.0649	9.53
Nitrosoheptamethyleneimine	C7 H14 N2 O	143.1181	7.504
N1-[4-(1,3-Oxazol-5-yl)phenyl]cyclopropane-1-carboxamide	C13 H12 N2 O2	229.0968	6.994
trans-Cinnamaldehyde	C9 H8 O	133.065	9.535
Nornicotine	C9 H12 N2	149.1074	0.99
Metamitron	C10 H10 N4 O	203.0926	1.052
trans-Anethole	C10 H12 O	149.0963	1.044
7-hydroxy-6-methoxy-2H-chromen-2-one	C10 H8 O4	193.0496	7.633
3-Hydroxy-3-methylbutanoic acid	C5 H10 O3	119.0705	7.211
trans,trans-2,4-Heptadienal	C7 H10 O	111.0803	6.988
N,N'-Diphenylurea	C13 H12 N2 O	213.1016	10.117
2,6-Dimethyl-γ-pyrone	C7 H8 O2	125.0599	1.146
NP-002336	C23 H36 O5	415.2433	11.845
NP-019360	C8 H12 O4	155.0705	6.026
NP-019360	C8 H12 O4	155.0704	5.928
PEG n7	C14 H30 O8	327.2012	8.259
1-(3-acetyl-2,4,6-trihydroxyphenyl)ethan-1-one	C10 H10 O5	211.0601	6.125
1-(2-furyl)pentane-1,4-dione	C9 H10 O3	167.0706	10.438
Metolachlor OXA	C15 H21 N O4	302.1361	10.333
N-(4-chlorophenyl)urea	C7 H7 Cl N2 O	171.0321	8.786
PEG n8	C16 H34 O9	371.2271	8.253
(7R,8S)-7,8-Dihydroxy-3,7-dimethyl-6-oxo-7,8-dihydro-6H-isochromene-5-carbaldehyde	C12 H12 O5	237.0753	9.029
Azobenzene	C12 H10 N2	183.0916	1.109
4-Chloro-1,2-diaminobenzene	C6 H7 Cl N2	143.0373	5.449
Mescaline NBOMe	C19 H25 N O4	332.1843	12.549

Name	Formula	m/z	RT [min]
4-(isopropylsulfonyl)-3-(methylthio)-1H-pyrazol-5-amine	C7 H13 N3 O2 S2	236.0526	5.974
NP-019988	C10 H10 O4	217.0465	1.139
N,N'-Dicyclohexylurea	C13 H24 N2 O	225.1957	11.183
2-methyl-2,3,4,5-tetrahydro-1,5-benzoxazepin-4-one	C10 H11 N O2	200.0682	7.382
Phthaldialdehyde	C8 H6 O2	135.0441	0.721
Melamine	C3 H6 N6	127.073	9.034
NP-019360	C8 H12 O4	195.0624	1.2
Citral	C10 H16 O	153.1276	7.38
4-Nitrosodiphenylamine	C12 H10 N2 O	199.087	8.589
Phthaldialdehyde	C8 H6 O2	135.0442	6.802
4-Phenyl-3-buten-2-one	C10 H10 O	147.0804	9.298
Maltol	C6 H6 O3	127.0392	1.997
(2E,4E,9Z)-1-(piperidin-1-yl)hexadeca-2,4,9-trien-1-one	C21 H35 N O	318.2783	13.48
5-(2,5-dihydroxyhexyl)oxolan-2-one	C10 H18 O4	225.1093	1.213
Dipropylene glycol dimethyl ether	C8 H18 O3	163.1328	10.203
Acridine	C13 H9 N	180.0808	10.471
Norharman	C11 H8 N2	169.0761	6.22
1,3-Divinyl-2-imidazolidinone	C7 H10 N2 O	139.0869	5.797
Vasicinone	C11 H10 N2 O2	203.0813	1.216
3-methoxy-1,13-dimethyl-9,11,12,13,14,15,16,17-octahydro-8H-cyclopenta[a]phenanthren-17-ol	C20 H26 O2	299.1993	11.838
4'-Methoxy-α-ethylaminovalerophenone	C14 H21 N O2	236.1642	9.235
N,N'-Diphenylurea	C13 H12 N2 O	213.1021	10.162
Desomorphine	C17 H21 N O2	272.1632	10.127
Phthaldialdehyde	C8 H6 O2	135.0442	8.021
N-(cyclopropylmethyl)-2-{[(1,2-dimethyl-1H-imidazol-4-yl)sulfonyl]amino}benzamide	C16 H20 N4 O3 S	349.1317	10.616
Cuminaldehyde	C10 H12 O	149.0961	11.508
4-Oxo-4-[(3-oxo-2-decanyl)amino]butanoic acid	C14 H25 N O4	272.1852	6.341
Phthaldialdehyde	C8 H6 O2	167.0706	9.705

Name	Formula	m/z	RT [min]
3-oxoindane-1-carboxylic acid	C10 H8 O3	177.0547	10.735
2-Methoxybenzaldehyde	C8 H8 O2	137.06	6.424
NP-007909	C13 H20 O3	207.1377	8.843
Memantine	C12 H21 N	180.1748	8.861
4-Phenylbutyric acid	C10 H12 O2	165.091	11.038
3-(4-chlorophenyl)-4-imino-7-(1-pyrrolidinyl)-3,4-dihydropyrimido[4,5-d]pyrimidin-2(1H)-one	C16 H15 Cl N6 O	343.1055	9.689
3-Acetyl-2,5-dimethylfuran	C8 H10 O2	139.0756	7.166
6-Quinolinecarboxylic acid	C10 H7 N O2	174.0545	6.697
D-(-)-Aspartic acid	C4 H7 N O4	134.0449	1.125
4,4'-Dihydroxydiphenylsulfone	C12 H10 O4 S	251.0368	8.309
Artemisinin	C15 H22 O5	283.1523	9.869
NP-016564	C16 H20 O6	331.1142	9.985
NP-019360	C8 H12 O4	173.0811	8.437
4-Piperidinecarboxamide	C6 H12 N2 O	129.1025	1.147
Sedanolide	C12 H18 O2	177.1273	9.1
L-Norleucine	C6 H13 N O2	132.1022	1.236
ethyl 4-amino-2-(methylsulfanyl)-1,3-thiazole-5-carboxylate	C7 H10 N2 O2 S2	219.0262	11.619
Trenbolone	C18 H22 O2	271.1684	10.828
Acetophenone	C8 H8 O	121.0651	5.91
2,3,4,9-Tetrahydro-1H-β-carboline-3-carboxylic acid	C12 H12 N2 O2	217.0967	6.038
2-methyl-1,2-dihydrophthalazin-1-one	C9 H8 N2 O	161.0709	6.629
DL-Arginine	C6 H14 N4 O2	175.1187	0.445
Harmine	C13 H12 N2 O	213.1021	6.705
N,N-Diisopropylethylamine (DIPEA)	C8 H19 N	130.1593	6.115
Gabapentin	C9 H17 N O2	172.1333	1.249
2-Methylcyclohexan-1,3-dione	C7 H10 O2	127.0757	8.57
Codeine	C18 H21 N O3	300.1587	1.315
2,4-Dimethylbenzaldehyde	C9 H10 O	135.0806	11.009
Pulegone	C10 H16 O	153.1274	10.624

Name	Formula	m/z	RT [min]
NP-003117	C13 H20 O4	263.1247	8.337
Lamivudine	C8 H11 N3 O3 S	230.0591	1.324
NP-022474	C16 H24 O3	265.1793	10.489
Piperonylonitrile	C8 H5 N O2	148.0395	6.624
4-heptyl-3-methyl-1H-pyrazol-5-ol	C11 H20 N2 O	197.1646	10.218
Decanamide	C10 H21 N O	172.1695	11.036
(2E,4E,9Z)-1-(piperidin-1-yl)hexadeca-2,4,9-trien-1-one	C21 H35 N O	318.2782	9.996
Cytosine	C4 H5 N3 O	112.051	1.307
NP-003117	C13 H20 O4	241.1431	9.412
DL-Lysine	C6 H14 N2 O2	129.1024	0.434
Lidocaine	C14 H22 N2 O	235.18	1.169
4,6-Dimethyl-2(1H)-pyrimidinone	C6 H8 N2 O	125.0713	1.239
1-propyl-1H-benzo[d]imidazole hydrobromide	C10 H12 N2	161.1074	6.623
ethyl 2-[(5-ethoxy-4-phenyl-4H-1,2,4-triazol-3-yl)thio]acetate	C14 H17 N3 O3 S	308.1056	7.838
1,3-Dimethylpteridine-2,4-dione	C8 H8 N4 O2	193.072	1.287
(±)15-HETE	C20 H32 O3	321.2411	11.609
2-aminoquinoline-3-carbonitrile	C10 H7 N3	170.0713	6.678
4-Hydroxyindole	C8 H7 N O	151.0867	1.216
N'-Cyclohexylidenaminomethanehydrazonamide	C7 H14 N4	155.1287	1.107
4-[(3S)-7-hydroxy-8-(3-methylbut-2-en-1-yl)-3,4-dihydro-2H-1-benzopyran-3-yl]benzene-1,3-diol	C20 H22 O4	327.1586	12.231
N'-Cyclohexylidenaminomethanehydrazonamide	C7 H14 N4	155.129	0.554
NP-020014	C15 H26 O3	237.1846	11.13
Cyclohexylamine	C6 H13 N	100.1124	5.255
PEG n5	C10 H22 O6	239.1484	6.797
Creatine	C4 H9 N3 O2	132.0771	11.585
5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one	C13 H22 O3	227.1639	10.495
2-[(3R,4S)-3-{[5-(Cyclohexylmethyl)-1,2-oxazol-3-yl]methyl}-4-piperidinyl]-N-(3-pyridinylmethyl)acetamide	C24 H34 N4 O2	433.2557	12.745
5,6,7,8-Tetrahydro-2-naphthol	C10 H12 O	149.0964	9.526

Name	Formula	m/z	RT [min]
4-Phenyl-3-buten-2-one	C10 H10 O	147.0805	9.629
NP-020082	C8 H12 O4	155.0704	7.203
1,2,3,4-Tetramethyl-1,3-cyclopentadiene	C9 H14	123.1171	9.395
NP-014924	C10 H12 O4	197.081	10.647
N-Amino(4-chloroanilino)methylideneguanidine	C8 H10 Cl N5	212.0696	5.255
Dimetridazole	C5 H7 N3 O2	142.0613	2.944
6-Pentyl-2H-pyran-2-one	C10 H14 O2	167.1067	8.878
NKK	C16 H32 N6 O5	389.2499	9.978
1-Adamantanamine	C10 H17 N	152.1435	5.918
NP-013210	C12 H14 O3	189.0911	10.559
NP-003399	C14 H12 O2	213.0906	7.572
NP-021018	C12 H18 O4	227.1277	10.867
2-Isopropyl-6-methyl-4-pyrimidinol	C8 H12 N2 O	153.1024	4.819
NP-007065	C8 H10 O3	155.0706	6.043
Apocynin	C9 H10 O3	167.0706	6.729
Apocynin	C9 H10 O3	167.0705	8.365
tetranor-12(R)-HETE	C16 H26 O3	267.1951	11.182
2-Methylcyclohexan-1,3-dione	C7 H10 O2	127.0755	5.858
Heptanophenone	C13 H18 O	191.1428	10.867
Cyclohexyl phenyl ketone	C13 H16 O	189.1272	11.724
Isophorone	C9 H14 O	139.1117	9.87
Oxprenolol	C15 H23 N O3	266.1744	10.613
[2-(hydroxymethyl)-5,5,8a-trimethyl-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-yl]methanol	C15 H26 O2	239.2004	12.236
Sedanolide	C12 H18 O2	195.1377	10.616
indoline-2-carboxylic acid	C9 H9 N O2	146.0602	5.38
trans-Cinnamaldehyde	C9 H8 O	133.065	8.684
2-Hydroxyatrazine	C8 H15 N5 O	198.1348	5.955
2-Methoxy-5-methylaniline	C8 H11 N O	138.0918	8.919
4-Acetamidoantipyrine	C13 H15 N3 O2	246.1233	5.882

Name	Formula	m/z	RT [min]
4-Phenylbutyric acid	C10 H12 O2	165.0913	8.521
Sedanolide	C12 H18 O2	195.1382	9.399
Bicyclo Prostaglandin E2	C20 H30 O4	357.2023	11.677
Sedanolide	C12 H18 O2	195.1379	9.571
NP-007909	C13 H20 O3	225.1484	9.737
Procyclidine	C19 H29 N O	288.2318	9.568
Eucalyptol	C10 H18 O	155.143	9.57
Isoferulic acid	C10 H10 O4	195.0652	7.617
2,6-Diaminotoluene	C7 H10 N2	123.092	11.878
4-Isobutylbenzoic acid	C11 H14 O2	179.1067	10.893
6-Pentyl-2H-pyran-2-one	C10 H14 O2	167.1068	8.997
N-Ethylamphetamine	C11 H17 N	164.1434	6.209
3-[(2-chloro-1,3-thiazol-5-yl)methyl]-5-methyl-1,3,5-oxadiazinan-4-ylideneamin	C8 H11 Cl N4 O S	247.0409	0.997
Prolinamide	C5 H10 N2 O	115.087	13.375
N,N-Diethylethanolamine	C6 H15 N O	118.123	13.418
4-(Diethylamino)salicylaldehyde	C11 H15 N O2	194.1176	7.727
NP-001846	C11 H20 O4	217.1431	10.736
N-Methyl-2-pyrrolidone	C5 H9 N O	100.0761	1.1
Meptazinol	C15 H23 N O	234.1848	0.99
5-Ethylcyclohexane-1,3-dione	C8 H12 O2	141.0911	8.509
Triethanolamine	C6 H15 N O3	150.1125	0.899
4-(Diethylamino)salicylaldehyde	C11 H15 N O2	194.1174	7.966
Efavirenz	C14 H9 Cl F3 N O2	338.0155	11.695
6-Methyl-2-pyridinemethanol	C7 H9 N O	124.076	6.94
NP-014287	C18 H32 O3	319.2234	12.755
PEG n5	C10 H22 O6	239.1486	5.573
Cyclohexyl phenyl ketone	C13 H16 O	189.1272	10.109
Dodecyltrimethylammonium	C15 H33 N	228.2681	11.542
Difenoxin	C28 H28 N2 O2	425.2242	8.602
Caprolactam	C6 H11 N O	114.0916	0.856

Name	Formula	m/z	RT [min]
NP-019491	C15 H22 O4	284.1849	10.483
Fexofenadine	C32 H39 N O4	502.2935	9.409
Chlorpheniramine	C16 H19 Cl N2	275.1305	8.025
Enilconazole	C14 H14 Cl2 N2 O	297.0552	9.433
1-Methoxymethyl-1H-benzotriazole	C8 H9 N3 O	164.082	8.783
cyclohexyl[4-(1H-indol-4-yl)piperazino]methanone	C19 H25 N3 O	312.2063	11.413
indoline-2-carboxylic acid	C9 H9 N O2	164.0705	7.188
2,6-Diaminotoluene	C7 H10 N2	123.0999	0.973
2-(1,3-benzodioxol-5-yl)-7-ethylimidazo[1,2-a]pyridine	C16 H14 N2 O2	267.1122	8.691
Nevirapine	C15 H14 N4 O	267.1234	8.402
Codeine	C18 H21 N O3	300.1586	0.982
Dodecylamine	C12 H27 N	186.2216	10.017
PEG Monolaurate n4	C20 H40 O6	399.2702	12.851
Valsartan	C24 H29 N5 O3	436.2327	11.165
Thiamine	C12 H16 N4 O S	265.111	0.864
NP-016928	C20 H28 O3	317.21	12.773
Hexadecanamide	C16 H33 N O	256.2625	13.104
Flurandrenolide	C24 H33 F O6	437.2339	7.141
Rhodamine 6G	C28 H30 N2 O3	443.2313	10.32
N-(2,4-Dimethylphenyl)formamide	C9 H11 N O	150.0915	8.468
5-Aminovaleric acid	C5 H11 N O2	118.0866	0.983
Tapentadol	C14 H23 N O	222.1848	11.675
Trimethoprim	C14 H18 N4 O3	291.1444	1.004
Cetirizine	C21 H25 Cl N2 O3	389.1614	10.304
Bis(2-ethylhexyl) amine	C16 H35 N	242.2837	11.405
1-Tetradecylamine	C14 H31 N	214.2526	10.711
6-Methyl-2-pyridinemethanol	C7 H9 N O	124.0761	0.975
Diphenhydramine	C17 H21 N O	256.169	8.499
(4S,5S,8S,10R)-4,5,8-trihydroxy-10-methyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	C10 H16 O5	217.1067	7.683

