THE ESTABLISHMENT OF A KNOWLEDGE HUB FOR CONTAMINANTS OF EMERGING CONCERN IN SOUTH AFRICAN WATER RESOURCES

Volume 1

Report to the
Water Research Commission

by

TL Botha[1,2], A Roopnarain[3], Z Ncube[3], G de Nysschen[3], B Ndaba[3], N Mokgalaka[4,5], M Bello-Akinosho[6], E Bamuza-Pemu[7], R Adeleke[8], A Mushwana[3], M van der Laan[3,9], P Mphahlele[3,5] and F Vilakazi[3,8]

[1]Department of Zoology, University of Johannesburg
[2]Water Research Group, Unit for Environmental Sciences and Management, North-West University
[3]Agricultural Research Council (ARC) – Natural Resources and Engineering
[4]University of Pretoria, Mamelodi Campus
[5]Tshwane University of Technology, Faculty of Science, Department of Chemistry
[6]Pathogenic Yeast Research Group, Department of Microbiology and Biochemistry Faculty of Natural and Agricultural Sciences, University of the Free State
[7]OptimalEnviro
[8]Unit for Environmental Sciences and Management, North-West University
[9]Department of Plant and Soil Sciences, University of Pretoria

WRC Report No. 3105/1/23
ISBN 978-0-6392-0562-5

December 2023

Obtainable from
Water Research Commission
Lynnwood Bridge Office Park, Bloukrans Building
4 Daventry Street
Lynnwood Manor
PRETORIA

orders@wrc.org.za or download from www.wrc.org.za

The publication of this report emanates from a project entitled *The Establishment of a Knowledge Hub for Contaminants of Emerging Concern in South African Water Resources* (WRC Project No. C2021/2022-00256)

This report forms part of a set of two reports. The other report is *The Establishment of a Knowledge Hub for Contaminants of Emerging Concern in South African Water Resources. Volume 2* (WRC Report No. 3105/2/23)

EXECUTIVE SUMMARY

BACKGROUND

The present Target Water Quality Guidelines only cover known contaminants; however, water professionals are already discovering novel pollutants in our water bodies that were previously at levels below detection limits. Some of these compounds are categorized as "emerging" pollutants or contaminants since they are not typically included on the list of pollutants that are monitored and regulated. These substances could have an adverse effect on the environment and human health. Examples of these include nanomaterials, flame retardants, microplastics, agricultural waste, microbial pollutants, heavy metals, and personal care products. Further environmental concerns could result from the prolonged, unregulated usage of these items. Emerging contaminants are discharged into the environment by a variety of human activities, and industrial effluent discharges. Some of these pollutants may well be mutagens, carcinogens, endocrine disruptors, or detrimental to the reproductive system. They may even persist in the environment and bioaccumulate. These suggest that the classification of emerging contaminants is neither uniform or complete, and that many of them may broadly fit into more than one classification type. A proper classification of the contaminant would only be possible with a greater comprehension of its makeup and toxicity.

AIMS

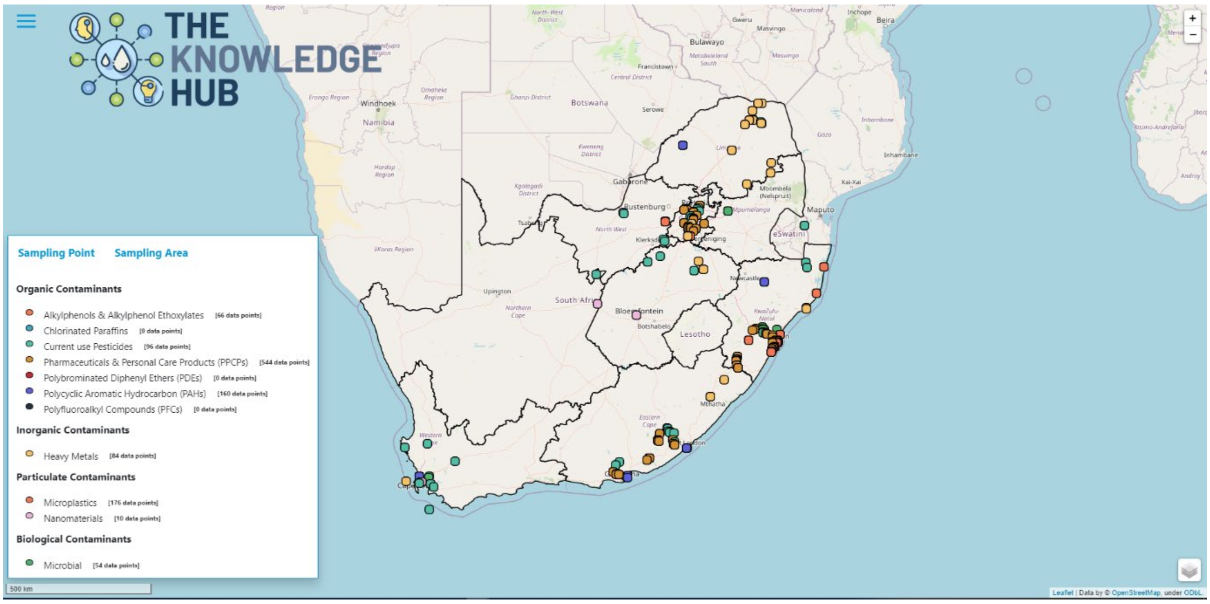
We may significantly improve research efforts by allowing for research collaborations between scientists in the same discipline by collecting research data. This would help uncover knowledge gaps and reduce the likelihood of duplication of research efforts. The creation of an interactive knowledge hub with databases for comprehensive information on growing pollutants of concern in South African surface water sources was the project's primary goal. Additionally, it sought to develop a platform for citizen science that would have fact sheets and brief videos that were supported by scientific evidence.

METHODOLOGY

The application developed can be found at https://www.ceckh.agric.za. The entire design was based on a web GIS (spatial data viewer) system that consists of a geodatabase, a map server, and a web viewer. Regular site visitors can view printable information sheets regarding Contaminants of Emerging Concern (CEC), as well as information on how to avoid CEC contamination and identify a lab for specialized CEC analyses. It is a web-based system with different modules that researchers use to upload specific information regarding CECs. This data is then processed and uploaded to a PostgreSQL instance running PostGIS extension and sent to an internal inbox for further approval by researchers. Once approved internally, the data is then served to the public as a map after being processed in the GeoServer. The Python script that is used to replicate this data from one DBMS to another also performs secondary quality checks (formatting and referencing) on the data before it is loaded into PostgreSQL as the data transfers from the MySQL instance to the PostgreSQL instance. Other considerations included making sure that only open-source software was used to build the entire system. No proprietary software or licenses would be necessary, making maintenance less expensive. Anyone with coding skills could easily develop it, and it would be simple to use for anyone with basic computer knowledge.

RESULTS AND DISCUSSION

The CEC Knowledge Hub's most recent update (March 2023) has drawn attention to knowledge gaps, including those in certain regions like the Northern Cape where no CEC data have been published. With the exception of the Free State, all provinces have been found to contain organic pollutants. Currently, only Limpopo, Mpumalanga, and KwaZulu-Natal have documented microbiological CECs. The majority of the provinces in South Africa have microplastic statistical data. Currently, there are 1190 data inputs in the compiled dataset, with 544 of them coming from pharmaceutical and personal care products, followed by 176 from microplastics, and the remaining inputs for CECs ranging between 54 and 160, with nanomaterials having the fewest at only five.



GENERAL CONCLUSIONS & RECOMMENDATIONS

A digital specimen bank of collected pollution data in South Africa has been established by the creation of a CEC Knowledge Hub. Even though the data already indicates where the majority of research has been done and areas of concern have been highlighted in South Africa, its strength will grow as more information is uploaded to the Hub. We anticipate that the Hub will be used more frequently in disciplines relevant to CECs in the environment as it becomes more populated as a first stop shop for CEC research efforts. Responsible scientific communication is vital and due to seasonal variations in data and probable limitations in the detection methods used, skilled researchers are required to interpret and understand the information collected from the hub.

To develop a categorization that is accurate and anchored in a high level of science, the toxicological evaluation is a significant undertaking that necessitates collaboration among numerous stakeholders. A proposed brief strategy for this project undertaking is included in the hub's current volume and is based on ongoing emerging research, which is currently being pursued internationally. This would class risk quotients into low, moderate and high risk by using measured or predicted concentrations to monitoring trigger values of CECs detected in aquatic ecosystems. Once the toxicology classing has been included, we will have a powerful tool to address emerging issues in water quality and is a major recommendation for future development of this CEC Knowledge Hub of which provisions for the inclusion have been made by adding an additional layer to the mapping points.

To our knowledge, neither South Africa nor the Southern African Development Community (SADC) have an interactive knowledge hub for CECs. It is advised that the SADC region, which regularly shares aquatic ecosystems, expand and create a regional knowledge hub to enhance regional data output and environmental monitoring campaigns.