Name	Formula	m/z	RT [min]
10,11-Dihydro-10,11-dihydroxycarbamazepine	C15 H14 N2 O3	271.1072	8.506
4-Methylbenzotriazole	C7 H7 N3	134.0716	8.85
3,5-di-tert-Butyl-4-hydroxybenzoic acid	C15 H22 O3	251.1636	11.506
NP-003553	C20 H34 O4	361.2336	11.772
Dodecyltrimethylammonium	C15 H33 N	228.2681	10.94
NP-002322	C18 H32 O4	295.2254	11.894
NP-019636	C9 H8 O4	163.039	8.748
4-tert-Butylcyclohexyl acetate	C12 H22 O2	199.169	12.502
2-(1,3-benzodioxol-5-yl)-7-ethylimidazo[1,2-a]pyridine	C16 H14 N2 O2	267.1123	9.521
trans,trans-2,4-Heptadienal	C7 H10 O	111.0809	1.176
NP-017152	C13 H23 N O2	226.1799	10.786
Prolinamide	C5 H10 N2 O	115.0869	1.111
Desomorphine	C17 H21 N O2	272.1638	8.8
Olomoucine	C15 H18 N6 O	299.1609	11.649
[(3R,4S)-3-[(6-Methoxy-3,4-dihydro-1-isoquinolinyl)methyl]-1-(4-morpholinylcarbonyl)-4-piperidinyl]acetic acid	C23 H31 N3 O5	430.2322	7.611
4-Ethylbenzaldehyde	C9 H10 O	135.0806	9.622
Ritalinic acid	C13 H17 N O2	220.1329	6.915
Carbamazepine 10,11-epoxide	C15 H12 N2 O2	253.0968	8.762
Dimetridazole	C5 H7 N3 O2	142.0614	1.704
Tropicamide	C17 H20 N2 O2	285.1602	7.828
3-(2,3-dihydro-1,4-benzodioxin-6-ylamino)-2-{[5-(trifluoromethyl)-2-pyridyl]sulfonyl}acrylonitrile	C17 H12 F3 N3 O4 S	412.056	10.683
(6E)-10-Heptyl-5,8,9-trihydroxy-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	C16 H28 O5	301.1999	11.642
NP-016582	C20 H35 N O	306.2784	11.431
Sulfapyridine	C11 H11 N3 O2 S	250.064	1.395
Ambrosic acid	C15 H20 O4	287.1248	10.759
Escitalopram	C20 H21 F N2 O	325.1712	8.501
Amitriptyline	C20 H23 N	278.1897	9.645
Urocanic acid	C6 H6 N2 O2	139.0505	11.599

Name	Formula	m/z	RT [min]
NP-002855	C12 H22 O4	231.1586	11.491
NP-016455	C11 H18 N2 O4	243.1348	11.957
Benzoylecgonine	C16 H19 N O4	290.1379	7.079
Oxybenzone	C14 H12 O3	229.0855	11.61
Sulfadimethoxine	C12 H14 N4 O4 S	349.0356	8.377
N1-mesityl-2-{[3,5-di(trifluoromethyl)phenyl]thio}acetamide	C19 H17 F6 N O S	422.0988	10.466
Urocanic acid	C6 H6 N2 O2	121.0399	12.683
Tropine	C8 H15 N O	142.1229	9.166
(2R,3R,4S,5S,6R)-2-[(3Z)-hex-3-en-1-yloxy]-6-(hydroxymethyl)oxane-3,4,5-triol	C12 H22 O6	285.13	8.825
Paracetamol	C8 H9 N O2	152.0707	1.192
NP-018661	C8 H16 O3	183.0989	9.712
NP-006656	C12 H22 O4	231.1587	11.286
2,4-Diaminotoluene	C7 H10 N2	123.0919	4.881
Atenolol	C14 H22 N2 O3	267.1697	0.98
1-propyl-1H-benzo[d]imidazole hydrobromide	C10 H12 N2	161.1074	0.965
6-Methoxyquinoline N-oxide	C10 H9 N O2	176.0706	8.343
Urocanic acid	C6 H6 N2 O2	139.0504	13.3
1-Tetradecylamine	C14 H31 N	214.2523	11.013
2-Aminobenzimidazole	C7 H7 N3	134.0716	1.01
Palmitoyl ethanolamide	C18 H37 N O2	300.2888	12.449
Metalaxyl	C15 H21 N O4	280.1535	10.207
L-Phenylalanine	C9 H11 N O2	166.0863	1.104
2,6-Dimethyl-γ-pyrone	C7 H8 O2	125.06	7.216
Diethanolamine	C4 H11 N O2	106.0866	10.146
N-{6-[(7-Chloro-4-quinazolinyl)oxy]-3-pyridinyl}-2-thiophenesulfonamide	C17 H11 Cl N4 O3 S2	419.0055	7.064
DEET	C12 H17 N O	192.1381	10.12
25T-NBOMe	C19 H25 N O3 S	348.1639	8.135
4-Methylbenzotriazole	C7 H7 N3	134.0715	8.386
PEG n5	C10 H22 O6	239.1484	1.125
Triethanolamine	C6 H15 N O3	150.1126	12.646

Name	Formula	m/z	RT [min]
4-(2,3-dihydro-1,4-benzodioxin-6-yl)butanoic acid	C12 H14 O4	245.0778	10.316
Triethanolamine	C6 H15 N O3	150.1126	13.336
PEG n6	C12 H26 O7	283.1746	6.152
Benzotriazole	C6 H5 N3	120.056	6.894
Triethyl phosphate	C6 H15 O4 P	205.0597	8.599
Carbamazepine	C15 H12 N2 O	237.1017	9.741
Lamivudine	C8 H11 N3 O3 S	230.0426	0.972
Tapentadol	C14 H23 N O	222.185	1.02
2-Methyl-5-propionylfuran	C8 H10 O2	139.0756	7.697
PPG n10	C30 H62 O11	599.434	12.563
5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one	C13 H22 O3	227.1637	11.217
N-Desmethyltramadol	C15 H23 N O2	250.1797	7.38
N,N-Diisopropylethylamine (DIPEA)	C8 H19 N	130.1593	1.027
NP-001596	C16 H30 O4	287.2209	12.507
Octadecanamine	C18 H39 N	270.3147	12.222
Dodecyltrimethylammonium	C15 H33 N	228.2682	10.774
Cotinine	C10 H12 N2 O	177.1022	0.979
Hexadecanamide	C16 H33 N O	256.2627	13.39
Tramadol	C16 H25 N O2	264.1953	7.018
1,5-Isoquinolinediol	C9 H7 N O2	162.0549	7.536
Lamotrigine	C9 H7 Cl2 N5	256.0146	7.408
Poly THF n5	C20 H42 O6	401.2856	12.598
PEG n10	C20 H42 O11	459.2784	7.405
PEG n11	C22 H46 O12	503.3045	7.631
Cetrimonium	C19 H41 N	284.3303	11.792
N-Methyldioctylamine	C17 H37 N	256.2991	11.412
Nicotine	C10 H14 N2	163.1229	0.992
Choline	C5 H13 N O	104.1073	0.896
Metformin	C4 H11 N5	130.1089	0.914
PEG n12	C24 H50 O13	547.3307	7.82

Name	Formula	m/z	RT [min]
Dodecyltrimethylammonium	C15 H33 N	228.2681	10.523
Thiacloprid	C10 H9 Cl N4 S	253.0305	8.328
PEG n7	C14 H30 O8	327.2006	6.267
Tramadol	C16 H25 N O2	264.1953	6.869
N-Methyldioctylamine	C17 H37 N	256.2992	11.256
Didecyldimethylammonium	C22 H47 N	326.377	11.778
PEG n13	C26 H54 O14	591.3567	7.989
Piperine	C17 H19 N O3	286.1429	11.176
Bis(2-ethylhexyl) amine	C16 H35 N	242.2837	11.517
Galaxolidone	C18 H24 O2	273.1842	12.21
PEG n14	C28 H58 O15	318.1951	8.139
Caffeine	C8 H10 N4 O2	195.0874	6.393
Cyclopropyl[(3S)-3-(5-phenyl-1,3,4-oxadiazol-2-yl)-1-pyrrolidinyl]methanone	C16 H17 N3 O2	284.1404	11.408
Triethanolamine	C6 H15 N O3	150.1127	11.603
Fluconazole	C13 H12 F2 N6 O	307.1106	7.89
5-Fluoro-3,5-AB-PFUPPYCA	C20 H26 F2 N4 O2	393.208	6.733
N-Methyl-2-AI	C10 H13 N	148.1122	1
α-Propylaminopentiophenone	C14 H21 N O	220.1694	1
NP-019547	C17 H26 O5	311.1845	10.738
Neotame	C20 H30 N2 O5	379.2232	12.883
PEG Monolaurate n6	C24 H48 O8	487.3221	12.853
Telmisartan	C33 H30 N4 O2	515.2423	10.276
Doxylamine	C17 H22 N2 O	271.1799	1.16
Valnemulin	C31 H52 N2 O5 S	565.368	13.109
4-(tert-butyl)phenyl 3,5-dimethylisoxazole-4-carboxylate	C16 H19 N O3	274.1432	7.228
N,N-dimethyl-9H-purin-6-amine	C7 H9 N5	164.0931	1.056
L-Isoleucine	C6 H13 N O2	132.1021	1.036
N-{4-[(2R,3R)-3-(Hydroxymethyl)-4-isobutyl-5-oxo-2-morpholinyl]phenyl}-3-methylbutanamide	C20 H30 N2 O4	363.2281	13.303
Solanidine	C27 H43 N O	398.3402	9.403

Name	Formula	m/z	RT [min]
Sulfamethoxazole	C10 H11 N3 O3 S	254.0588	7.189
Coniine	C8 H17 N	128.1437	0.996
PEG Monolaurate n7	C26 H52 O9	509.3662	12.85
PEG Monolaurate n5	C22 H44 O7	443.2962	12.851
Amisulpride	C17 H27 N3 O4 S	370.1784	0.995
Ecgonine	C9 H15 N O3	186.1124	7.906
N-Methyldioctylamine	C17 H37 N	256.2994	10.598
Terbuthylazine	C9 H16 Cl N5	230.1162	10.832
N-Methyldioctylamine	C17 H37 N	256.2989	11.229
Pseudoephedrine	C10 H15 N O	166.1225	1.038
Tebuthiuron	C9 H16 N4 O S	229.1114	9.53
O-Desmethyltramadol	C15 H23 N O2	250.1797	1.041
Methaqualone	C16 H14 N2 O	251.1173	9.962
Atrazine	C8 H14 Cl N5	216.1007	10.095
L-Tyrosine	C9 H11 N O3	182.081	1.237
Oxepanone	C6 H10 O2	115.0757	6.808
NP-011548	C18 H34 O3	299.2573	12.819
N-cyclooctylurea	C9 H18 N2 O	171.1491	8.718
Alphaprodine	C16 H23 N O2	262.1798	6.208
Methyl (2R,4S,6S,12bS)-2-[(2-acetamidoethyl)amino]-4-(3,4-difluorophenyl)-1,2,3,4,6,7,12,12b-octahydroindolo[2,3-a]quinolizine-6-carboxylate	C27 H30 F2 N4 O3	497.2339	7.414
Dodecyltrimethylammonium	C15 H33 N	228.2681	11.509
4-Acetamidobenzaldehyde	C9 H9 N O2	164.0706	7.439
Venlafaxine	C17 H27 N O2	278.2108	8.112
3-Hydroxy-2-methylpyridine	C6 H7 N O	110.0605	0.978
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	C15 H22 O2	235.1688	11.898
MPBP	C15 H21 N O	232.1693	1.019
L(-)-Carnitine	C7 H15 N O3	162.1124	0.911
Ecgonine methyl ester	C10 H17 N O3	200.1279	8.642
3-amino-2-phenyl-2H-pyrazolo[4,3-c]pyridine-4,6-diol	C12 H10 N4 O2	243.0871	9.004

Name	Formula	m/z	RT [min]
2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)	C9 H19 N O	158.154	10.463
5-Ethylcyclohexane-1,3-dione	C8 H12 O2	141.0912	8.974
Triethanolamine	C6 H15 N O3	150.1126	9.018
5-Hydroxymebendazole	C16 H15 N3 O3	298.1179	8.308
N-Methyl-2-phenylpropan-1-amine	C10 H15 N	150.1277	1.048
Dextrorphan	C17 H23 N O	258.1847	6.961
4-Methoxybenzaldehyde	C8 H8 O2	137.0599	7.365
Tetranor-12(S)-HETE	C16 H26 O3	267.1948	11.678
NP-020156	C9 H17 N O4	226.1047	9.411
4-chloro-1H-indazol-3-amine	C7 H6 Cl N3	168.0324	10.024
NP-007909	C13 H20 O3	225.1481	8.081
NP-007909	C13 H20 O3	225.1483	10.481
N-Desmethylvenlafaxine	C16 H25 N O2	264.1952	8.305
(2E)-2-(hydroxymethyl)-3-[3-oxo-5-(propan-2-yl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4-yl]prop-2-enoic acid	C15 H20 O5	303.1195	10.886
17α-Hydroxyprogesterone	C21 H30 O3	331.2257	10.563
PPG n10	C30 H62 O11	621.4155	12.417
Dodecyltrimethylammonium	C15 H33 N	228.2679	11.379
Dioctyldimethylammonium chloride	C18 H39 N	270.3148	10.756
5-Ethylcyclohexane-1,3-dione	C8 H12 O2	141.0912	8.223
(1aR,1bR,2R,3R,7R,7aS)-1b,2-dimethyl-7a-(prop-1-en-2-yl)-1aH,1bH,2H,3H,4H,5H,7H,7aH-naphtho[1,2-b]oxirene-3,7-diol	C15 H22 O3	251.1639	10.644
NP-018661	C8 H16 O3	183.0989	8.711
2-furyl[4-(1H-indol-4-yl)piperazino]methanone	C17 H17 N3 O2	296.1405	7.312
DL-Serine	C3 H7 N O3	106.0503	1.139
NP-012534	C15 H24 O5	307.1505	10.384
2,4-dihydroxyheptadec-16-en-1-yl acetate	C19 H36 O4	329.2676	13.29
NP-002322	C18 H32 O4	313.2364	11.887
3,4-Dimethoxy-α-pyrrolidinopentiophenone	C17 H25 N O3	292.1901	1.114
GRH	C14 H24 N8 O4	369.1978	8.67

Name	Formula	m/z	RT [min]
3,8,9-trihydroxy-10-propyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	C12 H20 O5	267.1195	9.615
10-Nitrooleate	C18 H33 N O4	350.2289	11.719
2-(1,3-benzodioxol-5-yl)-7-ethylimidazo[1,2-a]pyridine	C16 H14 N2 O2	267.1123	9.354
Diuron	C9 H10 Cl2 N2 O	233.024	10.461
NP-011548	C18 H34 O3	321.239	13.091
Valpromide	C8 H17 N O	144.1385	9.366
12-Aminododecanoic acid	C12 H25 N O2	216.1954	9.378
Ethyl sorbate	C8 H12 O2	141.0912	10.59
N,N'-Diphenylguanidine	C13 H13 N3	212.1179	1.164
N-(3-Chlorophenyl)-6,7-dimethoxyquinazolin-4-amine	C16 H14 Cl N3 O2	316.0858	8.13
Tropine	C8 H15 N O	142.1229	7.806
2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)	C9 H19 N O	158.1541	10.47
Mycophenolic acid	C17 H20 O6	343.1141	10.635
3-hydroxy-8-methoxy-3-methyl-1,2,3,4,7,12-hexahydrotetraphene-1,7,12-trione	C20 H16 O5	337.107	11.864
5-(2,5-dihydroxyhexyl)oxolan-2-one	C10 H18 O4	203.1275	10.098
Poly THF n4	C16 H34 O5	307.2469	9.745
Cinchophen	C16 H11 N O2	250.0855	12.941
Gabapentin	C9 H17 N O2	172.1331	7.775
NP-020632	C16 H20 O4	277.1425	10.34
6-(7-methyloctyl)-1H,3H,4H,6H-furo[3,4-c]furan-1-one	C15 H24 O3	253.1793	10.976
(7E,13E)-9,15-dihydroxy-4,10,16-trimethyl-1,5,11-trioxacyclohexadeca-7,13-diene-2,6,12-trione	C16 H22 O8	365.1193	8.131
2-(3,4-Dimethoxyphenyl)-5-methylamino-2-isopropylvaleronitrile	C17 H26 N2 O2	291.2059	8.355
Cyclohexanecarboxylic acid	C7 H12 O2	129.0913	6.689
Amitriptyline-d3	C20 H20 [2]H3 N	281.2079	13.348
Acetophenone	C8 H8 O	121.065	13.304
N2-(3-chloro-4-fluorophenyl)-3-(4-chlorophenyl)-4-cyano-5-(methylthio)thiophene-2-carboxamide	C19 H11 Cl2 F N2 O S2	436.9735	7.044
Flecainide	C17 H20 F6 N2 O3	415.144	8.669
Bisoprolol	C18 H31 N O4	326.2317	7.957