AKNOWLEDGEMENTS

- The Water Research Commission for financially supporting this research (WRC Project No. C2021/2022-00256).
- The Agricultural Research Council's Professional Development Programme (PDP) for supporting student interviews.
- Special thanks to Reference Committee Members who attended the Inaugural Meeting:

Full Name	Affiliation
Dr Eunice Ubomba-Jaswa	Water Research Commission – Research Manager
Ms Penny Jaca	Water Research Commission – Project Coordinator
Dr Nonhlanhla Kalebaila	Water Research Commission
Mr Stanley Nzama	Department of Water and Sanitation
Ms Tovhowani Nyamande	Department of Water & Sanitation
Mr Elijah Mogakabe	Department of Water and Sanitation
Mr Obed Baloyi	Department of Environmental Affairs
Ms Brenda Maphanga	Department of Environmental Affairs
Prof. Beatrice Opeolu	Cape Peninsula University of Technology
Prof. Jonathan Okonkwo	Tshwane University of Technology
Prof. Rialet Pieters	North-West University
Dr Edward Archer	Stellenbosch University
Mr Khangwelo KT. Rathogwa	Agricultural Research Council-Intellectual Property Unit
Dr Natalie Aneck-Hahn	University of Pretoria-Environmental Chemical Pollution
Ms Leanne Coetzee	Waterlab (Pty) Ltd
Ms Bettina Genthe	Private Consultant

CONTENTS

LIST OF FIGURES

LIST OF TABLES

ACRONYMS & ABBREVIATIONS

AP	Alkylphenols
APE	Alkylphenol Ethoxylates
AREC	Animal Research Ethics Committee
CEC	Contaminants of Emerging Concern
CP	Chlorinated Paraffin
CRM	Certified Reference Materials
DBP	Drinking Water Disinfection By-Products
DOI	Digital Object Identifier
EDC	Endocrine Disruptive Chemicals
EDS	Energy Dispersive x-ray Spectrometer
ENM	Engineered Nanomaterials
EP	Emerging Pollutants
FET	Fish Embryo Test
FT-IR	Fourier Transform Infrared Spectroscopy
GC-MS	Gas Chromatography – Mass Spectrometry
GHS	Globally Harmonized System
ICP-MS	Inductively Coupled Plasma – Mass Spectrometer
ICT	Information and Communications Technology
IT	Information Technology
KH	Knowledge Hub
KH DB	Knowledge Hub Database
LC50	Lowest concentration calculated to cause 50% of lethality
MP	Microplastics
OECD	Organisation for Economic Co-Operation and Development
PAH	Polycyclic Aromatic Hydrocarbon
PBDE	Polybrominated Diphenyl Ethers
PCB	Polychlorinated Biphenyls
PFOS	Perfluoroctane Sulfonate
PPCP	Pharmaceuticals and Personal Care Products
RQ	Risk Quotients
SEM	Scanning Electron Microscope
SPE	Solid Phase Extraction
TDS	Total Dissolved Solids
TEM	Transmission Electron Microscope
TSS	Total Suspended Solids
URL	Uniform Resource Locator
VOC	Volatile Organic Compounds

This page was intentionally left blank

CHAPTER 1: BACKGROUND

1.1. INTRODUCTION

Numerous compounds of various classes are now produced as a result of rapid population increase, urbanization, and industrialization and new ones are introduced on a daily basis. Unfortunately, our water bodies serve as an ultimate sink for most of these products and their degradates through various pathways with very serious adverse effects on ecological integrity and human health. Due to the fact that some of these substances are not on the typical list of pollutants that are monitored and regulated, they are classified as "emerging" pollutants or contaminants. Due to their great potential to enter the environment and widespread distribution throughout environmental matrices, these substances may have detrimental ecological and/or health effects on humans. (Necibi et. al., 2021; Daughton, 2005, Gavrilescu et. al., 2015). Some believe that “emerging pollutants” or “emerging contaminants” can be better described as “contaminants of emerging concern” (Sauvé and Desrosiers, 2014). Emerging pollutants are not just chemical pollutants; anthropogenic activities also cause water resources to become contaminated with biological micropollutants (bacteria and viruses). Waterborne diseases continue to be a leading cause of death worldwide and some of these are potentially pathogenic (Gavrilescu et. al., 2015) especially in developing and underdeveloped nations where there is a shortage of basic sanitation and potable water. Complicating matters is the fact that due to these compounds' chemical structural stability, traditional wastewater or drinking water treatment facilities are typically not suited to remove them. Furthermore, many of the microbial species used in the treatment train are sensitive to these chemicals (Gavrilescu et. al., 2015). Living systems have developed protective, defensive, or adaptive mechanisms for minimizing toxicity and exposure to many of the otherwise harmful, naturally occurring chemicals. The defence mechanisms of biological systems are occasionally insufficient for substances of developing concern that they have never been exposed to. (Daughton, 2005). There is an exceedingly significant variability in the quantities, complexity, and toxicities of emerging compounds in the environment (Daughton, 2005, Gavrilescu et. al., 2015) and pose problems for regulatory bodies (Sauvé and Desrosiers, 2014). Emerging contaminants are discharged into the environment by a variety of human activities, including agricultural practices, pharmaceutical and personal care product (PPCP) production, and industrial effluent discharges. Some of these pollutants may be endocrine disruptors, carcinogens, mutagens, or disruptive to reproductive systems. They may also bioaccumulate and/or persist in the environment. Based on these, emerging contaminants are not universally or fully categorized, and many of them may fall broadly into more than one classification type. Only with a deeper understanding of the nature and toxicity of the pollutant would a proper classification of that pollutant be achievable.

South Africa is a semi-arid country with unpredictable rainfall pattern having an average rainfall of 52% of the global average (DWAF, 1996). South Africa stands out as one of the most water scarce countries in the southern Africa region – a region that is considered the second region in the world to be confronted by a debilitating water deficit (Turton, 2000). As a consequence of its unpredictable rainfall pattern South Africa sometimes is faced with serious droughts, the most recent being in 2016. Reports from sources within the Department of Water and Sanitation (DWS) in South Africa indicate that the current water use practices in the country will not be sustainable beyond 2026 (DWAF, 1999). South Africa has no surplus water, and this would place some constrain on future economic growth and development. About 63% of water in South Africa is consumed by the agricultural sector and farmers will have to double their water use by 2050 if they are to meet growing food demands using current farming practices. Protecting South Africa's water resources safe is a task that is key to realising the vision and achieving the mission of both DWS and the UN Millennium Development Target 10 of Goal 7. Both of these goals rely on sufficient and high-quality water sources, and the water's quality ultimately determines whether it is suitable for a given end use. Both of these goals rely on sufficient and high-quality water sources, and the water's quality ultimately determines whether it is suitable for a given end use. The term water quality describes the physical, chemical, biological and aesthetic properties of water that determine its fitness for a variety of uses and for the protection of aquatic ecosystems. Many of these properties are controlled or influenced by constituents which are either dissolved or suspended in water (DWAF, 1996). It is appropriately stated in the National Water Act that “Recognizing that the protection of the quality of water resources is necessary to ensure sustainability of the nation’s water resources in the interest of all water users” (NWA, 1998). The negative impact of technological advancement to the water industry is the presence of contaminants of emerging concern in surface water resources. The current and future challenge is contaminant containment as well as reduction of their occurrence in water resources. To achieve these a better understanding of their nature, concentrations, fate in the environment and their toxic effects on organisms is required in order to adopt better management programs to minimize the risks to human health and the environment. The United States of America Environmental Protection Agency (US EPA) has 121 organic pollutants (US EPA, 2014) in its list of priority pollutants and the European Union (EU) has 45 organic compounds in its priority pollutants watch list (Carvalho et. al., 2015). Both lists are continuously being reviewed, and the inclusion of further compounds is being investigated. On the other hand, the South African Water Quality Guidelines (SAWQ) included only atrazine, phenol, and trihalomethanes (DWAF, 1996) as organic pollutants of concern. This indicates that presence of emerging chemical pollutants in our water resources and the danger they pose is unrecognized and/or grossly underestimated especially in light of the poor state of wastewater treatment facilities in South Africa and heavy agricultural activities in the country. The efficiency of municipal wastewater treatment is vital to the reduction of chemical pollutants in water as a number of these compounds emanate from domestic wastes that are channelled to wastewater treatment plants. Wastewater treatment facilities nationally are assessed by the Green Drop System (GDS) used to evaluate the entire value chain involved in the delivery of municipal wastewater services. The Green Drop assessment of the municipal wastewater treatment sector reveals the low compliance levels of Municipalities with the respective effluent quality standards. The Municipal wastewater treatment plants (WWTPs) are currently considered to be in an unacceptable state (DWS, 2022). The national average compliance figures in the past 12 months (July 2017-June 2018) is disturbing with a national average chemical compliance of 37.98% (Municipal Works), 34.12% (Public Works) and 3.8% (Private Works). Individual province scores ranged from very low scores of 1.46% to 61.08%. A total of 7 out of 9 provinces scored below 50%, with only 2 provinces (Western Cape (61.08%) and Gauteng (59.60%)) with compliance score above 50% (DWS, 2018). This is a far cry from the expected 80% minimum compliance. The low compliance levels is an indication of a high possibility of chemical pollutants of emerging concern passing through the treatment process and ultimately get discharged into surface water. South Africa's Constitution and Bill of Rights enshrine the basic human right to have access to sufficient water and a safe and healthy environment. Government fulfils these rights through the DWS assisted by several legislation including the National Water Act (NWA, 1998), the Water Service Act, 1997 (Act 108 of 1997), the Water Service Act, 1997 and more recently the National Water resource Strategy (NWRS2). The security of the water supply, environmental deterioration, and resource pollution are all addressed in the NWRS2, which also lays out the vision and strategic actions for effective water management. A database of pollutants found in South African water resources would serve as a central information hub, providing quick access to all known study results and details on pollutants that have been identified. The pollutants would be listed, along with all relevant scientific data, their prevalence, and their toxicity. There is currently no comprehensive database of data on contaminants in water resources in Africa. As a result, information about studies on CECs is not easily accessible, and it is challenging to pinpoint knowledge gaps as they emerge. This can sometimes result in duplicated research efforts and a delay in responding to pollution crises wherever they happen. Hence the need for a database containing information from all studies on CECs in waterways. While in the long run, there is opportunity for the database to grow to include information about the entire continent of Africa rather than just South Africa.

1.2 PROJECT AIMS

The main objective of the project is the establishment of an interactive knowledge hub with databases for all-inclusive information on emerging contaminants of concern in South Africa surface water sources. Six aims have been identified to achieve this objective. These include:

1.2.1 Assessment and collation of research conducted on emerging contaminants of concern in South African water resources

1.2.2 Compilation of identified emerging contaminants of concern in water, their occurrence including hotspots and their distribution in catchment areas in South Africa

1.2.3 Collation of available data on emerging contaminants of concern in South African Water Resources – analytical methods of identification

1.2.4 Compilation of possible correlations and seasonal variations of CECs in South African water resources

1.2.5 Identification of knowledge gaps

1.2.6 Establishment of an interactive knowledge hub with databases for all-inclusive information on emerging contaminants of concern in South Africa surface water sources

1.3 SCOPE AND LIMITATIONS

The main scope of the study was to create an interactive map with databases for emerging contaminants of concern in South Africa surface water sources and excluded marine water, estuarine and ground water. The aim would be supported by additional information related to collated data including site information, instrumentation used, and concentrations detected in the environment. This would allow for the identification of hotspots and areas of concern. A limitation of this study was the ability to include the toxicological information for the detected CECs present within the hub. A categorization strategy was established in the study based on Sutton et al. (2022) who performed risk assessment funded by the US EPA.

1.4 SUMMARY OF WORK TO DATE

The work conducted to date was separated into several phases as outlined below:

- Phase 1: Project planning – including recruitment of postgraduate research students (one doctoral, and one Master's student) and an intern (Computer Science/IT)
- Phase 2: Literature survey – Assessment and collation of research conducted on emerging contaminants of concern in South African water resources.
- Phase 3: Website/Database design including logo design and design of several layers within the database targeted at citizen, stakeholder and individuals in the agricultural sector. Compilation of identified emerging contaminants of concern in water, their occurrence including hotspots and their distribution in catchment areas in South Africa in a user-friendly online database.
- Phase 4: Inclusion of analytical methods of identification and levels of CECs in waterways. Initiation of a study to establish the fate of selected CECs and persistence. Testing of website/database.
- Phase 5: Population of interactive knowledge hub and database, retesting and restructuring based on feedback from experts in the reference group.
- Phase 6: Validation of selected analytical methods and protocols for identification of CECs in South Africa. Identification of knowledge gaps.

- Phase 7: Update of interactive knowledge hub with databases for all-inclusive information on emerging contaminants of concern in South Africa surface water sources. Publicity drive of the knowledge hub.
- Phase 8: Report writing and preparation of scientific and popular articles for publication. Presentation of the knowledge hub at several workshops, scientific conferences, via. radio interviews and at scientific publicity events/ roadshows.

CHAPTER 2: KNOWLEDGE HUB ACHITECTURE

2.1 LOGO DESIGN

The incorporation of a logo design for the CEC KH was seen as an extremely important output due to the continued promotion and recognisability of the site. By designing a logo it will give the KH a distinguishable look and feel and the aim is to grow the KH as a brand of its own (Foroudi et al., 2017). A logo design can be literal or figurative and the concept was to include water and knowledge processes within them in the design. To this end, three logos were designed and one was selected based on Team member appeal, usability, versatility and a voting process.

The logo aims to combine contaminated and non-contaminated water sites and eludes to how we are looking through water in order to find the answer. The theme is based on a corporate identity and can be altered to include icons and infographics. These could be used in order to allow for versatility in communication, i.e. bombs (bad quality), eye (loading), fish (target organism), this could be done by altering the water icon shapes.

The option selected as the preferred candidate logo was due to its popularity (8/10 votes) and versatility within the front-end website design. The logo was also decided as it was simple to use and could be altered according to specific bounds to maintain the logo identity. Each nodule could be used in order link different aspects to the website (Figure 1).

The colours used within the design are a blend of all five institutions (WRC, ARC, TUT, Unisa and NWU) involved within the CEC KH and the incorporation of green and blue are meant to invoke a feeling of calm rather than a panic or stress response. The imaging used which illustrates signal to brain shows how intellect was applied to resources in water that leads to thought and action (light bulb). The full image is not meant to resemble any specific contaminant but rather all of them: chemicals, contaminants bound to plastic, nanomaterials with functional groups.

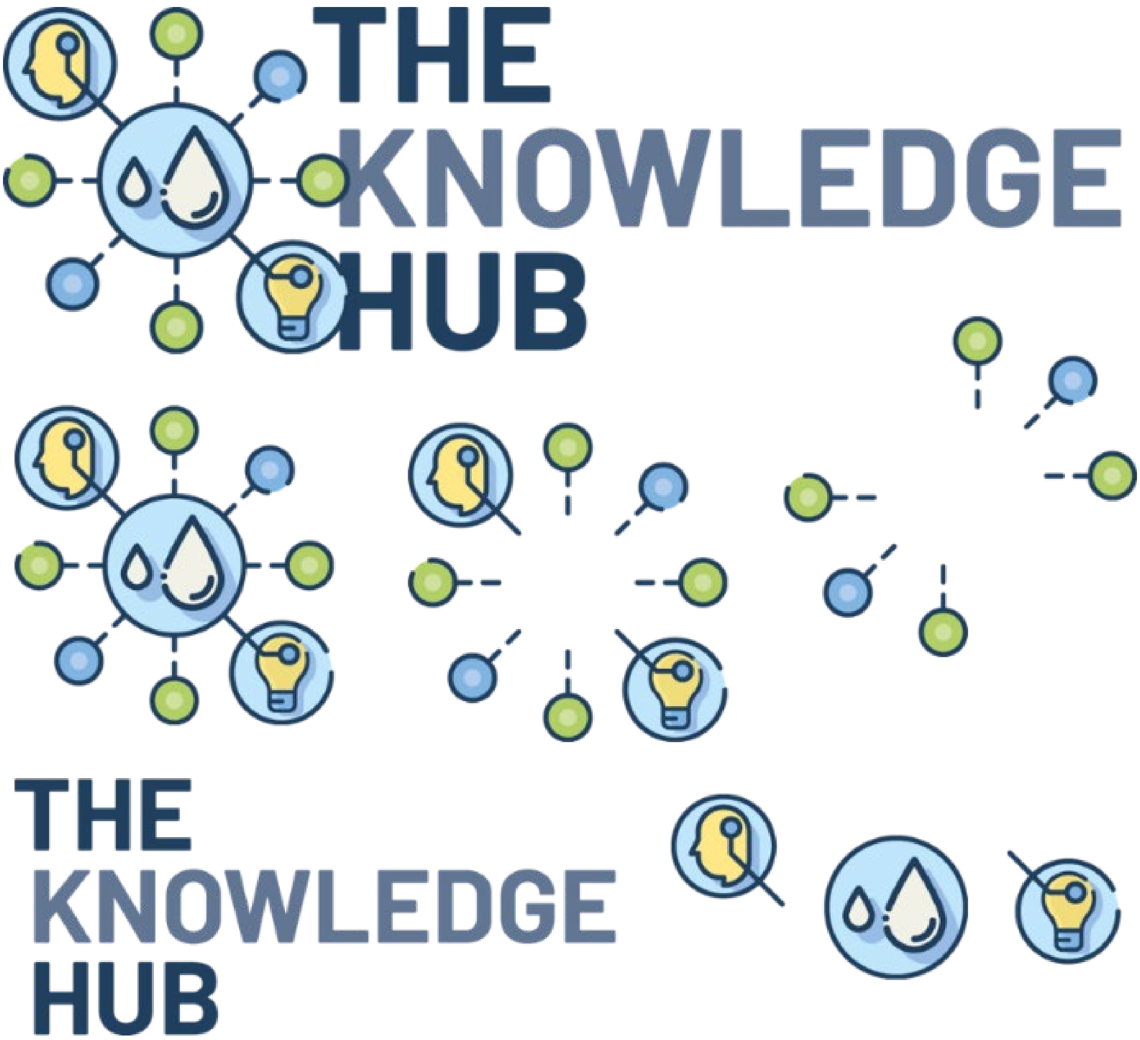


Figure 1: Selected logo design for the Contaminants of Emerging Concern Knowledge Hub

2.2 KNOWLEDGE HUB LAYOUT

The CEC KH domain was registered as www.ceckh.agric.za/ (Figure 1). The domain can be updated to a ".com" website at a later stage should this be necessary. The process was delayed by internal reviews at the ARC due to risks associated with potential cyber-attack and was only released at the end of June 2022. Now that this is approved the Team is allowed access off server. Security certificates are in the process of acquisition by ICT at the ARC, this will allow for the site to be accessed without the server being compromised.

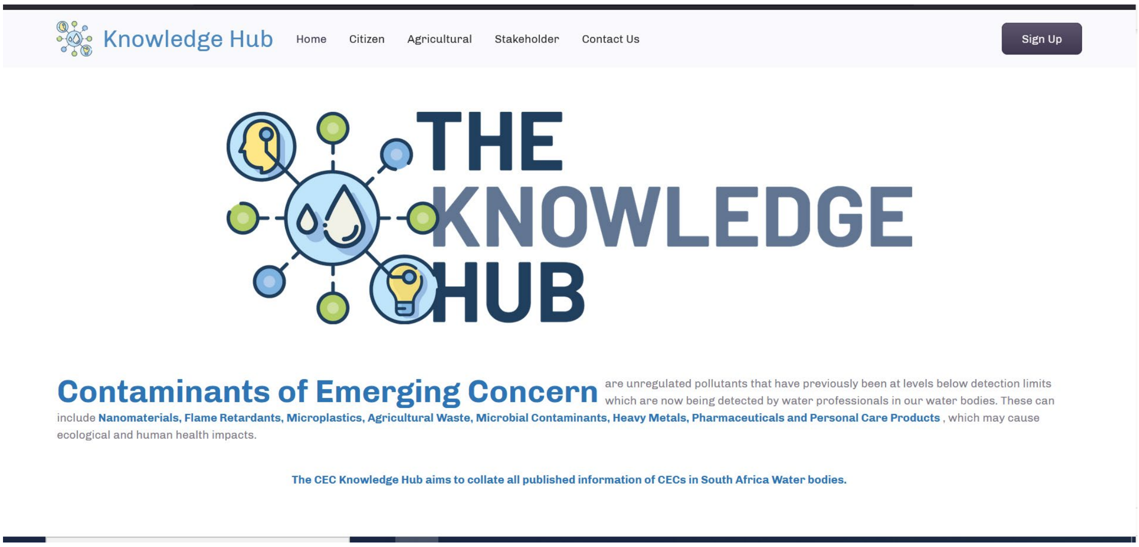


Figure 2: The new domain registered for the CEC Knowledge Hub

CITIZEN PAGE UPDATES

The citizen page has been updated to include a downloadable pdf document as well as a short video clip, approximately three minutes long, which describes each contaminant class and how they are able to enter the environment in layman's terms to ensure that it is understandable to anyone accessing the hub .