Name	Formula	m/z	RT [min]
3-{[4-(1,3-Benzodioxol-5-ylmethyl)piperazino]carbonyl}-6,7-dimethoxy-2H-chromen-2-one	C24 H24 N2 O7	453.1657	11.594
N,N'-Diphenylguanidine	C13 H13 N3	212.118	6.098
5-Methoxyindole	C9 H9 N O	148.0758	8.261
Palmitoleic Acid	C16 H30 O2	277.2131	13.314
Dihydromorphine	C17 H21 N O3	288.1585	10.527
(2E)-2-(hydroxymethyl)-3-[3-oxo-5-(propan-2-yl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4-yl]prop-2-enoic acid	C15 H20 O5	303.1197	11.026
β,β-Dimethyl-γ-methylene-γ-butyrolactone	C7 H10 O2	127.0756	7.745
NP-005394	C18 H30 O7	359.2051	11.144
(5E)-7-methylidene-10-oxo-4-(propan-2-yl)undec-5-enoic acid	C15 H24 O3	253.1793	8.546
1,5-Isoquinolinediol	C9 H7 N O2	162.055	7.253
Tetrahydrocortisone	C21 H32 O5	387.2126	10.788
Acridine	C13 H9 N	180.1799	6.575
Azoxystrobin acid	C21 H15 N3 O5	390.107	10.222
Thymine	C5 H6 N2 O2	127.0504	6.824
Dimethyl phosphate	C2 H7 O4 P	127.0157	1.155
2-amino-4-{[2-({[2,3-dihydroxy-2-(1-hydroxyethyl)butanoyl]oxy}methyl)-4-hydroxyphenyl]carbamoyl}butanoic acid	C18 H26 N2 O9	415.1718	9.358
(+/-)-Gingerol	C17 H26 O4	277.1786	10.809
mesityl (4-methylphenyl) sulfone	C16 H18 O2 S	275.1094	1.11
PPG n10	C30 H62 O11	621.4161	11.673
3-[3-(1,3-dimethyl-1H-pyrazol-4-yl)-1H-1,2,4-triazol-1-yl]-5-methylisoxazole	C11 H12 N6 O	245.1143	10.579
N-Methyldioctylamine	C17 H37 N	256.2991	13.286
1-Tetradecylamine	C14 H31 N	214.2526	10.959
Tapentadol	C14 H23 N O	222.185	7.315
3,3'-Dimethoxybenzidine	C14 H16 N2 O2	245.1279	10.285
Diethyl phosphate	C4 H11 O4 P	155.0468	8.609
Citalopram	C20 H21 F N2 O	325.1717	8.438
PPG n9	C27 H56 O10	563.3744	11.552
NP-001846	C11 H20 O4	239.1248	10.544

Name	Formula	m/z	RT [min]
NP-018660	C13 H22 O3	209.1533	8.949
3-(tert-butyl)-1-methyl-4,5-dihydro-1H-pyrazol-5-one	C8 H14 N2 O	155.1181	5.709
Citreoviridin	C23 H30 O6	403.2112	8.506
D-(+)-Proline	C5 H9 N O2	116.0709	0.419
4-heptyl-3-methyl-1H-pyrazol-5-ol	C11 H20 N2 O	197.1646	7.16
10-Hydroxycarbazepine	C15 H14 N2 O2	255.1124	9.511
Orphenadrine	C18 H23 N O	270.1846	9.027
Irbesartan	C25 H28 N6 O	429.2382	10.746
N,N-Diethyldodecanamide	C16 H33 N O	256.263	13.364
4-Piperidinecarboxamide	C6 H12 N2 O	129.1023	12.46
RMH	C17 H30 N8 O4 S	443.2177	10.202
Bis(2-ethylhexyl) amine	C16 H35 N	242.2838	7.837
Dextromethorphan	C18 H25 N O	272.2004	8.624
NP-005397	C18 H30 O6	365.1923	11.805
[(3R,4S)-3-[(6-Methoxy-3,4-dihydro-1-isoquinolinyl)methyl]-1-(4-morpholinylcarbonyl)-4-piperidinyl]acetic acid	C23 H31 N3 O5	430.2323	7.364
Nadolol	C17 H27 N O4	310.2003	8.923
4-Piperidinecarboxamide	C6 H12 N2 O	129.1025	13.279
Urocanic acid	C6 H6 N2 O2	139.0504	8.988
1-adamantyl(piperidino)methanone	C16 H25 N O	248.2007	8.797
Isoleucine	C6 H13 N O2	132.1021	13.042
5,6-Dimethylbenzimidazole	C9 H10 N2	147.0919	0.992
Neostigmine	C12 H18 N2 O2	223.1436	9.183
Gambogic acid	C38 H44 O8	323.6731	7.988
3-Hydroxybutyric acid	C4 H8 O3	105.055	7.167
Crotetamide	C12 H22 N2 O2	209.1643	9.553
1,4-dihydroxy-1,4-dimethyl-7-(propan-2-ylidene)-decahydroazulen-6-one	C15 H24 O3	275.161	11.134
N-Methyldioctylamine	C17 H37 N	256.2994	11.958
5-(2,5-dihydroxyhexyl)oxolan-2-one	C10 H18 O4	225.1092	9.934
Atazanavir	C38 H52 N6 O7	705.3944	11.373

Name	Formula	m/z	RT [min]
PPG n8	C24 H50 O9	483.3509	11.062
N-Benzylformamide	C8 H9 N O	136.0759	6.179
D-(+)-Maltose	C12 H22 O11	365.1039	0.86
(2R)-2-[(2R,5S)-5-[(2S)-2-hydroxybutyl]oxolan-2-yl]propanoic acid	C11 H20 O4	217.143	9.216
Bis(2-ethylhexyl) amine	C16 H35 N	242.2835	11.953
N-Desmethyltramadol	C15 H23 N O2	250.1797	6.769
4-Hydroxycoumarin	C9 H6 O3	163.0389	12.222
Oxepanone	C6 H10 O2	115.0757	5.712
(2E)-2-(hydroxymethyl)-3-[3-oxo-5-(propan-2-yl)-1,3,4,5,6,7-hexahydro-2-benzofuran-4-yl]prop-2-enoic acid	C15 H20 O5	298.164	10.62
Diethanolamine	C4 H11 N O2	106.0865	11.428
NP-014891	C11 H14 O3	177.0911	12.351
α-Pinene-2-oxide	C10 H16 O	153.1275	10.262
4-fluoro-N-[4-(4-methylpiperazino)phenyl]benzenesulfonamide	C17 H20 F N3 O2 S	350.1322	12.14
Choline	C5 H13 N O	104.1074	13.418
2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)	C9 H19 N O	158.154	9.99
Sulpiride	C15 H23 N3 O4 S	342.1472	0.975
4-chloro-1H-indazol-3-amine	C7 H6 Cl N3	168.0324	9.531
D-(+)-Proline	C5 H9 N O2	116.0709	1.08
4-tert-Butylcyclohexyl acetate	C12 H22 O2	199.1688	11.444
NP-004713	C15 H24 O2	219.1739	11.527
Cyclizine	C18 H22 N2	267.185	8.719
Creatine	C4 H9 N3 O2	132.077	0.956
Paracetamol	C8 H9 N O2	152.0707	7.608
1,10-Diamino-4,7-dioxadecane	C8 H20 N2 O2	177.1597	0.864
Coniine	C8 H17 N	128.1437	1.103
(1aR,1bR,2R,3R,7R,7aS)-1b,2-dimethyl-7a-(prop-1-en-2-yl)-1aH,1bH,2H,3H,4H,5H,7H,7aH-naphtho[1,2-b]oxirene-3,7-diol	C15 H22 O3	233.1533	10.31
Abacavir	C14 H18 N6 O	287.1606	1.037
5-[(1E)-3-hydroxy-3-methylbut-1-en-1-yl]-2-methylcyclohex-5-ene-1,2,4-triol	C12 H20 O4	229.1431	10.232

Name	Formula	m/z	RT [min]
2-Methyl-5-propionylfuran	C8 H10 O2	139.0757	7.371
(2,6-dimethylpiperidino)(3,4,5-trimethoxyphenyl)methanone	C17 H25 N O4	308.1847	8.657
Guanylurea	C2 H6 N4 O	103.0619	0.919
Hexamethoxymethyl melamine	C15 H30 N6 O6	391.2287	9.708
[(3R,4S)-1-[(4-Methoxyphenyl)acetyl]-3-{2-[4-(2-oxo-2,3-dihydro-1H-benzimidazol-1-yl)-1-piperidinyl]ethyl}-4-piperidinyl]acetic acid	C30 H38 N4 O5	535.2894	9.011
(11E,15Z)-9,10,13-trihydroxyoctadeca-11,15-dienoic acid	C18 H32 O5	311.2202	11.137
Tyrosylalanine	C12 H16 N2 O4	253.1194	10.136
2,2,6,6-Tetramethyl-1-piperidinol (TEMPO)	C9 H19 N O	158.1539	10.939
N,N'-Dicyclohexylurea	C13 H24 N2 O	225.1957	10.827
Crotonic acid	C4 H6 O2	87.04452	7.769
4-tert-Butylcyclohexyl acetate	C12 H22 O2	199.169	10.921
NP-021797	C12 H22 O3	237.1455	10.936
Guanine	C5 H5 N5 O	152.0568	0.979
Coenzyme Q2	C19 H26 O4	319.1893	10.99
1-Methoxymethyl-1H-benzotriazole	C8 H9 N3 O	164.082	8.67
Simazine	C7 H12 Cl N5	202.0852	9.273
NP-020454	C6 H13 N O	116.1073	7.904
Coenzyme Q2	C19 H26 O4	319.1894	9.813
NP-004713	C15 H24 O2	237.1846	11.124
Hydroxyterbuthylazine	C9 H17 N5 O	212.1503	7.248
(3aS,5aR,6R,9aS,9bS)-6-hydroxy-5a-methyl-3,9-dimethylidene-dodecahydronaphtho[1,2-b]furan-2-one	C15 H20 O3	249.1477	10.838
2,4-dihydroxy-6-methyl-3-[(2E)-3-methyl-5-[(1S,2R,6R)-1,2,6-trimethyl-3-oxocyclohexyl]pent-2-en-1-yl]benzaldehyde	C23 H32 O4	395.2179	12.619
Losartan	C22 H23 Cl N6 O	423.1679	10.528
Desmethylcitalopram	C19 H19 F N2 O	311.1547	8.707
2,3-dihydroxypropyl 12-methyltridecanoate	C17 H34 O4	325.2339	13.163
Bis(2-ethylhexyl) amine	C16 H35 N	242.2835	11.31
NP-016564	C16 H20 O6	331.1142	10.383
Tropine	C8 H15 N O	142.1229	8.809

Name	Formula	m/z	RT [min]
Urocanic acid	C6 H6 N2 O2	121.0399	1.165
AUDA	C23 H40 N2 O3	393.3097	11.47
Poly THF n5	C20 H42 O6	379.3041	10.551
Triphenylphosphine oxide	C18 H15 O P	279.0926	10.592
Didecyldimethylammonium	C22 H47 N	326.377	12.18
2,3-dihydroxypropyl 12-methyltridecanoate	C17 H34 O4	285.2417	12.799
NP-006888	C13 H24 O4	245.1742	11.415
5-amino-1-phenyl-1H-pyrazole-4-carbonitrile	C10 H8 N4	185.082	7.833
7-Methyladenine	C6 H7 N5	150.0776	0.974
Methocarbamol	C11 H15 N O5	242.1019	8.053
Dihydromorphine	C17 H21 N O3	288.1585	10.281
3,5-di-tert-Butyl-4-hydroxybenzaldehyde	C15 H22 O2	235.169	11.878
Decanophenone	C16 H24 O	233.1895	11.821
2'-fluoro-N-[3-(trifluoromethyl)phenyl][1,1'-biphenyl]-4-carboxamide	C20 H13 F4 N O	360.1002	8.095
3-(tert-butyl)-1-methyl-4,5-dihydro-1H-pyrazol-5-one	C8 H14 N2 O	155.118	0.982
N1-ethyl-4-methylbenzene-1-sulfonamide	C9 H13 N O2 S	200.0738	9.189
NP-021797	C12 H22 O3	215.1637	11.562
5-(6-hydroxy-6-methyloctyl)-2,5-dihydrofuran-2-one	C13 H22 O3	227.1637	10.916
PPG n7	C21 H44 O8	425.3095	10.543
Tropine	C8 H15 N O	142.1228	9.761
3-Hydroxybutyric acid	C4 H8 O3	105.055	7.989
NP-020214	C16 H32 O4	289.2364	12.861
Triethanolamine	C6 H15 N O3	150.1124	0.43
Meprylcaine	C14 H21 N O2	236.1641	1.093
(4S,5S,8S,10R)-4,5,8-trihydroxy-10-methyl-3,4,5,8,9,10-hexahydro-2H-oxecin-2-one	C10 H16 O5	217.1068	7.411
2-Isobutyl-3-methoxypyrazine	C9 H14 N2 O	167.1178	7.165
3-Acetamidophenol	C8 H9 N O2	152.0707	5.837
Mebendazole	C16 H13 N3 O3	296.1022	9.995
Nornicotine	C9 H12 N2	149.1076	6.083

Table A3-3: A list of compounds identified in water samples collected from d-DwTP and used in this cluster analysis

Name	Compound Class	Peak Area: Product water	Peak Area: Source water
(2E,4E)-N-(2-methylpropyl)dodeca-2,4-dienamide	Endogenous Metabolites; Natural Products/Medicines	509955.6639	918690.5509
(2S,5aS,8aR)-2-{3-[(2R)-2-(Methoxymethyl)-1-pyrrolidinyl]-3-oxopropyl}-1,6-dimethyloctahydropyrrolo[3,2-E][1,4]diazepin-5(2H)-one		3679980.658	3078160.642
1-(3,4-dichlorophenyl)ethan-1-one 1-(1H-1,2,4-triazol-3-yl)hydrazone		1042759.21	555366.8189
1,10-Diamino-4,7-dioxadecane		140734.8861	375204.7406
1,2,3-Benzotriazole	Industrial Chemicals	11312531.91	201549957.9
1,2-bis(2-methylphenyl)guanidine	Industrial Chemicals; Therapeutics/Prescription Drugs	240651.4546	348731.0195
1,3-Diphenylguanidine	Extractables/Leachables; Industrial Chemicals	1979793.226	46103553.35
12-Aminododecanoic acid		711278.8523	303719.168
1-Dodecyl-2-pyrrolidinone	Extractables/Leachables; Personal Care Products/Cosmetics; Textile Chemicals/Auxiliary/Dyes	43254043.68	147974177.2
1-Methylxanthine	Endogenous Metabolites	166748.3926	305993.2228
1-phenyl-2-[(2-{[4-(trifluoromethyl)pyrimidin-2-yl]amino}ethyl)amino]ethan-1-ol		7408064.863	6684508.765
1-PHENYL-2-BUTANONE		6012487.204	18642703.05
2-(2H-benzotriazol-2-yl)-4-tert-butylphenol	Extractables/Leachables	253750.5672	353379.8121
2-(3-chloro-2-methylanilino)benzoic acid		6857050.536	4091210.423
2,2,6,6-Tetramethyl-4-piperidinol	Extractables/Leachables; Industrial Chemicals	32579661.88	31983984.56
2-[(14E,16S,17S)-2-Oxo-8-(1-piperazinyl)-12-oxa-1,4-diazatricyclo[14.3.1.06,11]icosa-6,8,10,14-tetraen-17-yl]-N-(3-pyridinylmethyl)acetamide		1047314.929	10536509.26
2-[(3R,4S)-3-{[5-(Cyclohexylmethyl)-1,2-oxazol-3-yl]methyl}-4-piperidinyl]-1-(4-morpholinyl)ethanone		191729.0576	166607.6697

Name	Compound Class	Peak Area: Product water	Peak Area: Source water
2-aminoquinoline-3-carbonitrile		158719.8287	273269.948
2-Isopropyl-6-methyl-4-pyrimidinol		889951.6224	362496.856
2-methyl-1,2-dihydrophthalazin-1-one		3441224.4	2758920.288
2-sec-Butyl-3-methoxypyrazin	Excipients/Additives/Colorants	18661709.99	8536869.512
3,3'-Dimethoxybiphenyl-4,4'-diamine	Industrial Chemicals	7654905.07	336825.0408
3,6,9,12,15,18-Hexaoxaicosane-1,20-diol	Industrial Chemicals	40089190.2	74699325.46
3-Aminopyrrolidine		6086762.964	2082379.022
3-Hydroxypyridine	Endogenous Metabolites	1173250.124	2051244.765
4-(4,5-dihydro-1H-imidazol-2-yl)-2,6-dimethylmorpholine hydrobromide		5136814.475	9702762.231
4,6-dimethyl-2,7-diphenyl-3,7-dihydro-2H-pyrazolo[3,4-b]pyridin-3-one		239337.9568	231936.1466
4-Acetamidoantipyrine	Therapeutics/Prescription Drugs	464710.8017	2294227.071
4-Oxo-4-[(3-oxo-2-decanyl)amino]butanoic acid		202256.5137	2869577.575
5,6-Dimethylbenzimidazole	Endogenous Metabolites	4689507.312	12323719.61
5-[4-(2,5-dimethyl-1H-pyrrol-1-yl)phenyl]-4-(4-methylphenyl)-4H-1,2,4-triazole-3-thiol		709789.0868	244274.4235
5-Fluorocytosine	Therapeutics/Prescription Drugs	166248.1364	1695871.871
5-Methoxyindole		1032796.873	8273932.113
6beta-Naltrexol-d3	Drugs of Abuse/Illegal Drugs; Sports Doping Drugs	769207.9607	1228712.643
6-Chloro-5-methyl-1H-1,2,3-benzotriazole		4917294.969	198060.0747
8-Hydroxyquinoline	Therapeutics/Prescription Drugs; Endogenous Metabolites; Industrial Chemicals; Personal Care Products/Cosmetics; Pesticides/Herbicides	7550236.192	31454521.23
Abacavir	Therapeutics/Prescription Drugs	481663.5549	1025734.626
acenaphtho[1,2-b]quinoxaline		1128695.869	701755.2527
Acetylcholine	Endogenous Metabolites	1683842.915	10281746.88

Name	Compound Class	Peak Area: Product water	Peak Area: Source water
Acridine	Industrial Chemicals	7790350.122	11278597.83
Atazanavir	Therapeutics/Prescription Drugs	4031147.431	9026532.307
AUDA		2827712.502	13188582.83
Azoxystrobin acid	Pesticides/Herbicides	383233.9311	333440.4843
Berberine	Endogenous Metabolites; Natural Products/Medicines	1573812.297	4950515.931
Betaine	Endogenous Metabolites	24173866.09	23258017.63
Bezafibrate	Therapeutics/Prescription Drugs	703209.5714	220966.5302
Caffeine	Endogenous Metabolites; Natural Products/Medicines	2281194.328	3945726.806
Carbamazepine	Therapeutics/Prescription Drugs	76402446.11	106017370.2
Chlorpheniramine	Therapeutics/Prescription Drugs	4298944.155	11448210.62
Choline	Endogenous Metabolites	51603111.53	86544188.54
Cinchonine		154578.5762	385066.8787
Citalopram	Sports Doping Drugs	1900624.558	17107188.16
Climbazole	Therapeutics/Prescription Drugs	4407214.215	6429910.494
Cotinine	Endogenous Metabolites	3723478.251	17874680.07
Cyclohexylamine	Extractables/Leachables	8977720.497	49512988.17
Cyproheptadine	Therapeutics/Prescription Drugs	693395.4178	4071306.482
Cytosine	Endogenous Metabolites	1050153.979	2495528.295
Decanamide		2470273.194	1621005.744
Desmethylcitalopram	Therapeutics/Prescription Drugs; Sports Doping Drugs	2304915.182	5169985.388
Dextromethorphan	Sports Doping Drugs	2213734.694	3448380.325
Didecyldimethylammonium	Therapeutics/Prescription Drugs; Personal Care Products/Cosmetics; Textile Chemicals/Auxiliary/Dyes	30029613.58	81336211.96
Diethanolamine	Industrial Chemicals	14512376.73	11304028.91

Name	Compound Class	Peak Area: Product water	Peak Area: Source water
Diethyl phosphate	Pesticides/Herbicides	387782.4963	1469658.217
Diisodecyl phthalate	Extractables/Leachables; Textile Chemicals/Auxiliary/Dyes; Industrial Chemicals	53520156.72	16961543.36
diisopropylethylamine	Industrial Chemicals	10951121.54	143925468.3
Diltiazem	Therapeutics/Prescription Drugs; Drugs of Abuse/Illegal Drugs; Sports Doping Drugs	607305.4094	1769293.733
Dimethyl phosphate	Industrial Chemicals	2359939.321	1296556.281
Dimetridazole	Therapeutics/Prescription Drugs; Excipients/Additives/Colorants	17562319.47	4165836.429
Dimetridazole	Therapeutics/Prescription Drugs; Excipients/Additives/Colorants	2739157.175	4392702.424
Diuron	Pesticides/Herbicides; Industrial Chemicals	990944.3891	2670831.206
DL-Homoserine	Endogenous Metabolites	1563205.375	10474555.18
DL-Lysine	Endogenous Metabolites	28645859.39	30400114.49
DL-Serine	Endogenous Metabolites	52321501.12	47603910.9
DQH	Endogenous Metabolites	21486408.48	1206677.79
D-Serine	Endogenous Metabolites	134674401	60083572.3
Efavirenz	Therapeutics/Prescription Drugs; Drugs of Abuse/Illegal Drugs	10733872.74	23839171
Epinephrine	Therapeutics/Prescription Drugs; Endogenous Metabolites	3183669.729	12370604.1
ethyl 4-[2-(2-chlorophenyl)ethanehydrazonoyl]-5-methylisoxazole-3-carboxylate		1367193.028	2441364.193

Name	Compound Class	Peak Area: Product water	Peak Area: Source water
Fluocinolone Acetonide	Therapeutics/Prescription Drugs; Sports Doping Drugs	83381256.41	263623437.3
GNH	Endogenous Metabolites	149346767.5	130273941.8
Guanine	Endogenous Metabolites	567733.2623	3244990.943
hexadecandioic acid	Endogenous Metabolites; Natural Products/Medicines	76152640.59	48746189.73
Lamotrigine	Therapeutics/Prescription Drugs	61276995.95	41921266.07
L-Aspartic acid	Endogenous Metabolites	69759059.74	62721966.06
Lidocaine	Therapeutics/Prescription Drugs	348377.9766	1323852.682
Lidocaine	Therapeutics/Prescription Drugs	860849.6496	841244.0298
Macrosphelide D	Endogenous Metabolites; Natural Products/Medicines	251847.6725	467739.1479
Memantine	Therapeutics/Prescription Drugs; Sports Doping Drugs	827265.2521	1707098.011
Meprobamate	Therapeutics/Prescription Drugs; Sports Doping Drugs; Drugs of Abuse/Illegal Drugs	5157372.112	8898960.506
mesityl (4-methylphenyl) sulfone		4097619.896	12851014.19
Metformin	Therapeutics/Prescription Drugs	514382.6632	4659464.045
Methaqualone	Therapeutics/Prescription Drugs; Drugs of Abuse/Illegal Drugs; Sports Doping Drugs	40173012.95	72809736.77
Metronidazole	Therapeutics/Prescription Drugs	422754.5893	503906.8167
MPBP	Drugs of Abuse/Illegal Drugs	111777.2503	170861.7385
N-(1-Benzothiophen-3-yl)-N'-(3-cyclopropyl-1-methyl-1H-pyrazol-5-yl)urea		3386793.903	931815.5693
N-(2-Acetamidoethyl)-2-{(3R,4S)-3-[(5-butyl-1,2-oxazol-3-yl)methyl]-4-piperidinyl}acetamide		642121.0016	749353.47
N-(3-Chlorophenyl)-6,7-dimethoxyquinazolin-4-amine		13012293.93	5198807.714

Name	Compound Class	Peak Area: Product water	Peak Area: Source water
N,N,N',N',N'',N''-Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine	Extractables/Leachables; Industrial Chemicals; Textile Chemicals/Auxiliary/Dyes	4164340.625	10317574.41
N,N-Diethyl-3-methylbenzamide	Pesticides/Herbicides	11480070.46	32293265.41
N,N-dimethyl-9H-purin-6-amine		1818762.325	508891.0983
N-{6-[(7-Chloro-4-quinazolinyl)oxy]-3-pyridinyl}-2-thiophenesulfonamide		18178864.14	51795021.27
N2-(2,4-dimethylphenyl)-1,3-benzothiazol-2-amine		1795761.394	751122.0306
N-Amino(4-chloroanilino)methylideneguanidine		550931.7115	851675.4409
N-Arachidonoyl-L-serine	Endogenous Metabolites	500013.1399	1395744.362
N-Cyanoimido-S,S-dimethyl-dithiocarbonate		2299204.26	193778.252
N'-Cyclohexylidenaminomethanehydrazonamide		990826.3325	5096735.962
N-Methyl-2-AI	Drugs of Abuse/Illegal Drugs	1203839.915	35146440.74
Not named		189837.3622	265733.3237
NP-016582	Endogenous Metabolites; Natural Products/Medicines	105005.907	223056.9483
NP-021844	Endogenous Metabolites; Natural Products/Medicines	9323056.544	14274579.19
Ornithine	Endogenous Metabolites	69588292.68	65954356.36
Panthenol	Personal Care Products/Cosmetics	230437.7232	885879.9834
PEG Monolaurate n5	Extractables/Leachables; Industrial Chemicals	2151050.429	7096487.323
PEG Monolaurate n6	Extractables/Leachables; Industrial Chemicals	1503470.137	1031970.619
PEG n5	Industrial Chemicals	36846900.71	101251912.2
PEG n8	Industrial Chemicals	261061517.7	569847849.7
Piperine	Endogenous Metabolites; Natural Products/Medicines	1544535.357	2070862.302
PPG n5	Extractables/Leachables; Industrial Chemicals	19510423.48	22499245.97

Name	Compound Class	Peak Area: Product water	Peak Area: Source water
PPG n6	Extractables/Leachables; Industrial Chemicals	14919066.36	13993667.36
PPG n7	Extractables/Leachables; Industrial Chemicals	748587.5589	765268.1433
PPG n8	Extractables/Leachables; Industrial Chemicals	1146509.553	955177.7357
Quinine	Endogenous Metabolites; Natural Products/Medicines	174741.8279	2300590.958
Rhodamine 6G		436513.8876	10913743.68
Ricinine	Endogenous Metabolites; Natural Toxins	2303047.123	3086956.084
Sodium [dodecanoyl(methyl)amino]acetate	Extractables/Leachables; Personal Care Products/Cosmetics; Textile Chemicals/Auxiliary/Dyes; Industrial Chemicals	335860.7469	485465.3303
Solanidine	Natural Toxins; Endogenous Metabolites	193434.1456	283594.2235
Sorbic acid	Extractables/Leachables; Excipients/Additives/Colorants; Industrial Chemicals; Endogenous Metabolites; Personal Care Products/Cosmetics	22756522.64	23683102.93
Sulfadimethoxine	Therapeutics/Prescription Drugs	201583.9065	330021.7503
Sulfamethoxazole	Therapeutics/Prescription Drugs; Endogenous Metabolites	5133815.325	96937291.43
Sulfapyridine	Therapeutics/Prescription Drugs; Pesticides/Herbicides	3628388.997	35470235.27
Tebuthiuron	Pesticides/Herbicides	2038251.269	3702565.154
TMK	Endogenous Metabolites	163716.7832	190572.2787

Name	Compound Class	Peak Area: Product water	Peak Area: Source water
tolytriazole	Textile Chemicals/Auxiliary/Dyes; Endogenous Metabolites	64190962.39	1143959074
Tributyl phosphate	Industrial Chemicals	3808531.784	4801754.312
Triethyl citrate	Extractables/Leachables; Excipients/Additives/Colorants; Personal Care Products/Cosmetics; Industrial Chemicals	19641419.82	17377308.68
Triethylene glycol monobutyl ether	Industrial Chemicals	6945930.708	8575637.544
Triethylphosphate	Industrial Chemicals	5231883.762	8914210.347
Triisopropanolamine	Extractables/Leachables; Industrial Chemicals; Textile Chemicals/Auxiliary/Dyes; Personal Care Products/Cosmetics; Pesticides/Herbicides	6227382.426	14153389.15
Trimethoprim	Therapeutics/Prescription Drugs	96774.87497	3756563.027
Triphenylphosphine oxide		17757465.14	27636918.78
Tris(2-butoxyethyl) phosphate	Extractables/Leachables; Textile Chemicals/Auxiliary/Dyes; Industrial Chemicals	130429482.3	129344436.2
Tyroscherin		1007553.969	1704862.001
Valsartan	Therapeutics/Prescription Drugs	1731896.638	1275135.509
Vatalanib dihydrochloride		159658.1609	187594.9425

Table A3-4: List of detected compounds from the Trace finder targeted screening workflow of downstream, upstream, and effluent extracts.

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Metolcarb_M-C2H2NO	9.04	109.0645	113540582
Esprocarb	7.43	266.1584	78327290
Tiocarbazil	7.79	280.1740	53012777
Diaminotoluene	1.17	123.0911	50282577
Guaifenesin	9.1	199.0956	43431496
Ethyl Paraben	8.99	167.0695	28808151
Morphine-D3	8.69	289.1631	24314878
Tiemonium	7.89	318.1528	11425497
Penicillic-Acid	9.01	171.0644	11037310
Dimepiperate	7.74	264.1429	9874520
Ethiofencarb_M-C4H8NOS	0.04	107.0489	9501722
Propargite	7.61	368.1895	8661313
1-Methylamino-1-(3,4-Methylenedioxyphenyl)Propane	10.38	194.1167	6241029
Methedrone	10.38	194.1167	6241029
MDMA	10.38	194.1167	6241029
Isoprocarb	10.38	194.1167	6241029
Trimethacarb, 2,3,5-	10.38	194.1167	6241029
3,4,5-Trimethacarb	10.38	194.1167	6241029
Dimidium	9.45	300.1507	4935268
Cycluron	9.81	199.1796	4682578
Acetaminophen	13	152.0701	4651509
2-Acetamidophenol	13	152.0701	4651509
3-Acetamidophenol	13	152.0701	4651509
Bis(2-Ethylhexyl) Phthalate	8.96	391.2823	4456957
Dibutyl Succinate	9.69	231.1579	4108882
4-Aminophenol	12.67	110.0598	3600501
L-Isoleucine	12.65	132.1013	3591684
Metolcarb	13	166.0855	3554400

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Benzocaine	13	166.0855	3554400
4-Aminobiphenyl	12.55	170.0957	3500655
Diphenylamine	12.55	170.0957	3500655
Flumethasone	10.69	411.1970	3279334
Aldicarb	4.16	116.0523	3170610
Hymexazol	0.08	100.0391	2919283
Dexamethasone	6.93	393.2072	2840425
Betamethasone	6.93	393.2072	2840425
Bufexamac	12.79	224.1270	2835321
Gabapentin	8.99	172.1324	2744439
Pentamidine	8.04	341.1971	2706114
Sumatriptan	11.1	296.1430	2574201
Flurandrenolide	7.3	437.2332	2465167
Ecgonine	12.86	186.1116	2306242
Maleic hydrazine	11.78	113.0342	1978415
Maleic Hydrazide	11.78	113.0342	1978415
Glutamic Acid	12.96	148.0598	1963172
Propham_M-C3H5	10.38	138.0545	1959035
Cycloxydim	7.01	326.1787	1902363
Propoxur_M-C3H5	6.64	168.0648	1898079
gamma-Aminobutyric Acid	12.67	104.0704	1857709
Prohexadione	8.57	213.0748	1853119
Bioresmethrin	11.63	339.1938	1758796
Resmethrin	11.63	339.1938	1758796
Spironolactone	9	417.2089	1682261
L-Histidine	9.34	156.0762	1525979
Furmecyclox	12.2	252.1583	1399659
Phthalic Acid, Bis-Propyl Ester	8.08	251.1266	1323160
Triadimenol	8.11	296.1174	1318018