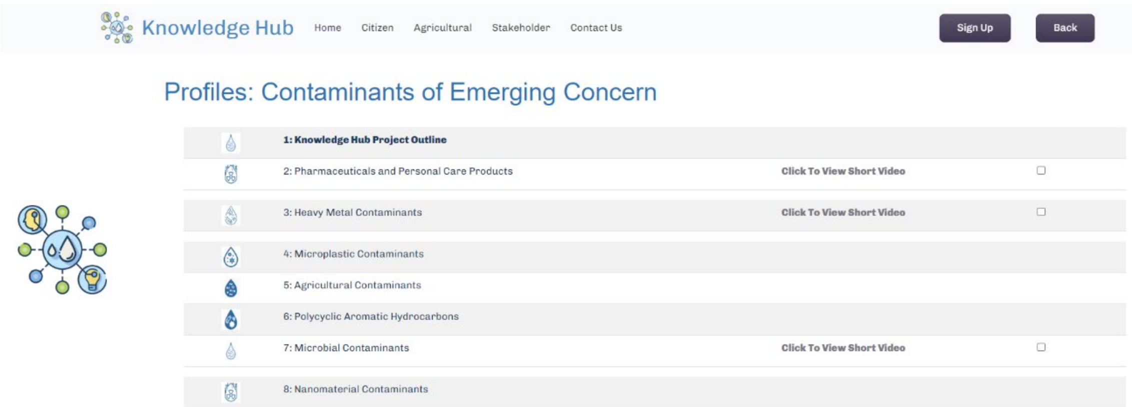


Figure 3: The Citizen page for the CEC Knowledge Hub

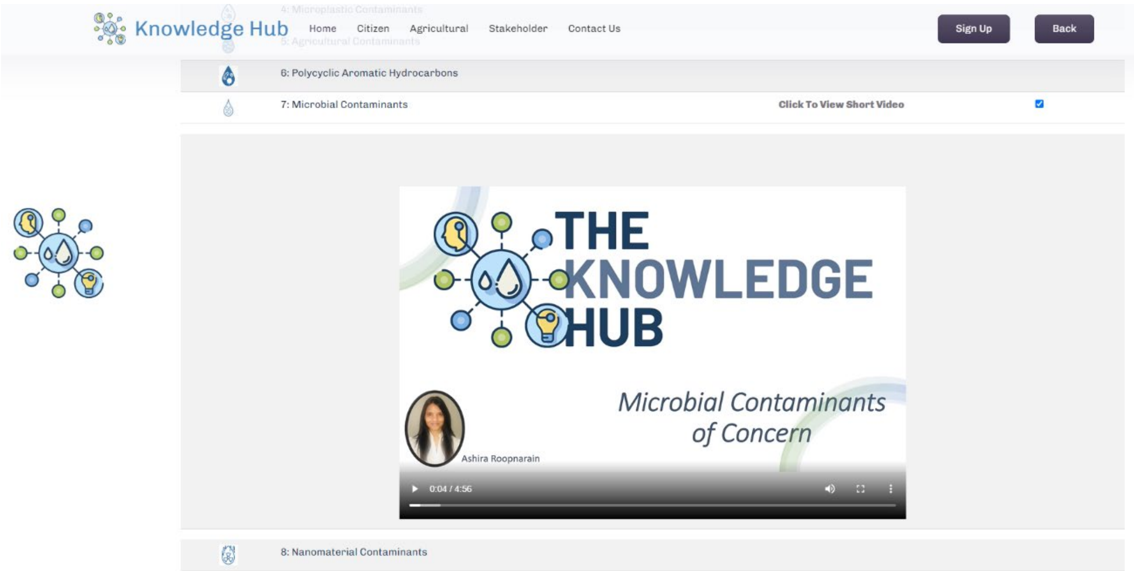


Figure 4: The Citizen page when clicked to show short video for the CEC Knowledge Hub

AGRICULTURAL PAGE UPDATES

The Agricultural Page has been finalized and focus was placed on *how* CECs enter the environment, *where* the potential input could come from and *when* they would be deposited into aquatic ecosystems. The page has been updated to reflect an agricultural scenario with various possible contaminant sources to be aware of, it also shows where soil or water samples should be collected. All media used was created in Canva pro. The idea is that this page could be expanded upon to reflect emerging issues, such as how poor water quality affects precision agriculture, which uses various sensors prior to dosing.

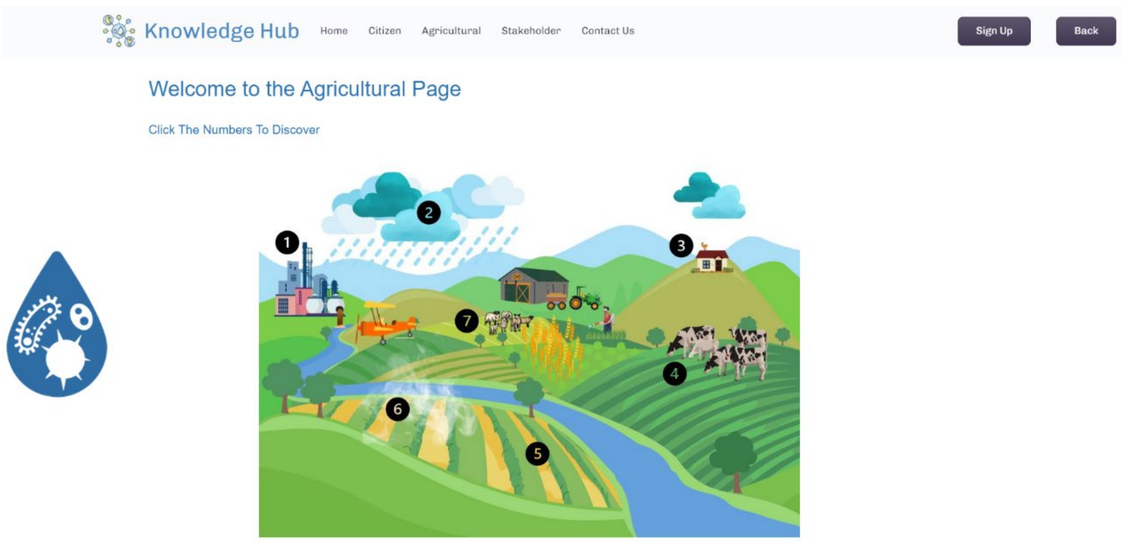


Figure 5: The landing page for the Agricultural page of the CEC Knowledge Hub

STAKEHOLDER PAGE UPDATES

The Stakeholder Page has been updated as suggested in the Reference group meetings. The data when imported now includes a DOI checker, which ensures no data duplication takes place. Where available CAS numbers are included per contaminant in the CEC Knowledge Hub. Bulk importing is possible to ensure minimal time is used to upload data and the data can be exported in an excel format for further processing by the user. The map interface remains unchanged but ICT is working on the best way to include the number count of contaminants per class within the HUB. Currently we have 590 data points, which are being updated by researchers within the project prior to the final reporting period, this will ensure that the report is not misrepresented by not including all available literature. The data search has therefore been expanded upon beyond SCOPUS to include other DHET accredited journals.

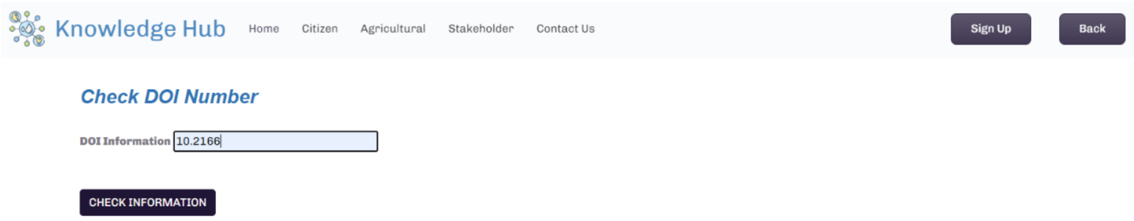
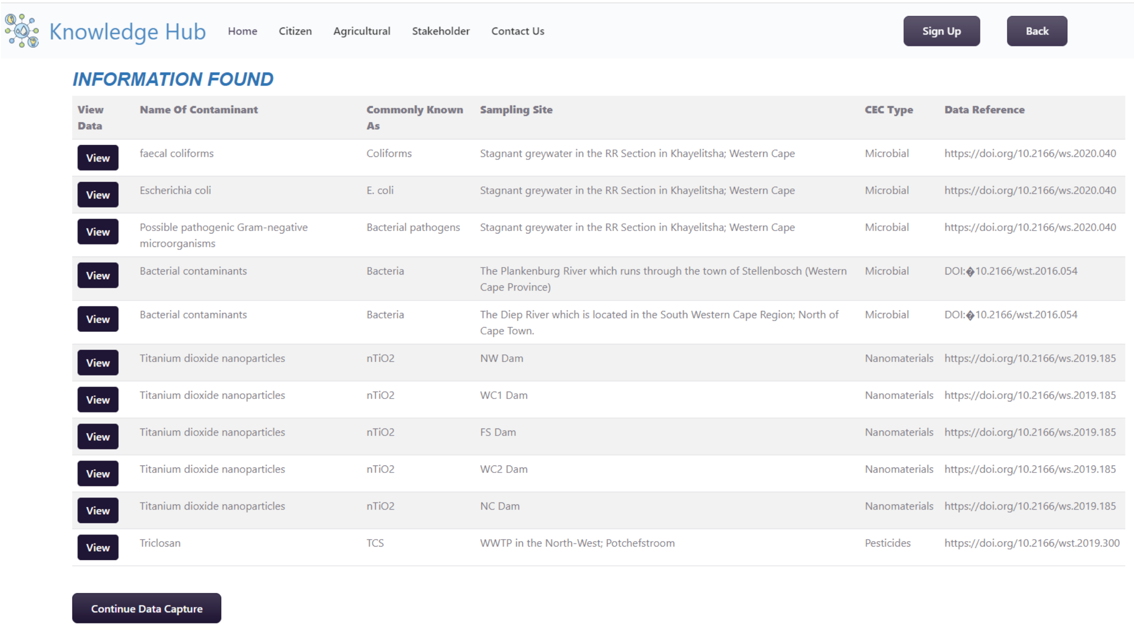