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Propoxyphene	11.63	340.2254	1302437
Dextropropoxyphene	11.63	340.2254	1302437
Hypoglycin A	12.92	142.0857	1231691
Furathiocarb	10.63	383.1654	1163826
3-Amino-2-Oxazolidinone (AOZ)	12.04	103.0500	1162675
Dimethyl Phthalate	8.79	195.0644	1089690
Strophanthidin	7.83	405.2289	1085601
Prosulfocarb	6.53	252.1429	1059517
Glibornuride	10.98	367.1703	1051785
Mevinphos	9.86	225.0532	1027681
Mevinphos-Cis/Trans	9.86	225.0532	1027681
1-Aminocyclohexanecarboxylic Acid	12.41	144.1013	1012420
6-beta-Hydrocortisol	10.61	379.2127	1001622
Phthalic Acid, Bis-Iso-Butyl Ester	12.33	279.1577	994902
Dibutyl Phthalate	12.33	279.1577	994902
Valpromide	9.85	144.1377	990683
Tranexamic Acid	11.02	158.1168	939759
Picaridin	8.72	230.1740	925744
Mescaline	12.8	212.1271	827855
Alminoprofen	8.26	220.1322	747289
Azaperone	9.83	328.1821	699504
7-Aminoflunitrazepam	7.47	284.1188	693237
L-Tyrosine	9.48	182.0803	691178
Clemastine	9.61	344.1769	661705
Metanephrine	9.06	198.1117	644506
Tenuazonic-Acid	9.06	198.1117	644506
Dopamine	12.37	154.0856	606485
Xylylcarb	12.84	180.1012	604303
XMC	12.84	180.1012	604303

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Propham	12.84	180.1012	604303
Phenacetin	12.84	180.1012	604303
Propoxur	11.55	210.1117	604249
Anhydroecgonine Methyl Ester	9.12	182.1167	603885
Sethoxydim	6.86	328.1943	597873
Verrucarol	8.56	267.1578	596836
Butylone	8.69	222.1114	555207
Ethylone	8.69	222.1114	555207
Carbofuran	8.69	222.1114	555207
Mycophenolic-Acid_M+Na	9.28	343.1136	554163
Cathinone	9.2	150.0906	545255
Norepinephrine	11.02	170.0805	520481
Chlordiazepoxide	6.57	300.0909	483997
Benzophenone	10.68	183.0796	477919
20-beta-Dihydroprednisolone	9.95	363.2181	471856
Kadethrin	8.91	397.1456	467653
Fenpyroximate	7.95	422.2095	430130
Bufencarb	12.57	222.1478	424937
Fluocinolone Acetonide	9.48	453.2076	395043
Metazachlor	7.1	278.1067	393938
Epinephrine	11.03	184.0960	392768
Ricinine	6.71	165.0664	387070
2-NP-AOZ-D4	12.9	240.0910	372400
Betamethasone 21-Acetate	7.76	435.2199	365726
Triamcinolone Acetonide	7.76	435.2199	365726
Amphetamine	12.47	136.1115	363403
Methoprotryne	8.28	272.1547	355608
Dinotefuran-metabolite-UF	12.96	159.1122	351375
Paroxetine	7.2	330.1512	335387

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Nithiazine	9.28	161.0382	331288
Anhydroecgonine	12.47	168.1011	330254
3-Methoxytyramine	12.47	168.1011	330254
Diethofencarb	9.09	268.1532	329131
Imidacloprid,desnitro-olefin	8.53	209.0590	327396
Acetamiprid-metabolite-IM-2-1	8.53	209.0590	327396
Vardenafil	9.06	489.2286	323239
Danofloxacin	7.74	358.1546	319564
Crotoxyphos	5.78	315.0997	313374
Hydrocortisone Aceponate	9.5	461.2528	312785
Cortisone	9.05	361.2021	306094
Enrofloxacin	8.5	360.1714	290955
15-Acetyldeoxynivalenol_M+Na	7.87	361.1240	285215
Trimethoxyamphetamine	8.02	226.1427	280702
Terbutaline	8.02	226.1427	280702
Fluconazole	7.5	307.1129	276202
Viloxazine	8.31	238.1426	274643
Ametryn	9.7	228.1289	273466
Piracetam	12.77	143.0808	258378
Alprenolol	7.58	250.1789	258157
Miglitol	12.81	208.1172	239251
20-beta-Dihydrocortisol	9.39	365.2340	233591
Pioglitazone	7.79	357.1285	220661
Northiaden	6.57	282.1298	215983
Physostigmine	7.42	276.1699	199635
Salbutamol	9.13	240.1583	185866
Albuterol	9.13	240.1583	185866
Benperidol	9.44	382.1916	183495
Propaphos	12.97	305.0974	181126

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Cafeine	6.7	195.0869	165551
Propoxycaine	10.74	295.2028	152220
Clomipramine	10.31	315.1638	150767
Tropicamide	9.65	285.1586	139820
O-Desmethylvenlafaxine	7.98	264.1946	137521
Tramadol	7.98	264.1946	137521
N-Desmethylvenlafaxine	7.98	264.1946	137521
MBDB	10.25	208.1322	124256
MDEA	10.25	208.1322	124256
Fenobucarb	10.25	208.1322	124256
Promecarb	10.25	208.1322	124256
Methcathinone	9.34	164.1062	118052
DEF	12.06	315.1037	117135
Phenmetrazine	12.69	178.1219	112509
Buphedrone	12.69	178.1219	112509
Dimethylcathinone	12.69	178.1219	112509
Mephedrone	12.69	178.1219	112509
AZT	8.91	268.1040	110219
Neosolaniol_M+NH4	7.74	400.1948	107253
Ecgonine d3	0.69	189.1304	105204
Atraton	12.72	212.1497	101643
L-(-)-Norephedrine	12.96	152.1063	101438
Norephedrine	12.96	152.1063	101438
Hippuric Acid	8.16	180.0649	100376
Chlormequat Chloride	8.61	122.0725	99252
Ciprofloxacin	9.48	332.1418	95583
Methylone	8.94	208.0961	94255
Atrazine	7.1	216.1009	92672
Cyclohexamide	9.43	282.1686	89636

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Risperidone	6.8	411.2205	85285
Carbaryl	8.78	145.0642	83213
Ethoprophos	9.38	243.0641	74738
Methomyl_M-C2H2NO	8.69	106.0321	74307
Halofenozide	10.1	331.1199	73305
Prazosin	9.69	384.1684	72339
Promethazine	9.5	285.1425	71546
Creatine	12.85	132.0761	70939
Fenbuconazole	8.35	337.1230	69029
Tentoxin	8.53	415.2321	68849
Sulfamethoxazole	6.11	254.0581	68195
DMST	7.86	215.0847	67336
Bendiocarb	11.99	224.0907	65947
Dioxacarb	11.99	224.0907	65947
Ancymidol	6.76	257.1280	65054
Methylprednisolone	9.26	375.2182	64322
Iprobenfos	7.62	289.1028	62699
Clofibrate	8.69	243.0794	62452
Sulfacetamide	6.59	215.0486	59328
Karbutilate	7.02	280.1643	53448
Valethamate	10.76	306.2412	53228
Duloxetine	7.78	298.1263	49609
Phthalic Acid, Bis-Hexyl Ester	8.22	335.2209	49477
Prometryn	9.6	242.1445	49359
Terbutryn	9.6	242.1445	49359
3,4-DMMC	9.94	192.1375	48879
4-EMC	9.94	192.1375	48879
N-Ethylbuphedrone	9.94	192.1375	48879
Pentedrone	9.94	192.1375	48879

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Phendimetrazine	9.94	192.1375	48879
Diethyl Toluamide	9.94	192.1375	48879
Asulam	6.87	231.0430	48640
Prednisone	7.71	359.1866	48183
Chlorproethazine	11.99	347.1326	48022
Pyrazinamide	10.03	124.0511	47316
Desoximetasone	8.48	377.2140	47306
Fluorometholone	8.48	377.2140	47306
HT2-Toxin	8.46	425.2156	47219
6-Phenyl-2-Thiouracil	12.6	205.0439	46660
Paxilline	7.65	436.2495	46022
Atrazine-Desethyl	7.91	188.0691	45219
Carbofuran, 3OH-	11.35	238.1065	45117
Azaperol	10.48	330.1973	44838
Penicillin-G	8.38	335.1075	43919
Dicrotophos	7.78	238.0832	43892
Desmetryn	7.06	214.1122	43748
Simetryn	7.06	214.1122	43748
Imidacloprid,desnitro	10.78	211.0744	43600
Ephedrine	12.55	166.1219	43029
Pseudoephedrine	12.55	166.1219	43029
Methoxyamphetamine	12.55	166.1219	43029
Edrophonium	12.55	166.1219	43029
Tebuconazole	9.89	308.1534	42931
Trimipramine	5.33	295.2173	40194
MPBP	12.41	232.1686	39893
Hydroxyzine	8.79	375.1815	39496
Paclobutrazol	9.26	294.1380	38415
Triadimefon	7.37	294.1016	38253

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Fluspirilene	9.39	476.2485	38055
Zilpaterol	6.94	262.1547	37791
Pyrinuron	9.61	273.0993	36677
Propyphenazone	8.51	231.1494	36351
Amoxapine	10.24	314.1043	34995
Aldicarb-sulfoxide_M-C2H4NO2	10.5	132.0471	34657
Dibutylone	12.53	236.1271	34642
Pentylone	12.53	236.1271	34642
Phenyltoloxamine	7.57	256.1684	34093
Flurazepam	7.39	388.1571	32880
Loxapine	8.95	328.1223	32393
Isoniazide	9.56	138.0667	32161
Sulfamethazine	10.46	279.0919	32134
Sulfisomidine	10.46	279.0919	32134
Cortisol-21-Hemisuccinate	8.96	463.2335	32124
Triamterene	11.14	254.1146	31575
Perazine	9.05	340.1831	31376
Formoterol	11.63	345.1807	31203
Probenecid	6.78	286.1116	30872
Tebutam	11.68	234.1841	30735
Imiprothrin	8.98	319.1641	30733
Thiabendazole	6.12	202.0425	29637
Nifedipine	9.7	347.1241	29253
Sildenafil Citrate	9.6	475.2128	28833
Metalaxyl-M	7.08	280.1531	27821
Metalaxyl	7.08	280.1531	27821
D-Trans-Allethrin	10.02	303.1960	27258
Allethrin	10.02	303.1960	27258
Testosterone Benzoate	10.64	393.2440	27100

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
T-2-Toxin	9.64	467.2257	25774
Methylphenidate	9.45	234.1478	25664
Normeperidine	9.45	234.1478	25664
Metronidazole-OH	12.97	188.0658	24894
N-Desmethyl Mephenytoin	10.1	205.0979	24634
Sparfloxacin	8.65	393.1717	24600
Flamprop Isopropyl	7.42	364.1105	24318
Flamprop-M-isopropyl	7.42	364.1105	24318
Dosulepin	12.92	296.1463	24041
Homocysteine	8.12	136.0423	23907
Ouabain	9.27	585.2884	23566
Cyproconazole	8.75	292.1216	22752
Uniconazole	8.75	292.1216	22752
Benzofenap	7.35	431.0935	22631
Aldicarb-sulfone	10.52	223.0745	20602
Butoxycarboxim	10.52	223.0745	20602
Acetamiprid	10.52	223.0745	20602
Pregabalin	12.47	160.1326	20165
Cyamemazine	7.51	324.1519	19640
Fluoxymesterone	9.44	337.2189	19587
TFMPP	10.8	231.1094	19227
Bumetanide	7.45	365.1182	19224
Bendroflumethiazide	7.59	422.0460	19001
Fludrocortisone	8.46	381.2085	18975
Dimefuron	7.32	339.1206	18866
Droperidol	9.49	380.1750	18535
Butralin	6.41	296.1607	18434
Fluocinonide	9.56	495.2191	18376
Famphur-oxon	6.74	310.0499	17617

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Alloxydim	7.04	324.1795	17380
Thiamine	7.38	265.1116	17081
Difenoxuron	12.17	287.1391	16593
Iproniazid	8.9	180.1130	16514
Ethiofencarb	6.81	226.0890	16489
Methiocarb	6.81	226.0890	16489
Quinidine	7.86	325.1899	15859
Quinine	7.86	325.1899	15859
Isopropalin	7.87	310.1755	15791
Perphenazine	11.32	404.1559	15736
Propizepine	12.85	297.1725	15592
Propericiazine	12.86	366.1651	15460
Felbamate	10.07	239.1028	15344
Cimbuterol	11.73	234.1608	15072
Amodiaquine	11.41	356.1521	14994
Isoxaflutole	7.66	360.0499	14883
10-Hydroxycarbazepine	8.25	255.1116	14794
Betamethasone 17-Valerate	9.77	477.2657	14778
Noroxymorphone	9.81	288.1216	14543
Buflomedil	7.53	308.1844	14301
Sedaxane	9.72	332.1585	14214
Trenbolone	11.54	271.1680	14170
L-Methionine Sulfoxide	12.77	166.0525	14071
Pipotiazine	7.61	476.2058	14040
Citreoviridin	8.94	403.2120	13504
6beta-OH-Budesonide	9.2	447.2386	13359
Fensulfothion	7.54	309.0381	13353
Fenspiride	7.92	261.1595	13331
Zearalenone	8.61	319.1548	13268

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Fluvoxamine	9.31	319.1630	13186
2-NP-AMOZ	7.32	335.1334	13067
Pimozide	9.33	462.2358	12799
Cis-Mefentanyl	6.2	351.2424	12797
Alpha-Methylfentanyl	6.2	351.2424	12797
Azinphos-methyl_M-C2H6O2PS2	11.02	160.0505	12665
Etoricoxib	12.33	359.0610	12508
15-Acetyldeoxynivalenol_M+NH4	8.25	356.1719	12325
Lidocaine	7.91	235.1810	12310
Dimethenamid	7.04	276.0822	12251
Buphedrine	11.77	180.1376	12183
Methylephedrine	11.77	180.1376	12183
Methoxymethamphetamine	11.77	180.1376	12183
Mexiletine	11.77	180.1376	12183
Imidacloprid	7.32	256.0600	12178
Sulindac Sulfide	6.76	341.0989	12040
Metofluthrin	6.93	361.1432	12020
Ethofumesate	5.75	287.0960	11749
Imazamethabenz-methyl	8.58	289.1536	11721
Isoxsuprine	7.26	302.1754	11638
Ractopamine	7.26	302.1754	11638
Dobutamine	7.26	302.1754	11638
Sebuthylazine-Desethyl	9.1	202.0848	11557
Simazine	9.1	202.0848	11557
Flutolanil	7.31	324.1199	11492
Lacidipine	8.47	456.2401	11486
Dichlorvos	3.51	220.9522	11485
Zimelidine	8.75	317.0656	11362
Clethodim-sulfoxide	7.15	376.1353	11157

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Uradipil	10.78	388.2325	11075
Bensulfuron-methyl	7.26	411.0970	11050
3-Indoleacetic Acid	12.73	176.0698	10988
Desmedipham_M+NH4	6.91	318.1437	10915
Phenmedipham_M+NH4	6.91	318.1437	10915
Bifenazate	6.36	301.1537	10831
Thiazafluron	8.99	241.0374	10755
Piperonyl-butoxide	9.62	356.2414	10747
Clozapine	12.13	327.1384	10739
Desmedipham	4.64	301.1195	10684
Phenmedipham	4.64	301.1195	10684
Dimethoxybenzidine	8.37	245.1279	10619
Etomidate	8.37	245.1279	10619
Nandrolone Decanoate	6.81	429.3344	10513
Valsartan	10.78	436.2354	10499
Meprednisone	8.83	373.2022	10495
Pyrethrinii	8.83	373.2022	10495
Isothipendyl	12.97	286.1386	10305
3-Methyl-2-Quinoxalinecarboxylic Acid	9.07	189.0667	10253
Dazomet	6.73	163.0350	10223
Methacrifos	12.96	241.0284	10066
Famoxadone	7.05	392.1590	9963
Sulfoxaflor_M-C2H3N2SO	13	174.0518	9911
Pyrithiobac	6.46	327.0201	9897
Ethyl Loflazepate	6.9	361.0758	9753
Decoquinate	6.7	418.2600	9470
Melatonin	12.03	233.1287	9348
Pirimiphos-methyl	6.69	306.1023	9327
Pyriftalid	11.14	319.0732	9225

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Aflatoxin-G2	10.08	331.0819	8932
Demexiptiline	5.23	279.1484	8910
Mefloquine	6.56	379.1257	8876
Pyridate	6.56	379.1257	8876
Nebivolol	8.69	406.1839	8703
Carbimazole	6.63	187.0531	8642
Nitenpyram	10.39	271.0952	8286
Cadusafos	10.39	271.0952	8286
Propylene Thiourea	7.06	117.0480	8212
Phosfolan	9.29	256.0224	8183
Sulfathiazole	5.93	256.0218	8183
Valdecoxib	5.83	315.0811	7965
Diltiazem	9.56	415.1698	7948
Fenthion-sulfoxide	6.71	295.0229	7888
Milbemectin A3	6.38	511.3047	7746
Norbenzoylecgonine	6.33	276.1223	7673
Diacetoxyscirpenol_M+NH4	8.61	384.1999	7468
Ceftriaxone	11.63	555.0519	7442
Zonisamide	0.69	213.0326	7364
Trihexyphenidyl	6.25	302.2480	7110
Parathion-methyl-oxon	0.13	248.0325	6951
Triazoxide	0.13	248.0325	6951
Fenpyrazamine	9.48	332.1418	6946
Propiconazole	5.64	342.0755	6936
Clenpenterol	5.6	291.1017	6775
Fuberidazole	6.01	185.0704	6575
Etoposide	5.75	589.1925	6547
Harmine	12.81	213.1030	6513
Neburon	5.58	275.0701	6506

Wastewater Up Stream			
Compound Name	**RT**	**m/z**	**Peak Area**
Phthalic Acid, Bis-N-Pentyl Ester	10.08	307.1889	6448
Dimethachlor	5.41	256.1105	6426
Prazepam	10.59	325.1107	6338
Norketamine	5.88	224.0837	6305
Ebastine	12.04	470.3068	6265
Coniine	11.06	128.1429	6225
Beclomethasone	12.6	409.1794	6047
Alimemazine	9.33	299.1583	6036
Fenthion	5.47	279.0283	6008
Oxprenolol	9.43	266.1743	5979
Cyclanilide	5.29	274.0022	5782
Aicar	6.37	259.1049	5779
Methohexital	11.21	263.1386	5629
Clotiazepam	8.58	319.0668	5623
Bentranil	10.02	224.0696	5616
Fluazifop-Butyl	5.15	384.1410	5519
Fluazifop-P-butyl	5.15	384.1410	5519
Penicillin-V	0.37	351.1024	5460
Triflumizole	5.02	346.0937	5394
Lactofen	5.15	479.0833	5238
Clozapine N-Oxide	1.2	343.1334	5228
7-(2,3-Dihydroxypropyl)Theophylline	8.59	255.1079	4799
Simeconazole	5.14	294.1444	4550

Table A3-4: List of detected compounds from the Trace finder targeted screening workflow of downstream, upstream, and effluent extracts (continues)

Wastewater Down Stream				Wastewater Effluent Discharge			
Compound Name	**RT**	**m/z**	**Peak Area**	**Compound Name**	**RT**	**m/z**	**Peak Area**
1-(4-Chlorophenyl)piperazine (p-CPP)	12.27	272.2005	2576	Netilmicin	7.72	476.3062	160388793
1-Methyl-3-Phenylpiperazine	10.25	330.0608	4371	Dexamethasone	7.21	393.2090	148459236
21-Desacetyl Deflazacort	5.46	253.0316	4504	Betamethasone	7.21	393.2090	148459236
3,4-DMMC	10.72	352.1475	4650	Flurandrenolide	7.49	437.2353	137443579
3-Amino-2-Oxazolidinone (AOZ)	5.42	162.0142	4666	Bis(2-Ethylhexyl) Phthalate	0.03	391.2837	118628144
3-Hydroxystanozolol	6.53	188.0827	4792	Diaminotoluene	0.77	123.0917	49736491
3-Indoleacetic Acid	9.14	190.1266	4848	Phthalic Acid, Bis-Iso-Butyl Ester	11.97	279.1588	42026361
4-Acetamidoantipyrine	11.83	180.1382	4863	Dibutyl Phthalate	11.97	279.1588	42026361
4-Aminoantipyrine	11.83	180.1382	4863	Dimethyl Phthalate	7.85	195.0652	24373632
4-Aminobiphenyl	11.83	180.1382	4863	Alfentanyl	7.49	417.2589	15744826
4-Aminophenol	11.83	180.1382	4863	Metolcarb_M-C2H2NO	12.65	109.0649	15332583
4-EMC	11.11	489.2296	4919	Cycluron	7.21	199.1803	14369294
5-Hydroxy Omeprazole	6.48	124.0507	4932	4-Aminobiphenyl	11.07	170.0963	10671188
6beta-OH-21-Desacetyl Deflazacort	9.77	311.0403	4953	Diphenylamine	11.07	170.0963	10671188
6beta-OH-Budesonide	10.74	282.1455	4991	1-Methylamino-1-(3,4-Methylenedioxyphenyl)Propane	0.77	194.1174	10353071
7-Aminonitrazepam	10.71	415.2322	5004	Methedrone	0.77	194.1174	10353071
Acetalozamide	5.43	890.5231	5031	MDMA	0.77	194.1174	10353071
Aconitine	5.94	293.0706	5068	Isoprocarb	0.77	194.1174	10353071
Aicar	9.58	117.0476	5173	Trimethacarb, 2,3,5-	0.77	194.1174	10353071
Albendazole	12.93	315.2306	5184	3,4,5-Trimethacarb	0.77	194.1174	10353071
Alminoprofen	12.93	315.2306	5184	Bufexamac	0.75	224.1280	10313043
Alprenolol	9.66	275.1321	5198	Penicillic-Acid	12.65	171.0654	9704000
Anabasine	3.51	273.1842	5288	Ethiofencarb_M-C4H8NOS	10.49	107.0493	8420197
Anisotropine Methylbromide	10.89	312.1158	5310	Sumatriptan	0.05	296.1439	7852194
Articaine	5.74	480.2108	5340	Valethamate	9.93	306.2423	6844442
Atorvastatin	5.48	230.1177	5413	Fluocinolone Acetonide	7.49	453.2092	6798966

Azatadine	5.48	230.1177	5413	L-Isoleucine	1.01	132.1019	6569879
Bamifylline	5.48	230.1177	5413	Guaifenesin	8.6	199.0964	6110366
Beclomethasone	5.48	230.1177	5413	Metolcarb	12.98	166.0863	6036767
Benazepril	5.48	230.1177	5413	Benzocaine	12.98	166.0863	6036767
Benoxinate	12.77	209.1284	5473	Ethyl Paraben	10.51	167.0704	5337851
Bensultap	12.77	209.1284	5473	Glutamic Acid	0.72	148.0603	5085046
Bentranil	6.43	429.2382	5476	L-Histidine	0.68	156.0768	4286164
Benzedrone	8.39	167.1038	5495	Tranexamic Acid	12.79	158.1175	4104857
Benzobicyclon	4.83	299.0620	5566	Acetaminophen	12.95	152.0707	3838186
Benzthiazuron	4.83	299.0620	5566	2-Acetamidophenol	12.95	152.0707	3838186
Benzydamine	12.92	128.1433	5621	3-Acetamidophenol	12.95	152.0707	3838186
Benzylfentanyl	12.77	199.0458	5764	Ethoprophos	7.22	243.0634	3299339
Betamethasone 17-Valerate	12.74	360.1769	5801	Maleic hydrazine	0.75	113.0347	3232858
Betanechol	6.67	305.1480	5802	Maleic Hydrazide	0.75	113.0347	3232858
Bis(2-Ethylhexyl) Phthalate	7.72	256.1100	5808	Propham_M-C3H5	12.9	138.0550	2884794
Boldenone	7.35	122.0269	5889	Hymexazol	0.79	100.0396	2783489
Bromperidol	12.75	324.1527	5897	Propentofylline	6.99	307.1750	2708528
Buphedrine	6.61	213.1859	5909	Butylone	8.79	222.1125	2625487
Butroxydim	10.75	236.0916	6026	Ethylone	8.79	222.1125	2625487
Butylone	7.55	408.1710	6124	Carbofuran	8.79	222.1125	2625487
Carbamazepine	7.05	441.0388	6149	gamma-Aminobutyric Acid	12.89	104.0708	2434911
Carbofuran-3-Keto	11.31	343.1169	6179	4-Aminophenol	12.23	110.0602	2237401
Carbophenothion	10.38	212.1021	6441	Hypoglycin A	12.71	142.0862	2207172
Cephalomannine	6.95	295.0410	6577	3-Amino-2-Oxazolidinone (AOZ)	12.45	103.0504	1966584
Chloranocryl	9.51	344.1764	6588	Ecgonine	7.93	186.1124	1943440
Chlorethoxyfos	11.46	233.1507	6609	L-Tyrosine	0.83	182.0810	1938516
Ciclesonide	11.79	259.1032	6610	Furmecyclox	12.21	252.1594	1849417
Cimaterol	7.95	406.1837	6651	Cafeine	6.57	195.0876	1780883
Cis-Mefentanyl	12.02	206.1539	6661	1-Aminocyclohexanecarboxylic Acid	12.95	144.1019	1719096
Clanobutin	9.97	275.0900	6688	AZT	0.77	268.1036	1710911
Clenpenterol	6.97	315.0676	6711	Benzophenone	10.75	183.0804	1571389

Clenproperol	6.97	315.0676	6711	Propoxur_M-C3H5	12.28	168.0654	1519770
Clidinium	12.83	282.1310	6851	Butachlor	7.02	312.1731	1460037
Clobetasol Propionate	10.58	273.0973	6889	Pretilachlor	7.02	312.1731	1460037
Clobetasone Butyrate	6.92	285.0204	6928	Imidacloprid,desnitro-olefin	11.17	209.0596	1459125
Clofilium Tosylate	11.95	267.1712	6971	Acetamiprid-metabolite-IM-2-1	11.17	209.0596	1459125
Colistin	11.95	267.1712	6971	Thiabendazole	6.34	202.0432	1303800
Convallatoxin	11.51	316.0346	6975	Piracetam	12.95	143.0814	1260211
Cortisol-21-Hemisuccinate	10.51	268.1541	6999	Miglitol	7.58	208.1180	1167452
Cortivazol	9.6	230.0237	7062	Xylylcarb	12.84	180.1019	1149796
Cymarin	2.02	226.1674	7091	XMC	12.84	180.1019	1149796
Cytisine	2.02	226.1674	7091	Propham	12.84	180.1019	1149796
Deiquat	2.02	226.1674	7091	Phenacetin	12.84	180.1019	1149796
Deoxycorticosterone Acetate	11.06	231.1589	7107	N-Desmethyl Mephenytoin	6.32	205.0968	1088074
Desonide	7.37	338.0460	7151	Valpromide	10.02	144.1382	1044402
Desoximetasone	7.35	328.0603	7316	Atraton	12.84	212.1505	1028436
Desoxycortone	12.94	234.1848	7344	Kojic-Acid	7.24	143.0339	957345
Despropionyl p-Fluoro Fentanyl	10.81	231.0868	7346	Gabapentin	9.07	172.1331	922930
Detomidine	7.31	258.1852	7391	3-Indoleacetic Acid	8.37	176.0706	861693
Dibutylone	0.68	142.0089	7516	Fenpyroximate	7.65	422.2075	840636
Dichlorisone Acetate	7.72	292.1223	7696	Atrazine-D5	9.95	221.1322	831358
Digoxin	7.72	292.1223	7696	Dodemorph	12.95	282.2789	797128
Dihydro Capsaicin	5.78	456.2364	7781	Pefloxacin	7.04	334.1551	792334
Dimethoxybenzidine	11.03	332.1443	7782	Bufencarb	12.89	222.1487	756215
Dimethylamylamine	11.67	296.1842	7934	Aldicarb	12.85	116.0531	743991
Doxapram	12.8	495.2186	7952	Theobromine	8.76	181.0711	737989
Drospirenone	11.77	282.2423	7972	Paraxanthine	8.76	181.0711	737989
Ebastine	13	305.2462	8188	Betamethasone 21-Acetate	7.76	435.2196	719690
Emetine	6.36	393.1729	8267	Triamcinolone Acetonide	7.76	435.2196	719690
Epitestosterone	12.49	239.1019	8374	Albendazole Sulfoxide	7.76	282.0904	620126
Eplerenone	2.28	161.0387	8377	Triazoxide	7.7	248.0341	617382
Estrendione	12.75	203.1136	8453	MBDB	11.25	208.1329	615069

Etamiphylline	7.88	415.1304	8762	MDEA	11.25	208.1329	615069
Ethacrynic Acid	9.58	259.0592	8812	Fenobucarb	11.25	208.1329	615069
Ethyl Loflazepate	12.78	259.0577	8812	Promecarb	11.25	208.1329	615069
Ethylone	12.78	259.0577	8812	Norepinephrine	12.61	170.0812	585251
Etoricoxib	12.78	259.0577	8812	Atrazine-Desethyl	12.48	188.0706	581357
Famprofazone	7.57	360.0498	8947	Ofurace	7.76	282.0904	580090
Fexofenadine	12.93	397.1455	9037	Dopamine	12.59	154.0861	555520
Firocoxib	12.98	308.1844	9144	Dinotefuran-metabolite-UF	12.71	159.1127	528173
Flephedrone	13	318.1535	9237	Epinephrine	12.96	184.0967	507330
Fludrocortisone	11.81	280.1756	9811	Creatine	12.27	132.0767	491280
Flumazenil	7.69	325.1275	10359	Methotrexate	7.21	455.1794	485767
Fluorometholone	12.24	205.0786	10464	Rabenzazole	9.24	213.1125	422888
Fluspirilene	12.24	310.1265	10930	MPBP	11.87	232.1696	410981
Fluticasone	7.15	360.1899	11216	3,4-DMMC	10.05	192.1381	407567
Formoterol	12.84	237.1237	11498	4-EMC	10.05	192.1381	407567
gamma-Aminobutyric Acid	12.86	280.1743	11821	N-Ethylbuphedrone	10.05	192.1381	407567
Gelsemine	10.16	266.1739	12208	Pentedrone	10.05	192.1381	407567
Glycopyrrolate	8.03	327.1373	12274	Phendimetrazine	10.05	192.1381	407567
Guanabenz	7.84	286.1384	12513	Diethyl Toluamide	10.05	192.1381	407567
Guanfacine	13	282.1687	12683	Metronidazole-OH	12.01	188.0664	394993
Halcinonide	12	365.1454	13477	Guanfacine	7.72	246.0185	348372
Harmine	10.65	225.0525	13551	Clidinium	6.85	352.1909	343506
Hydrocortisone Aceponate	10.65	225.0525	13551	Amphetamine	12.88	136.1120	330841
Hydroxyfentanyl	12.38	161.1286	14093	Cathinone	0.75	150.0914	330358
Indapamide	12.31	188.1108	14137	Metanephrine	12.38	198.1124	309231
Indoprofen	8.69	326.1608	14297	Tenuazonic-Acid	12.38	198.1124	309231
Ipratropium	12.46	341.1681	14461	Imidacloprid,desnitro	11.21	211.0752	264079
Isopropamide	6.76	231.0273	14554	Phenmetrazine	12.8	178.1225	252272
Isoxicam	6.76	231.0273	14554	Buphedrone	12.8	178.1225	252272
Isoxsuprine	12.35	390.2119	15435	Dimethylcathinone	12.8	178.1225	252272
Jervine	6.77	241.0368	16235	Mephedrone	12.8	178.1225	252272