Figure 6: The DOI precheck in Stakeholder page of the CEC Knowledge Hub



View Data	Name Of Contaminant	Commonly Known As	Sampling Site	CEC Type	Data Reference
View	faecal coliforms	Coliforms	Stagnant greywater in the RR Section in Khayelitsha; Western Cape	Microbial	https://doi.org/10.2166/ws.2020.040
View	Escherichia coli	E. coli	Stagnant greywater in the RR Section in Khayelitsha; Western Cape	Microbial	https://doi.org/10.2166/ws.2020.040
View	Possible pathogenic Gram-negative microorganisms	Bacterial pathogens	Stagnant greywater in the RR Section in Khayelitsha; Western Cape	Microbial	https://doi.org/10.2166/ws.2020.040
View	Bacterial contaminants	Bacteria	The Plankenburg River which runs through the town of Stellenbosch (Western Cape Province)	Microbial	DOI:�10.2166/wst.2016.054
View	Bacterial contaminants	Bacteria	The Diep River which is located in the South Western Cape Region; North of Cape Town.	Microbial	DOI:�10.2166/wst.2016.054
View	Titanium dioxide nanoparticles	nTiO2	NW Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Titanium dioxide nanoparticles	nTiO2	WC1 Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Titanium dioxide nanoparticles	nTiO2	FS Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Titanium dioxide nanoparticles	nTiO2	WC2 Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Titanium dioxide nanoparticles	nTiO2	NC Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Triclosan	TCS	WWTP in the North-West; Potchefstroom	Pesticides	https://doi.org/10.2166/wst.2019.300

Figure 7: An example of the DOI precheck search results in Stakeholder page of the CEC Knowledge Hub

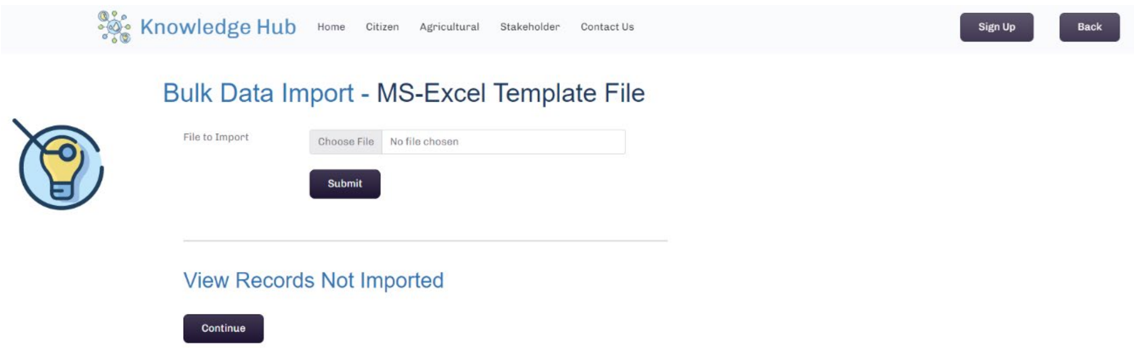


Figure 8: The bulk import function using the Excel template in the Stakeholder page of the CEC Knowledge Hub

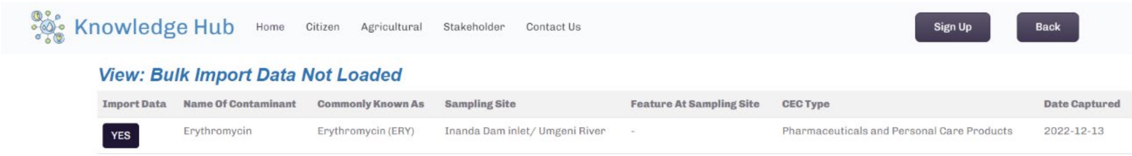


Figure 9a: The bulk import precheck function in the Stakeholder page of the CEC Knowledge Hub

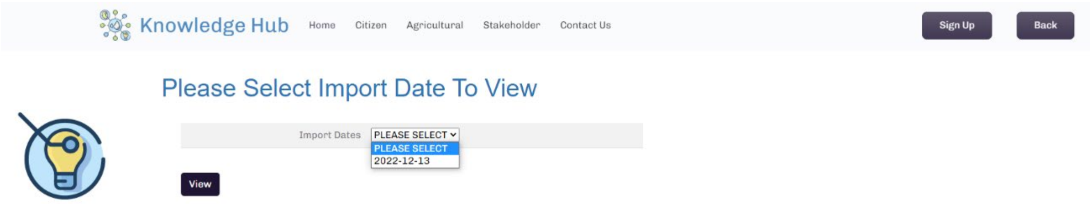


Figure 9b: The data export function in the Stakeholder page of the CEC Knowledge Hub

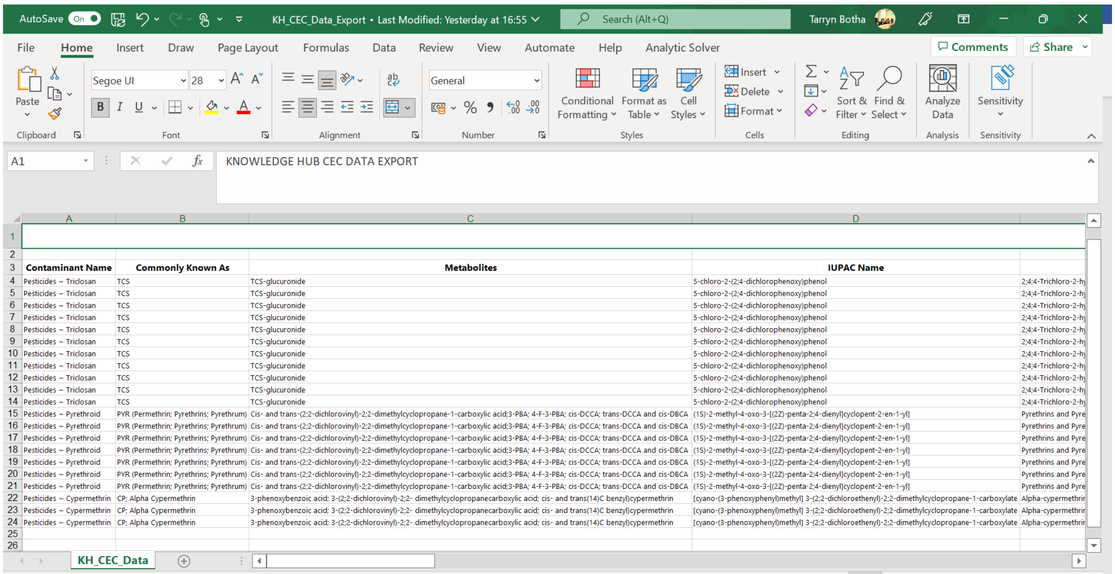


Figure 10: An example of the Excel template used for data export in the Stakeholder page of the CEC Knowledge Hub

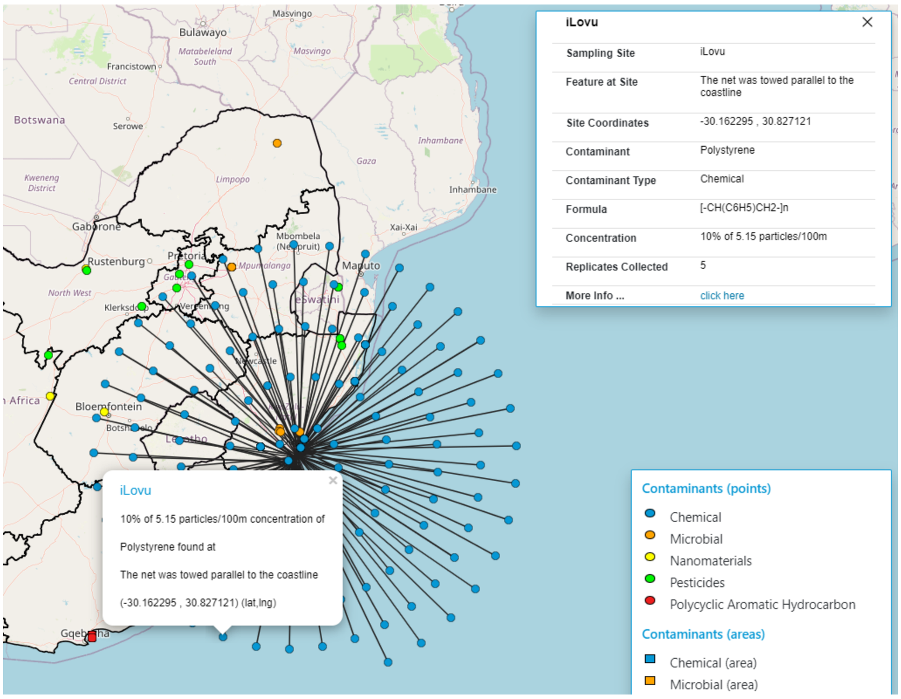


Figure 11: The final map of the data on the Stakeholder page of the CEC Knowledge Hub, legends will include the number of points per contaminant

2.3 APPLICATION DEVELOPMENT/KNOWLEDGE HUB FRAMEWORK

The framework of the knowledge hub is setup into three distinct areas.

1- Data Input
2- Data Processing
3- Visualization

The framework will stay the same but the underlying technologies used to make the system will be modified or changed when the system is built to its final version. The idea is to keep it as simple as possible whilst allowing scalability and modularity to allow the ease of plugging in or removing technologies as newer and better possibilities are considered or found.