Kavain	8.34	299.1576	16910	2-NP-AOZ-D4	8.91	240.0920	244839
Ketamine	7.54	256.0146	17110	Propoxur	11.56	210.1127	237035
Lansoprazole	8.01	585.2877	17930	L-Methionine Sulfoxide	0.72	166.0531	227620
L-Histidine	9.82	150.0585	18227	O-Desmethylvenlafaxine	12.24	264.1954	222587
L-Methionine	12.78	411.1986	18283	Tramadol	12.24	264.1954	222587
L-Methionine Sulfoxide	12.29	203.0918	18753	N-Desmethylvenlafaxine	12.24	264.1954	222587
Lornoxicam	9.31	319.1532	19084	Simetone	6.79	198.1349	215837
L-Thyronine	7.65	320.0378	19273	Mescaline	12.93	212.1280	206423
L-Tyrosine	7.22	146.0633	19291	Morphine-D3	10.68	289.1638	195307
Mabuterol	11.25	275.1493	19859	Prothioconazole	6.86	344.0398	184993
Mapenterol	9.93	297.1703	20271	Norfloxacin	6.1	320.1392	184483
MDPBP	10.52	321.0822	20343	Picaridin	10.19	230.1749	180836
MDPV	7.45	416.2814	21341	Sotalol	7.89	273.1265	180135
Medroxyprogesterone	12.58	186.0873	21345	Alprenolol	11.94	250.1800	173563
Megestrol Acetate	12.21	238.1429	21509	Methomyl_M-C2H2NO	12.15	106.0324	171590
Meloxicam	12.87	253.1651	22320	Prohexadione	8.37	213.0759	160094
Mepenzolate	12.91	243.1085	22753	Anhydroecgonine	12.93	168.1018	151189
Meprednisone	11.94	160.0507	22762	3-Methoxytyramine	12.93	168.1018	151189
Mesterolone	12.54	181.0974	23203	Hippuric Acid	11.97	180.0656	150933
Methazolamide	11.18	279.0922	23379	Isocarbamid	12.24	186.1237	149577
Methenolone	11.18	279.0922	23379	Indoprofen	7.89	282.1134	147348
Methoxetamine	6.77	344.0399	23605	Pregabalin	12.27	160.1332	146825
Methylephedrine	8.31	335.2222	23976	Furaltadone	12.59	325.1153	145090
Methylone	11.22	165.0659	24308	Aflatoxin-B1	5.31	313.0722	138684
Methyltestosterone	10.97	223.0737	24549	Enrofloxacin	7.05	360.1714	132522
Methysticin	10.97	223.0737	24549	Sparfloxacin	6.89	393.1729	122214
Metolazone	10.97	223.0737	24549	Oxadixyl	11.76	279.1346	110545
Mifepristone	12.42	189.1311	25213	Phthalic Acid, Bis-Propyl Ester	10.89	251.1276	104841
Miglitol	7.41	233.0904	25254	Sulfamethoxazole	7.18	254.0594	104595
Mitragynine	10.61	253.1067	25609	Dimetilan	12.88	241.1295	98733
Mometasone Furoate	0.8	137.0458	25838	Pirbuterol	12.24	241.1547	96560

Monocrotaline	7.48	418.2608	26071	Danofloxacin	7.09	358.1561	89562
MPBP	11.09	219.1349	26187	Aldicarb-sulfoxide_M-C2H4NO2	9.62	132.0479	87146
N,N-Dimethyltryptamine	12.66	142.0610	29397	Anhydroecgonine Methyl Ester	10.79	182.1175	86246
Nabumetone	12.91	284.1186	32713	Methylone	8.05	208.0969	69486
Nafronyl Oxalate	10.51	280.1539	33691	Bentranil	10.06	224.0704	65539
Nandrolone Decanoate	10.51	280.1539	33691	Ephedrine	12.98	166.1227	64948
Naphyrone	12.31	304.1389	38434	Pseudoephedrine	12.98	166.1227	64948
N-Butylscopolamine Bromide	12.82	128.0454	40350	Methoxyamphetamine	12.98	166.1227	64948
N-Desmethylclobazam	10.53	240.1592	41493	Edrophonium	12.98	166.1227	64948
Neostigmine	10.53	240.1592	41493	L-(-)-Norephedrine	12.93	152.1070	64345
Neriifolin	8.01	303.1268	46774	Norephedrine	12.93	152.1070	64345
N-Ethylbuphedrone	6.96	360.1717	47856	Sethoxydim	7.14	328.1956	64309
Nifenazone	8	430.2727	48073	Ipronidazole	12.92	170.0925	63188
Nikethamide	6	320.1392	48113	Metronidazole	11.98	172.0716	62266
Nimesulide Reduced	7.85	282.1128	48375	Butylate	0.05	218.1568	61950
N-Methylscopolamine Bromide	8.33	220.1332	50209	Methcathinone	12.79	164.1070	59542
Norbormide	12.74	212.1393	51262	Dimethylamylamine	0.77	116.1435	59134
Norfenfluramine	6.99	358.1552	52924	Metalaxyl-M	10.48	280.1538	56472
Nor-LSD	12.24	236.1271	53098	Metalaxyl	10.48	280.1538	56472
Normethylfentanyl	12.24	236.1271	53098	Bendiocarb	12.31	224.0913	55912
Norpropoxyphene	12.34	172.0718	54875	Dioxacarb	12.31	224.0913	55912
Ohmefentanyl	10.29	267.1587	57849	Fluconazole	7.85	307.1115	53752
Oleandrin	0.14	224.0339	58269	Heptenophos	7.58	251.0225	52699
omega-Hydroxynorfentanyl	7.06	254.0589	59845	Cymoxanil_M-C3H4NO	6.86	128.0457	50929
Omeprazole Sulphone	11.45	313.0718	60040	Carbofuran, 3OH-	11.67	238.1071	49967
Ormetoprim	12.47	180.0659	64864	Lamotrigine	7.62	256.0150	46953
ortho-Chlorophenylpiperazine (oCPP)	12.94	164.1069	75055	Alminoprofen	8.37	220.1333	45747
Ouabain	12.31	250.1798	75679	Sulfallate	0.04	224.0340	45417
Oxabetrinil	12.96	170.0924	76702	Verrucarol	10.25	267.1588	45194
Oxaziclomefone	7.68	241.1284	79195	Trinexapac-ethyl	10.58	253.1069	43767
Oxine-Copper	12.84	218.1026	82918	Pipemidic Acid	7.19	304.1391	43129

Oxitropium	12.54	116.1437	84257	Pymetrozine	12.72	218.1026	41680
Oxolinic Acid	12.79	152.1070	84885	Zearalenone	9.43	319.1531	40462
Oxyclozanide	12.79	152.1070	84885	Ethaboxam	12.17	321.0839	40324
Oxyphenonium	12.54	226.1438	84894	Trimethoxyamphetamine	12.9	226.1436	38712
Paclitaxel	12.54	226.1438	84894	Terbutaline	12.9	226.1436	38712
Patulin	7.84	218.1566	86870	Ipronidazole-OH	12.28	186.0873	36972
Pendimethalin	7.87	273.1262	90662	Desoxycarbadox	6.44	231.0867	36210
Penfluron	12.96	238.1067	92154	Dibutylone	12.25	236.1274	35835
Pentanochlor	11.43	132.0478	93756	Pentylone	12.25	236.1274	35835
Pentedrone	12.91	160.1331	94887	Isothipendyl	7.9	286.1359	35282
Pentylone	12.42	224.0913	96769	Viloxazine	11.65	238.1434	34317
PFHxDA	12.42	224.0913	96769	Salbutamol	10.49	240.1592	33529
PFODA	11.36	224.0707	99985	Albuterol	10.49	240.1592	33529
Phalloidin	10.84	182.1177	103714	Isouron	12.27	212.1392	31535
Phenisopham	7	328.1954	107693	Hexazinone	12.44	253.1657	30879
Phthalic Acid, Bis-Iso-Butyl Ester	6.7	198.1348	109092	Phthalic Acid, Bis-Hexyl Ester	8.34	335.2222	30763
Phthalic Acid, Bis-N-Pentyl Ester	10.94	251.1276	112947	Fluocinonide	11.65	495.2193	29888
Phthalic Acid, Bis-Propyl Ester	10.25	106.0325	123712	Zalcitabine	0.77	212.1027	29407
Phthalic Acid,Bis-N-Heptyl Ester	12.26	264.1956	128352	Ormetoprim	11.2	275.1489	28805
Physostigmine	12.26	264.1956	128352	Pyridostigmine	12.4	181.0970	27832
Pilocarpine	12.26	264.1956	128352	Azaconazole	7.73	300.0292	27457
Pindone	7.49	251.0226	135255	Demeton-O-Methyl	6.71	231.0263	27280
Pipenzolate	11.81	279.1346	136804	Demeton-S-methyl	6.71	231.0263	27280
Piperalin	6.76	352.1904	137441	Dimetridazole	12.4	142.0613	26367
Pirbuterol	5.15	325.1128	141747	Metamitron	10.68	203.0919	25601
Pridinol	12.29	208.0972	141888	Tetramisole	7.7	205.0795	24953
Prifinium	12.84	166.1227	144483	Diethofencarb	10.48	268.1541	21929
Primidone	12.84	166.1227	144483	Propizepine	9.89	297.1698	21770
Probenecid	12.84	166.1227	144483	Aldicarb-sulfone	10.52	223.0750	21758
Procyazine	12.84	166.1227	144483	Butoxycarboxim	10.52	223.0750	21758
Prodiamine	12.82	289.1622	146931	Acetamiprid	10.52	223.0750	21758

Prolintane	12.78	241.1542	153418	Carbofuran-3-Keto	12.64	236.0907	21184
Propantheline	12.62	212.1279	174587	Meprobamate	11.06	219.1349	20972
Propentofylline	11.24	211.0754	188578	Phosmet	6.45	318.0032	20896
Propionyl Promazine	11.6	210.1124	197360	Acibenzolar-S-methyl	7.21	211.0001	20593
Propoxycaine	9.05	213.0759	213195	Mefloquine	6.89	379.1244	19664
Propoxyphene	9.27	213.1125	215034	Pyridate	6.89	379.1244	19664
Propyphenazone	10.22	230.1749	218289	Mevinphos	10.69	225.0520	19230
Proscillaridin A	0.74	166.0532	218316	Mevinphos-Cis/Trans	10.69	225.0520	19230
Pseudocapsaicin	12.94	168.1020	237215	7-(2,3-Dihydroxypropyl)Theophylline	12.51	255.1091	19221
Pyrazolynate	12.94	168.1020	237215	Etamiphylline	12.67	280.1756	18520
Pyrimethamine	12.65	178.1226	270164	Tebutam	11.54	234.1848	18463
Pyrinuron	12.65	178.1226	270164	Methamidophos	0.65	142.0091	18147
Quinclorac	12.65	178.1226	270164	7-Aminoflunitrazepam	12.23	284.1181	17784
Quizalofop-Methyl	12.65	178.1226	270164	Ecgonine d3	12.23	189.1315	16287
Remifentanyl	12.84	186.1237	275317	Tiemonium	12.06	318.1530	16206
Rescinnamine	0.75	150.0914	282749	Carbetamide	11.54	237.1231	16202
Retrorsine	8.89	240.0922	295879	Thiofanox Sulfoxide	9.73	235.1110	16071
Ricinine	7.69	282.0904	304490	Nithiazine	0.33	161.0387	16064
Rofecoxib	7.69	282.0904	304490	Imidacloprid-olefin	7.92	254.0439	15677
Romifidine	7.12	455.1795	339518	Ciprofloxacin	7.95	332.1409	15295
Salbutamol	7.13	246.0183	342860	Triazophos	7.88	314.0735	15191
Salmeterol	7.6	422.2076	348078	Florfenicol_M+Na	7.9	379.9915	15047
Salvinorin A	6.93	334.1548	349572	Clofibrate	7.39	243.0792	15007
Sebuthylazine-Desethyl	7.41	248.0340	362595	Flumethasone	12.27	411.1984	14713
Senecionine	12.41	198.1122	385714	Propaphos	12	305.0979	14609
S-Metolachlor	12.41	198.1122	385714	Propanil	12.13	218.0126	14532
Solanidine	12.41	232.1694	392270	Sulfachloropyridazine	7.01	285.0205	13717
Solanine	12.65	181.0712	416005	Fluphenazine	7.65	438.1815	13671
Sparteine	12.65	181.0712	416005	Felbamate	11.58	239.1038	13299
Sudan 1	12.7	136.1120	436368	3-Methyl-2-Quinoxalinecarboxylic Acid	7.32	189.0652	13089
Sudan 2	13	188.0665	467258	Isopyrazam	7.83	360.1865	12949

Sudan 3	8.01	285.1606	470970	Azinphos-methyl_M-C2H6O2PS2	0.64	160.0504	12638
Sudan 4	10.09	192.1382	484672	Carbaryl	9.13	145.0648	12148
Sulcofuron	10.09	192.1382	484672	Chlorpheniramine	7.55	275.1313	12044
Sulfisoxazole	10.09	192.1382	484672	Dimepiperate_M-C9H9	5.81	146.0632	11576
Sulindac Sulfide	10.09	192.1382	484672	Buflomedil	12.98	308.1848	11518
Sumatriptan	10.09	192.1382	484672	Etrimfos	5.93	293.0706	10831
SWEP	10.09	192.1382	484672	Dazomet	9.54	163.0358	10811
TCMTB	12.86	159.1128	487267	Thifensulfuron-methyl	7.18	388.0391	10495
Testosterone	8.31	176.0704	516224	Sulfadoxine	10.86	311.0804	10453
Testosterone 17-Enanthate	12.98	188.0704	551566	Sulfadimethoxine	10.86	311.0804	10453
Testosterone 17-Isocaproate	12.92	132.0768	564879	Desmethylcitalopram	8.17	311.1569	10366
Testosterone 17-Phenylpropionate	12.22	184.0968	566965	Clonidine	7.32	230.0235	9770
Testosterone 17-Undecanoate	12.23	170.0811	616459	Propionyl Promazine	11.64	341.1695	9735
Testosterone Acetate	7.26	116.0530	624835	Phenthoate	7.78	321.0389	9471
Testosterone Benzoate	12.23	154.0862	630907	Ofloxacin	7.61	362.1495	9346
Testosterone Cypionate	11.95	208.1329	636073	Chlortoluron	7.34	213.0780	9336
Testosterone Decanoate	11.95	208.1329	636073	Alfuzosine	12.43	390.2121	9247
Testosterone Propionate	11.95	208.1329	636073	L-Methionine	0.8	150.0582	9178
TFMPP	11.95	208.1329	636073	Imidacloprid,urea	7.55	212.0595	9057
THC	7.72	435.2199	651290	Sulfapyridine	7.98	250.0643	8886
Thiazafluron	7.72	435.2199	651290	Tropicamide	8.06	285.1607	8651
Thifluzamide	6.93	312.1730	658343	Penflufen	8.45	318.1961	8243
Thiocolchicoside	6.93	312.1730	658343	Tobramycin	12.05	468.2648	8217
Thiram	12.84	282.2791	670824	Tropatepine	11.22	334.1611	8146
Tiletamine	6.24	202.0433	711547	Carfentrazone-ethyl	7.85	412.0453	8118
Tiotropium	9.97	221.1323	763556	Mesterolone	12.13	305.2470	7948
Torsemide	9.02	172.1331	838871	Pipamperone	6.95	376.2408	7880
Trenbolone	12.75	222.1487	873206	Duloxetine	12.71	298.1254	7867
Trichloronat	6.81	307.1750	902531	MDPV	12.31	276.1581	7827
Triclocarban	7.13	143.0338	936012	Oxabetrinil	11.36	233.0930	7666
Trimethoxyamphetamine	12.83	212.1506	971342	Nalidixic Acid	11.36	233.0930	7666