Core technologies used here are

- HTML – HTML is the abbreviation for Hypertext Mark-up Language. It is the standard mark-up language for documents designed to be displayed in a web browser. It can be assisted by technologies such as Cascading Style Sheets (CSS) and scripting languages such as PHP or JavaScript
- CSS – CSS is the abbreviation for Cascading Style Sheets. It is a style sheet language used for describing the presentation of a document written in a mark-up language such as HTML. It is a cornerstone technology of the World Wide Web, alongside HTML and JavaScript.

- PHP – PHP is the abbreviation for Hypertext Pre-Processor. It is downloadable freeware software (http://www.php.net). It is a general-purpose scripting language especially suited to web development
- MySQL – MySQL 8 is the latest version of the open-source relational database management system and will be the primary DBMS used for the backend database. MySQL is especially suited for internet/cloud based systems such as the knowledge hub. [https://www.mysql.com/ accessed 2021]
- Python 3.8 – Python is a programming language that lets you work more quickly and integrate your systems more effectively. Its role in this project is mainly for systems integration.
- Windows server 2019 machine (which is a virtual machine on Microsoft Virtual Server)
- GeoServer 2.17 – GeoServer is an open source server for sharing geospatial data. Designed for interoperability, it publishes data from any major spatial data source using open standards [http://geoserver.org/ accessed 2021/01/05] (Figure 5).

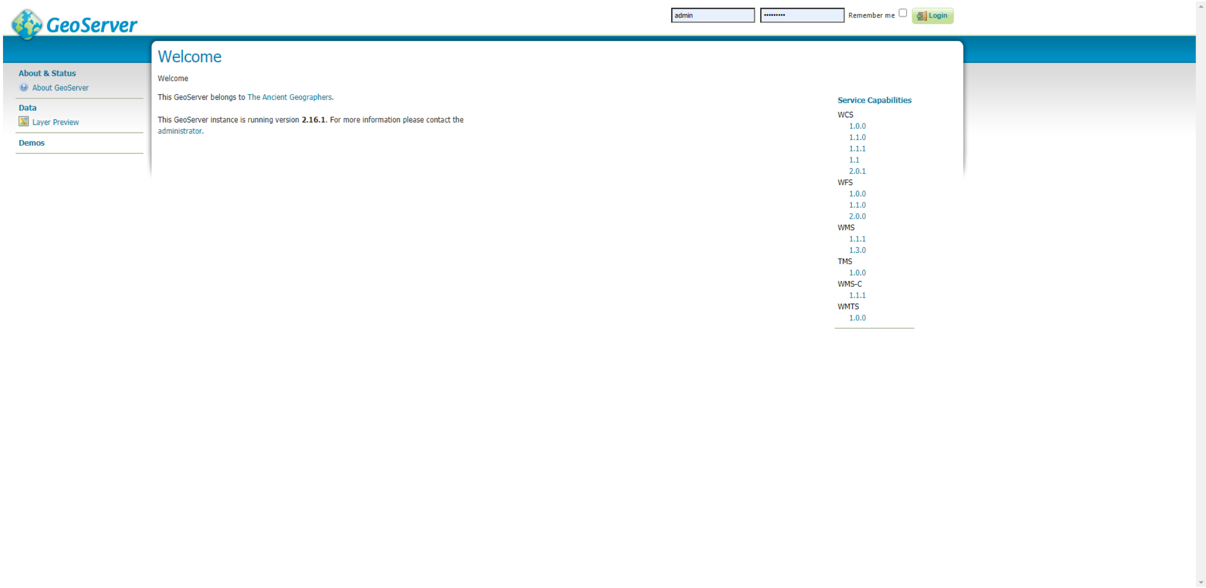


Figure 12: The GeoServer start page

- Apache Tomcat 9 – is the open source implementation of the Java Servlet, JavaServer Pages, Java Expression Language and Java WebSocket technologies. With Tomcat, you can power large-scale, mission-critical web applications [https://www.techrepublic.com/article/how-to-install-apache-tomcat-on-ubuntu-server-16-04/ accessed 2021/01/05] (Figure 6).

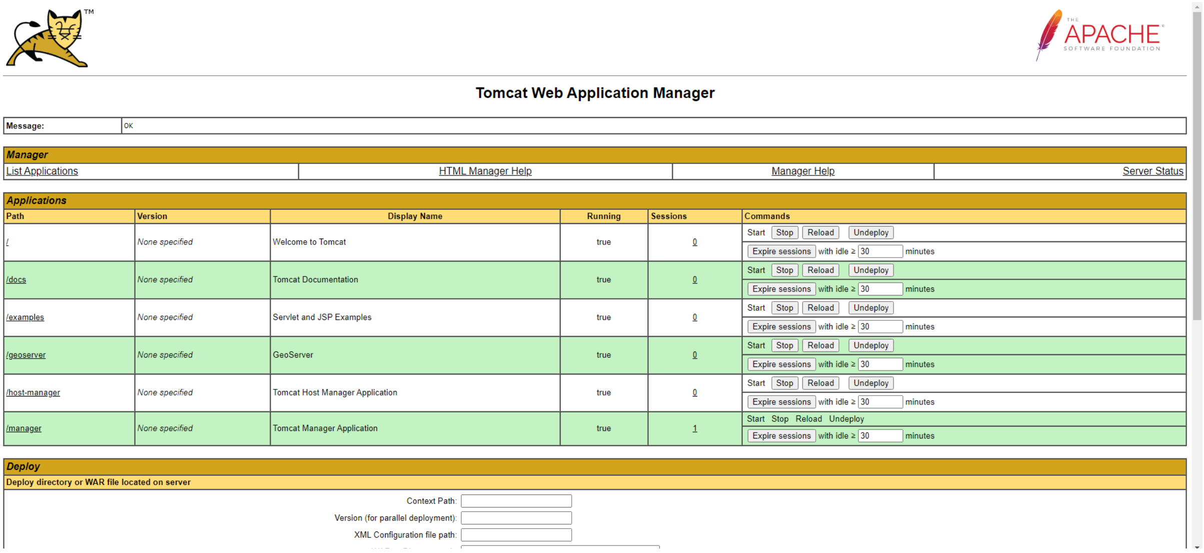


Figure 13: The Tomcat Web Application Manager used for development of the Contaminant of Emerging Concern Knowledge Hub

- Leaflet 1.7.1 – Leaflet is the leading open-source JavaScript library for mobile-friendly interactive maps. [https://leafletjs.com/ accessed 2021/01/05]. The viewer itself uses HTML 5 and Leaflet, Ajax and plain old JavaScript.

The core of the system is built on a virtual machine hosted by the Agricultural Research Council ICT infrastructure and service delivery division. Currently hosting of the system is done on a virtual server only accessible from within the ARC network. On launch, once the system goes live, it will be hosted on a virtual server accessible from outside the ARC as well.

2.3.1 Data input

Technologies used in the beta version are Microsoft Excel Spreadsheets and scripts written in python 3.8, which at the time of writing was the most stable latest release of python, and MS Excel was being used to test the whole build concept. The Spreadsheet sits in a shared directory on the ARC network at SCW and the researchers can edit or change it at will. There are currently no checks and quality checks built in as the system is still being developed. The idea is to move this into an online database with quality checks and approval processes.

Currently data input into the system entails a network-based spreadsheet that the researchers edit, this is replicated to another excel spreadsheet that sits on windows server on the virtual machine which is then exported as a csv into the PostgreSQl database on the virtual machine (Figure 7).

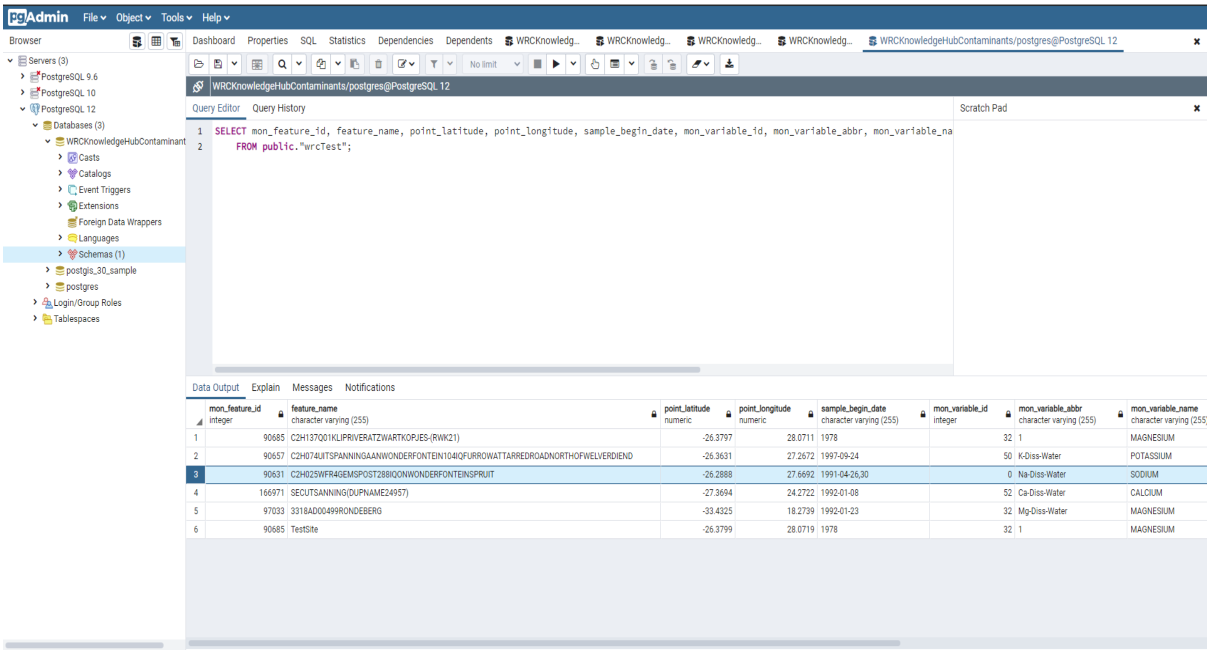


Figure 14: A screenshot of the PostgreSQL Database with test data

The production version, i.e. the next iteration of the system when the database backend is created will be a MySQL database replicating to a PostgreSQL database. We have created the database schema (Figure 8) and are well on our way to creating the database itself. MySQL is downloadable freeware software (https://dev.mysql.com/downloads/mysql/. It is an open-source relational database management system