Tripelennamine	10.06	144.1383	1024640	Sedaxane	11.29	332.1565	7537
Valdecoxib	12.92	180.1021	1051015	Orphenadrine	6.81	270.1842	7514
Valethamate	12.92	180.1021	1051015	Ancymidol	7.82	257.1290	7505
Verrucarol	12.92	180.1021	1051015	Meleagrin	10.22	434.1839	7473
Xipamide	12.92	180.1021	1051015	Cevadine	7.02	592.3489	7458
Xylazine 4-Hydroxy	6.27	205.0972	1089079	Methylphenidate	12.23	234.1493	7409
Xylometazoline	6.49	195.0876	1128195	Normeperidine	12.23	234.1493	7409
Zilpaterol	12.96	143.0815	1419969	Retrorsine	8.45	352.1752	7357
Zolazepam	7.54	208.1178	1445505	Fluroxypyr	6.31	254.9736	7332
Tranexamic Acid	9.97	209.0598	1534330	Promethazine	8.73	285.1431	7310
Diaminotoluene	9.97	209.0598	1534330	Pimozide	12.4	462.2331	7097
Ecgonine d3	11.95	168.0656	1703030	Ergocristine	6.95	610.3033	7038
Maleic hydrazine	0.75	268.1038	1725009	Ergocristinine	6.95	610.3033	7038
Daminozide	10.79	183.0804	1761381	Nitrofurazone	12.12	199.0462	7028
Aminocyclopyrachlor	12.87	144.1020	1778167	Rescinnamine	7.85	635.2979	7012
Bialaphos	7.87	186.1123	1866188	Buturon	9.53	237.0780	6948
Chlormequat Chloride	0.81	182.0812	1988251	Amfepramone	12.39	206.1538	6908
Cyromazine	12.22	252.1593	1994382	Norfluoxetine	6.69	296.1247	6716
Dinotefuran-metabolite-UF	12.73	103.0505	2213588	Cycloxydim	11.21	326.1800	6585
Methamidophos	12.75	142.0861	2277218	TEPP	5.4	291.0753	6582
Nicotine	12.82	110.0602	2312606	Flephedrone	7.56	182.0967	6461
Aminopyralid	12.83	104.0709	2654813	Pyridaben	7.34	365.1464	6427
Propylene Thiourea	8.75	222.1124	2810734	Tilidine	12.06	274.1794	6176
Acephate	8.75	222.1124	2810734	Atorvastatin	6.71	559.2606	6010
Acephate_M-C2H2N	8.75	222.1124	2810734	Coniine	12.85	128.1434	6004
Acetamiprid-metabolite-IM-1-4	12.91	138.0550	2927997	Fenamiphos	12.06	304.1145	5977
Dalapon	12.26	100.0396	3030845	Phorate-Oxon-Sulfoxide	11.83	261.0370	5972
Kojic-Acid	12.61	113.0347	3298604	Tiocarbazil	9.72	280.1740	5741
Maleic Hydrazide	12.61	113.0347	3298604	Norfluvoxamine	10.95	305.1484	5702
Ethylenethiourea	7.42	417.2588	3339050	Lacidipine	8.6	456.2366	5682
Benzophenone	0.07	243.0633	3451241	Propiconazole	6.78	342.0755	5640

Florfenicol Amine	7.41	453.2091	3516583	Amicarbazone	12.23	242.1610	5616
Glutamic Acid	12.77	152.0706	4040864	Detomidine	6.29	187.1225	5606
Acamprosate	12.77	152.0706	4040864	THC	12.96	315.2312	5601
Cysteine	12.77	152.0706	4040864	Cannabidiol	12.96	315.2312	5601
Homocysteine	12.79	158.1173	4089247	Clenpenterol	11.49	291.1012	5592
Norepinephrine	0.66	156.0767	4439096	Allopurinol	0.8	137.0457	5440
Tobramycin	10.53	167.0704	5176181	Thiophanate	5.96	371.0832	5312
PFBA	0.74	148.0604	5253866	EPTC	6.79	190.1269	5158
Ecgonine	10.92	306.2426	6369616	Quinoxyfen	5.07	308.0025	4942
Epinephrine	8.36	199.0964	6449735	Norflurazon-desmethyl	5.51	290.0291	4789
Kanamycin	12.96	166.0864	6491111	Furathiocarb	5.19	383.1653	4720
Metformin	12.96	166.0864	6491111	Anabasine	0.74	163.1228	4706
Ribavirin	12.98	132.1019	6871421	Nicotine	0.74	163.1228	4706
Metronidazole-OH	10.52	107.0493	8367142	Thiencarbazone-methyl	5.1	391.0378	4692
Nivalenol_M+CH3OO	7.65	296.1438	8640513	Minaprine	8.24	299.1865	4666
Nivalenol_M+HCOO	12.37	171.0655	9965672	Isoxaflutole	5.1	360.0508	4641
Netilmicin	11.12	170.0964	10121042	Chlorprothixene	5.87	316.0907	4493
Clopyralid	11.12	170.0964	10121042	Cimetidine	11	253.1221	4457
Hymexazol	12.86	194.1178	10366572	2-NP-SEM	10.25	209.0660	4430
Nithiazine	12.86	194.1178	10366572	Methacrifos_M-CH3O	5.67	209.0025	4374
Acetaminophen	12.86	194.1178	10366572	Medazepam	8.09	271.1001	3455
Acetaminophen-D4	12.86	194.1178	10366572	Demeton-S-Methyl-Sulfone	4.8	263.0166	2143
Oxamyl-oxime	12.86	194.1178	10366572	Demeton-S-sulfone	4.8	263.0166	2143
Formetanate	12.86	194.1178	10366572				
Omethoate	0.75	224.1280	10523591				
Pymetrozine	0.05	199.1802	13535076				
Anhydroecgonine	12.3	109.0650	15650824				
Aminocarb	7.8	195.0651	25693916				
Aldicarb-sulfoxide	12	279.1588	41408591				
Aldicarb-sulfoxide_M-C2H4NO2	12	279.1588	41408591				
Asulam	0.77	123.0918	53350236				

Dinotefuran	7.41	437.2351	74081667				
Isoniazide	7.12	393.2089	91348854				
Piracetam	7.12	393.2089	91348854				
Thiamine	7.65	476.3062	93525319				
Imidacloprid,desnitro	0.03	391.2837	113460866				

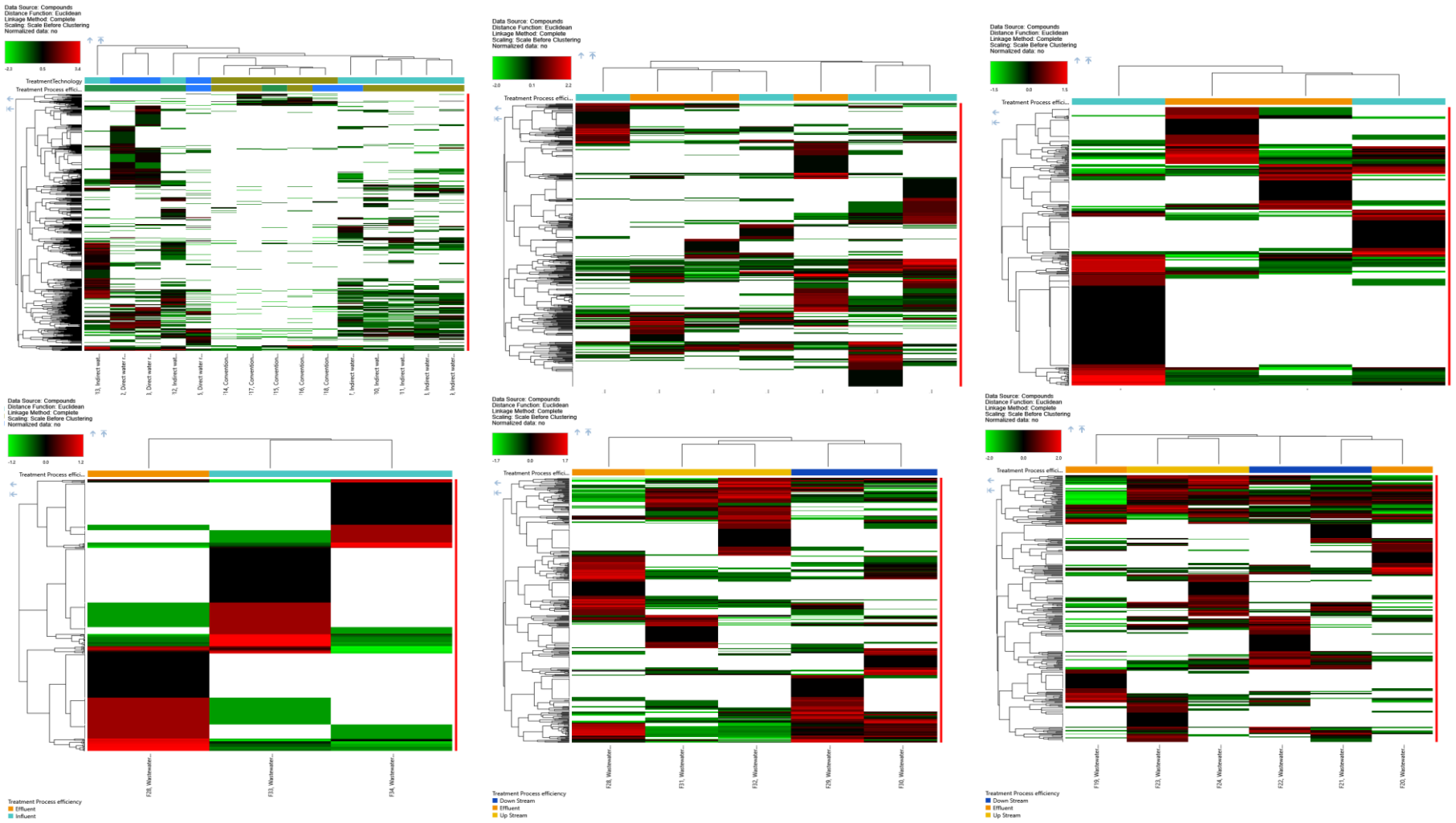

Figure A1: Hierarchical Cluster plots of three-source waters from conventional, indirect, and direct reuse treatment technologies.

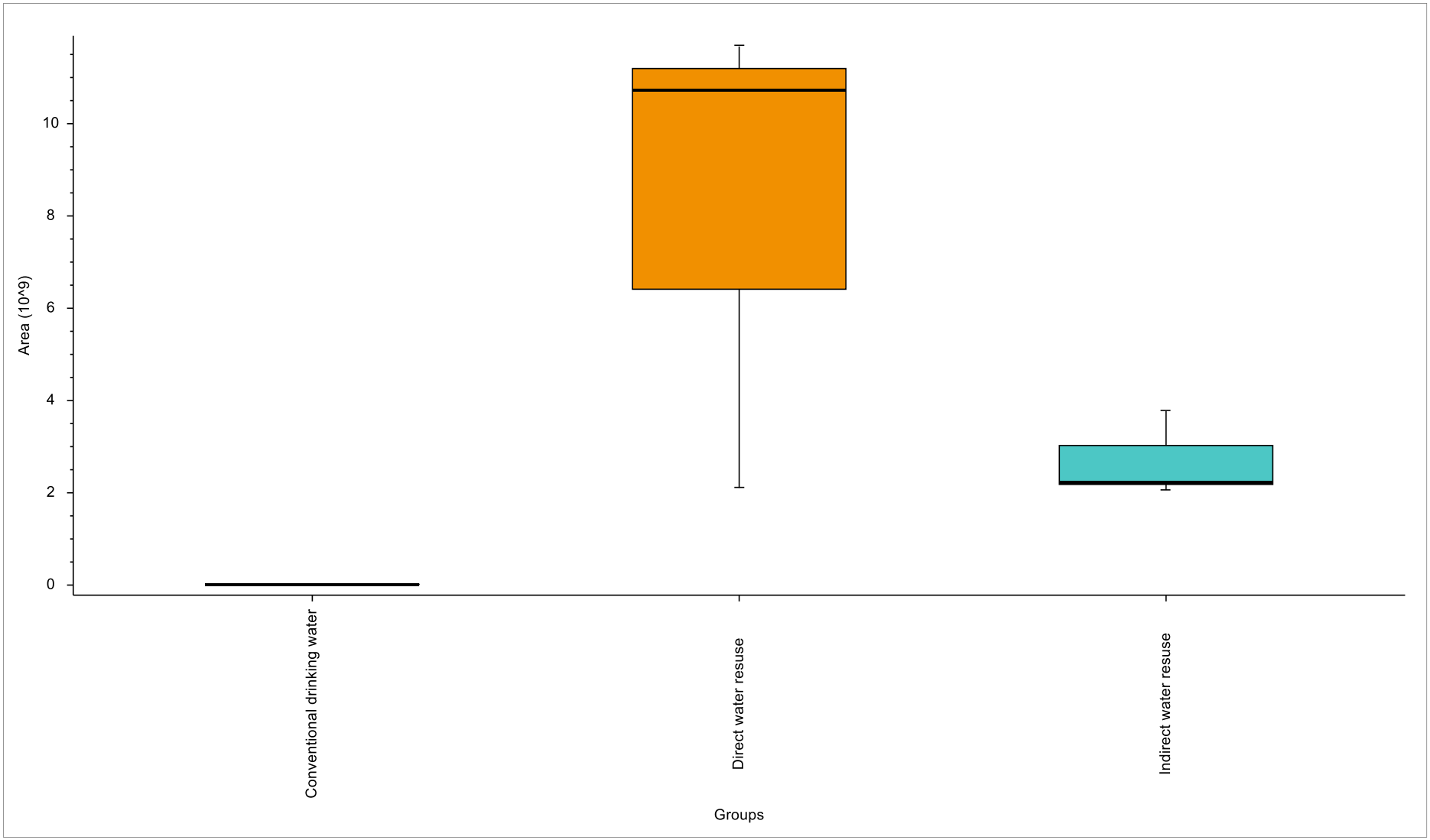

Figure A2 Shows the whisker box plot illustrating the distribution of compound levels across the potable treatment plants

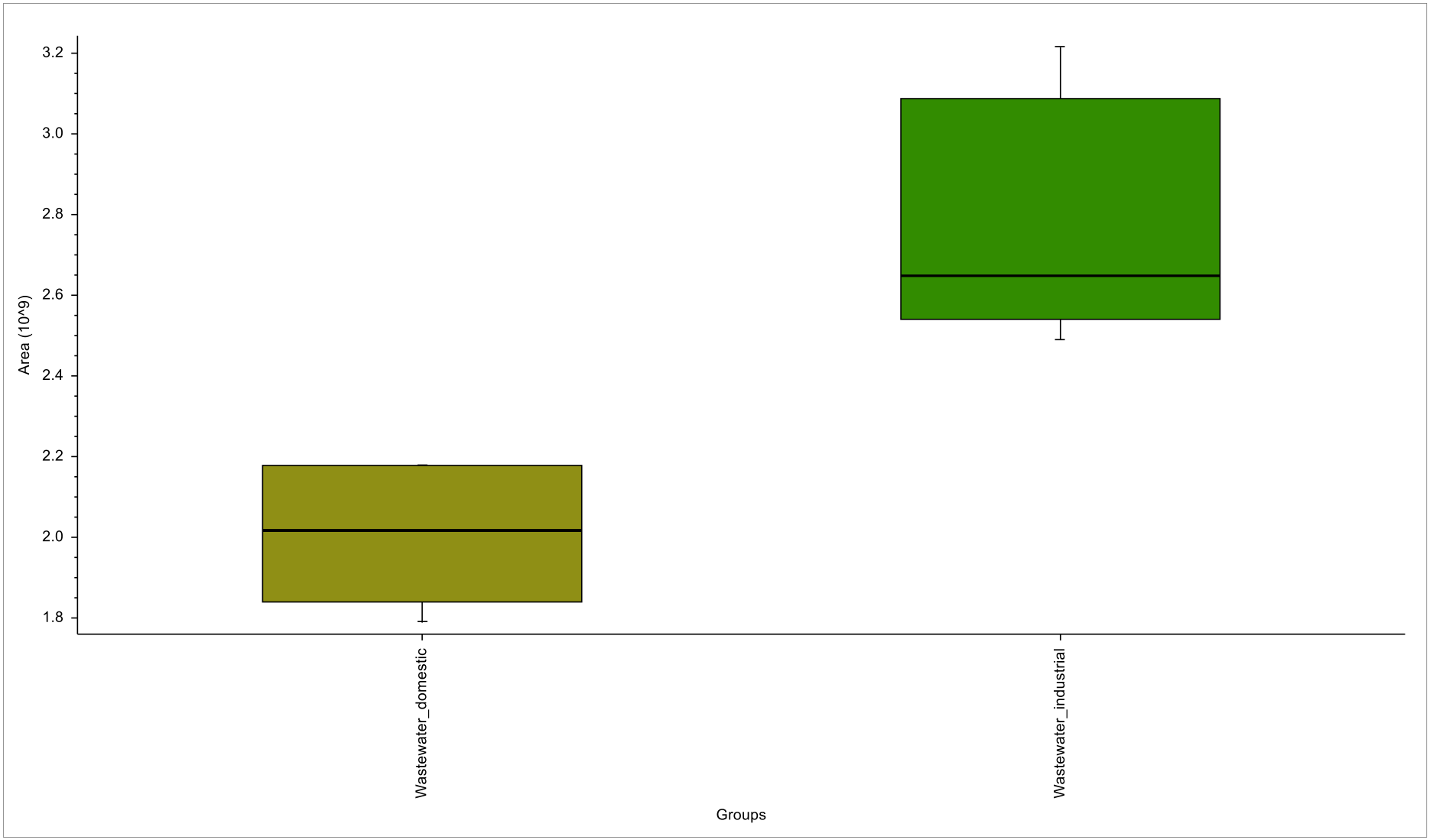

Figure A3 Shows the whisker box plot illustrating the distribution of compound levels across the wastewater treatment works