Excel-File-Field-Name	MySQL-Field-Name	Data Type	Comment
	KH_ID	BigInt	Primary key for the table
Solubility in water	Sol_Water	decimal(13,10)	Solubility of contaminant in water
Sampling site	Samp_Site	varchar(255)	Drop down field with options for different contaminants
Feature at sampling site	Samp_Site_Feat	varchar(255)	Unique features recorded at sampling site
point_latitude	Lat	decimal(13,10)	Sampling point latitude
point_longitude	Long	decimal(13,10)	Sampling point longitude
Coordinate-Status	Coord_Status	varchar(255)	Differentiate between actual site coordinates or sampling site general coordinates
Sample collection notes	Samp_Coll_Notes	varchar(255)	Other sample collection notes
Instrument used	Inst_Used	varchar(255)	Details regarding the instruments used for the sampling
Concentration detected in sample	Dect_Con_Samp	varchar(255)	Concentration detected in sample
Detection limit of machine	Mac_Detect_Lim	varchar(255)	Detection limit of machine
Reference for analysis method	Analysis_Meth_Ref	varchar(255)	Reference for analysis method
Replicates collected	Rep_Coll	varchar(255)	Replicates collected
Unit of measure	Meas_Unit	varchar(255)	Unit of measure
Unit of measure_full name	Meas_Unit_full	varchar(255)	Unit of measure_full name
Data Reference / DOI	Data_Ref	varchar(255)	Data Reference / DOI
Chemical abundance in the sample	Samp_Chem_Abun	varchar(25)	Chemical abundance in the sample
Name of contaminant	ContaName	varchar(255)	Name of contaminant
Contaminant-Type	ContaType	varchar(25)	Contaminant-Type
Commonly known as	AKA	varchar(255)	Commonly known as
Metabolites	Metabolites	varchar(255)	Metabolites
IUPAC Name	IUPAC_Name	varchar(255)	IUPAC Name
Synonym	Synonym	varchar(255)	Synonym
Formula	Formula	varchar(255)	Formula
Molar mass	Molar_Mass	varchar(255)	Molar mass
Density	Density	varchar(255)	Density
Melting point	Melt_Point	decimal(3,5)	Melting point
Boiling point	Boil_Point	decimal(3,5)	Boiling point

Figure 15: The MySQL database table design information extracted from the developed excel spreadsheet

This database will consist mainly of data gathered and then used in the detection and monitoring of contaminants of emerging concern (CEC's) in South African water resources.

2.3.2 Data processing

Currently to test the concepts that the developers implemented, python scripts have been written to export the spreadsheet data into the PostgreSQL database that is then published on GeoServer as a web mapping service (WMS) ready to be consumed by GIS internet technologies. GeoServer uses PostgreSQL database with the PostGIS extension as its native database or database of choice for spatial data.

The python script creates a copy of the spreadsheet on the virtual machine and copies all relevant data from the network spreadsheet. It will then export all the data into the postgreSQl database (Figure 9).

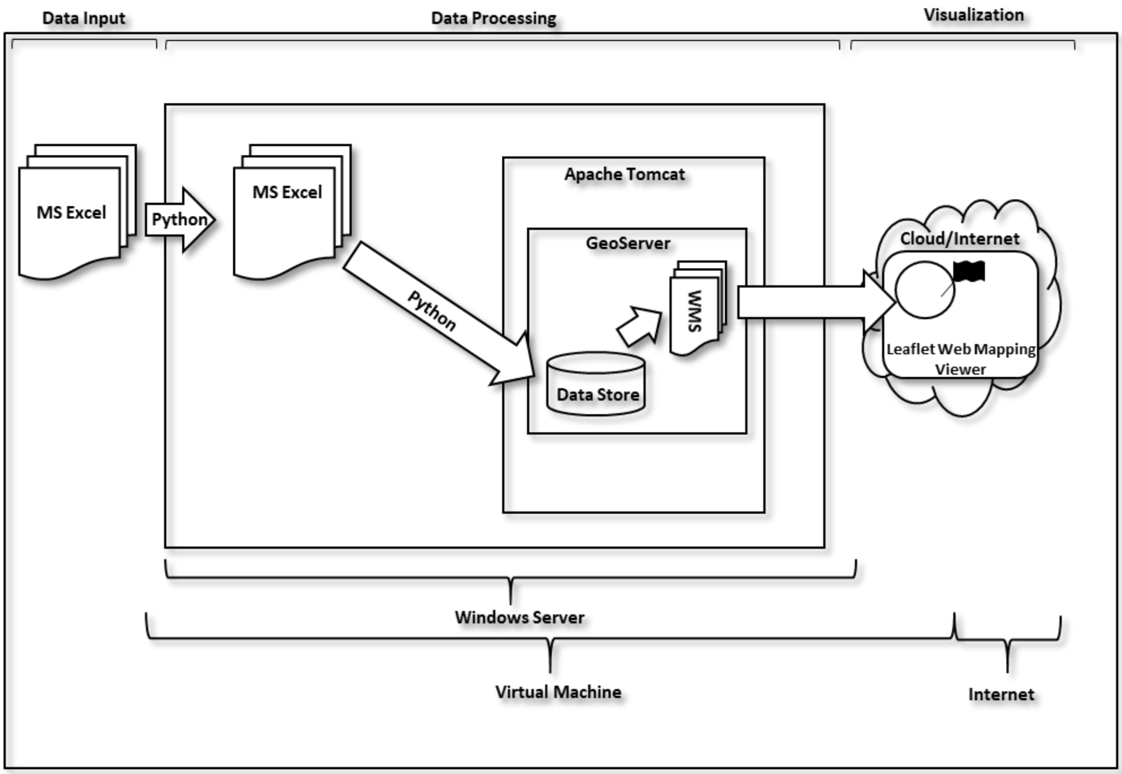


Figure 16: An overall summary of the Contaminant of Emerging Concern Knowledge Hub Beta

This part of the system is set up to run the update scripts twice a day to check for new edits/additions/changes on the original excel spreadsheet, these are then pushed to the shapefile to be populated with these new updates.

The same methods are going to be used in the final version were the database that users interact with will replicate to a posgreSQl database. Ultimately, what is envisaged is that the spreadsheets will be replaced by a web-based database interface that will allow registered users to enter into the system. The revised version (Figure 10) will not use spreadsheets but web pages for entering data into a MySQL database which will replicate to an instance of PostgreSQL database running a PostGIS extension.

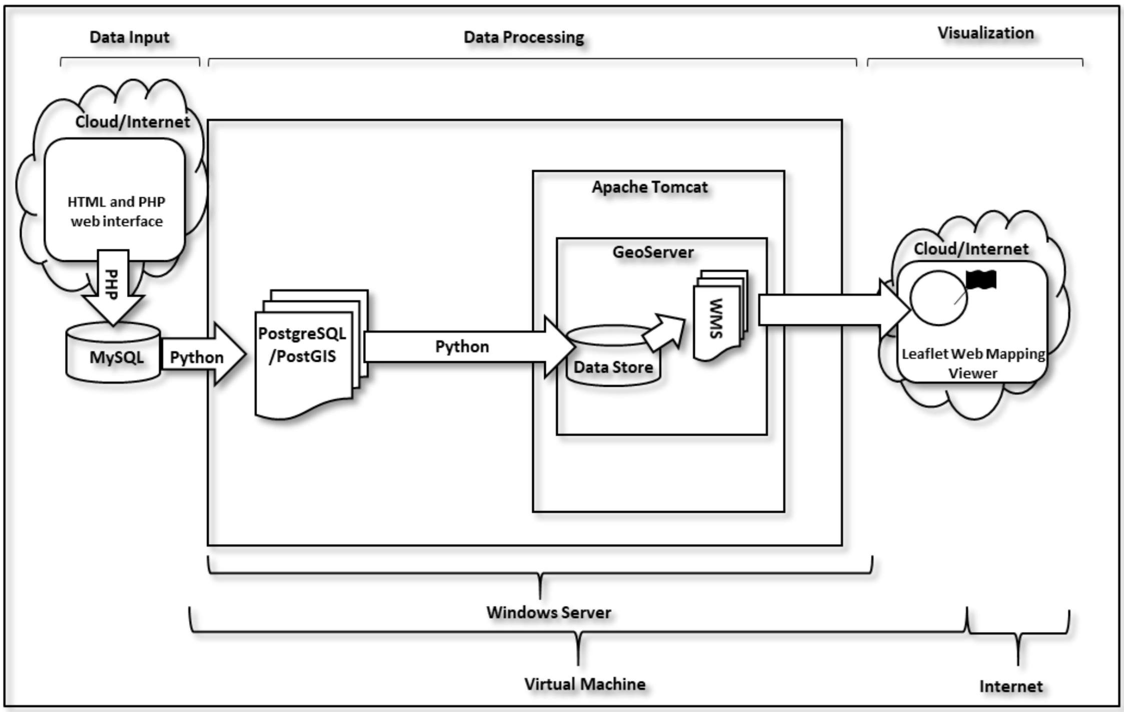


Figure 17: The envisaged final ICT system for the Contaminant of Emerging Concern Knowledge Hub

From the exported data in PostgreSQL database the latitude and longitude fields are used to plot each record spatially/on a map and thus better visualize it for better decision making. The move from plain database records to a map layer is managed in GeoServer.

2.4 Data visualization

Technically there are two visualization modules of the project but these are merged into one seamless experience for the end user. The user interface and data entry is developed in HTML, CSS, JavaScript and Php.

User interface

Development of the system's user interface/front-end will be done using the latest versions of PHP in combination with HTML, CSS, JavaScript and Php. The above-mentioned technologies will be used to develop the different pages of the system. These include a page where researchers can upload certain information regarding CECs. This info will be available on the system as soon as a quality control process used to verify the info supplied, has completed

Geospatial Visualization

A SQLView layer is published on GeoServer as a WMS/WFS service. A SQL View layer is a dynamic layer in GeoServer created from a SQL script to be executed on each request for data that queries the Postgres database in our case. It utilizes the latitude and longitude data to create a point. A SQL View layer can be used to perform complex database queries to derive content for a layer (Figure 11).

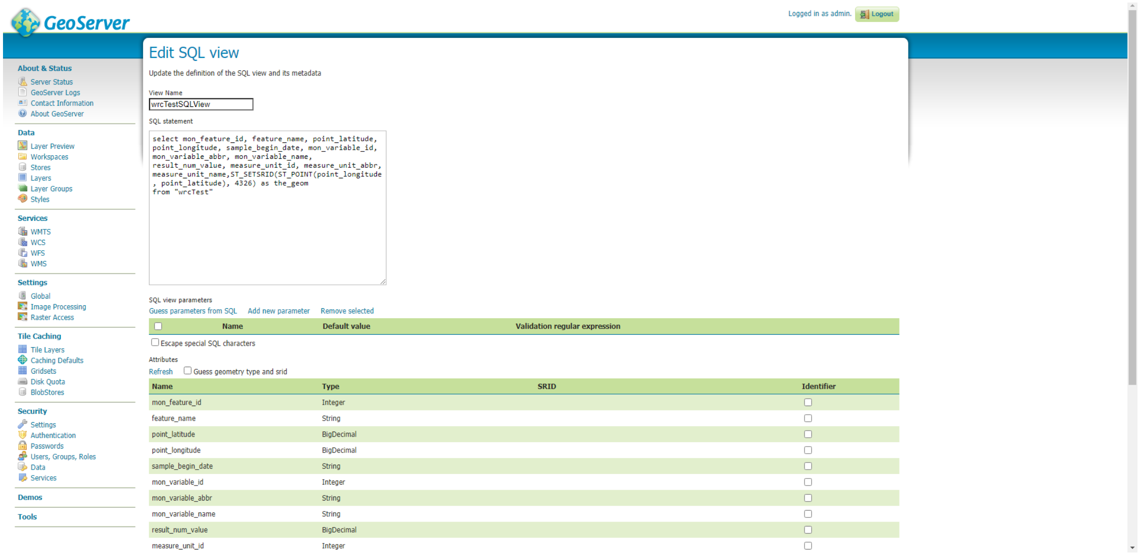


Figure 18: SQLView Layer definition in GeoServer

Custom styling and custom icons, created by developers at ARC-SCW are then applied to the layer before it is published as a service (Figure 12).

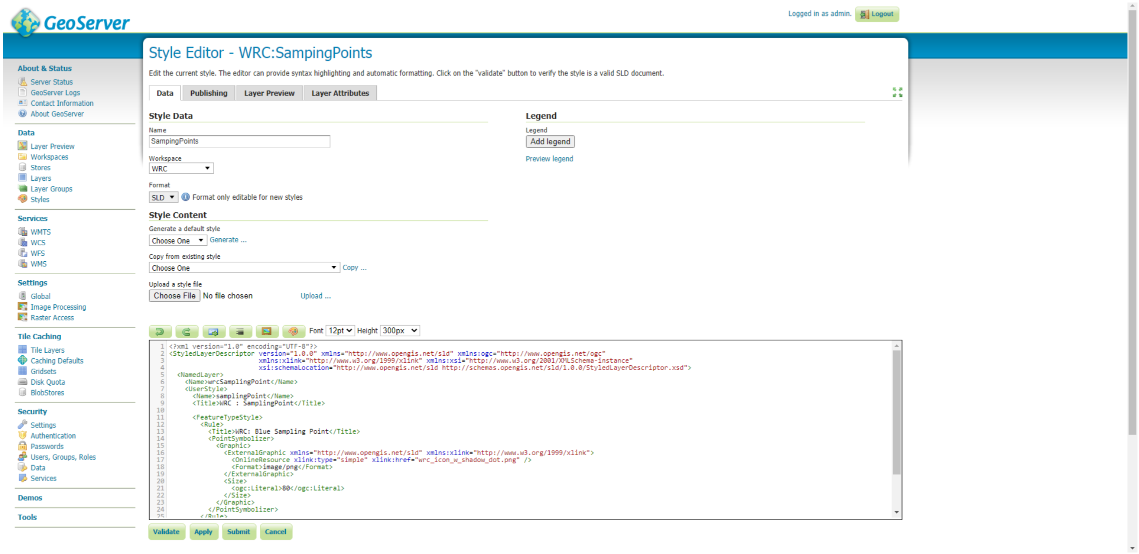


Figure 19: Custom Layer Styling

Icons are created in GIMP (GNU Image Manipulation Program), an open source image editing software. A color palette from the WRC logo is used in the creation of these icons (Figure 13).

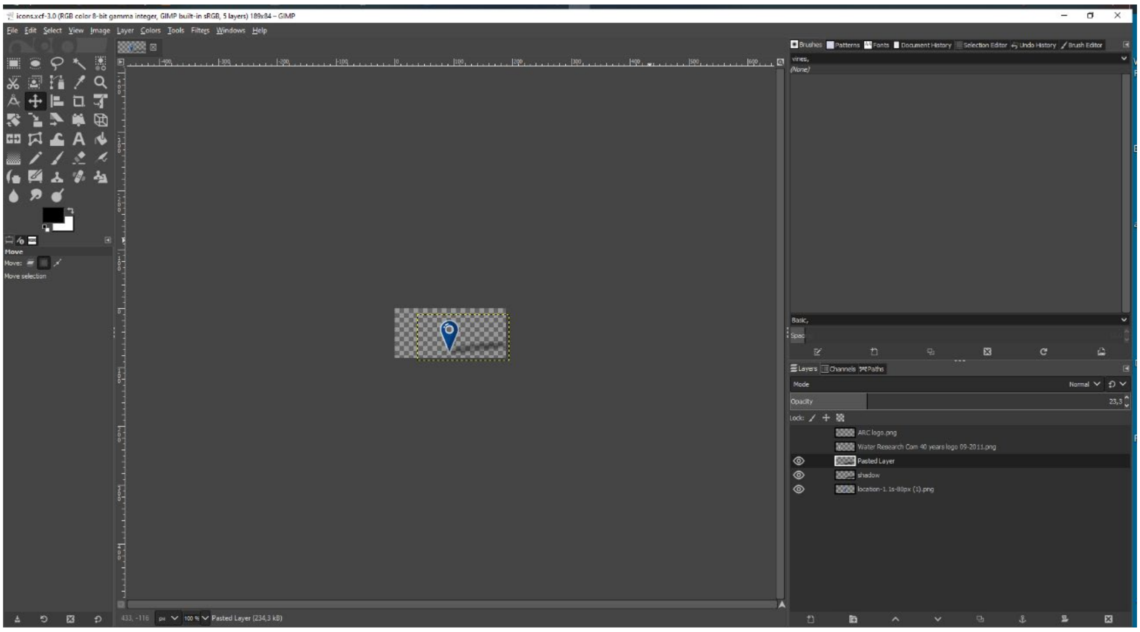


Figure 20: Creating custom icons in GIMP

The WMS is consumed using Leaflet. The leaflet web-mapping viewer shows some context layers and sampling sites as points on a dynamic map (Figure 14).

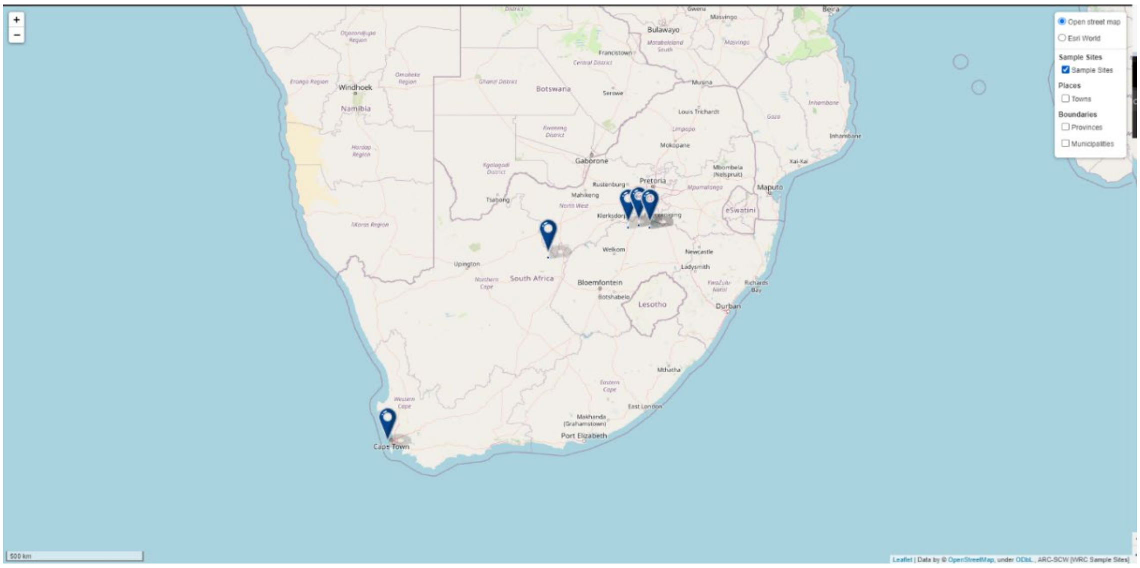


Figure 21: Sample points in Leaflet viewer

Leaflet allows for dynamic map capabilities on the data, the ability to zoom in and out of points, add different context layers, and turn layers on or off. It creates an environment with a myriad of valuable options that can be used to further unlock the data and get more information from it (Figure 15).

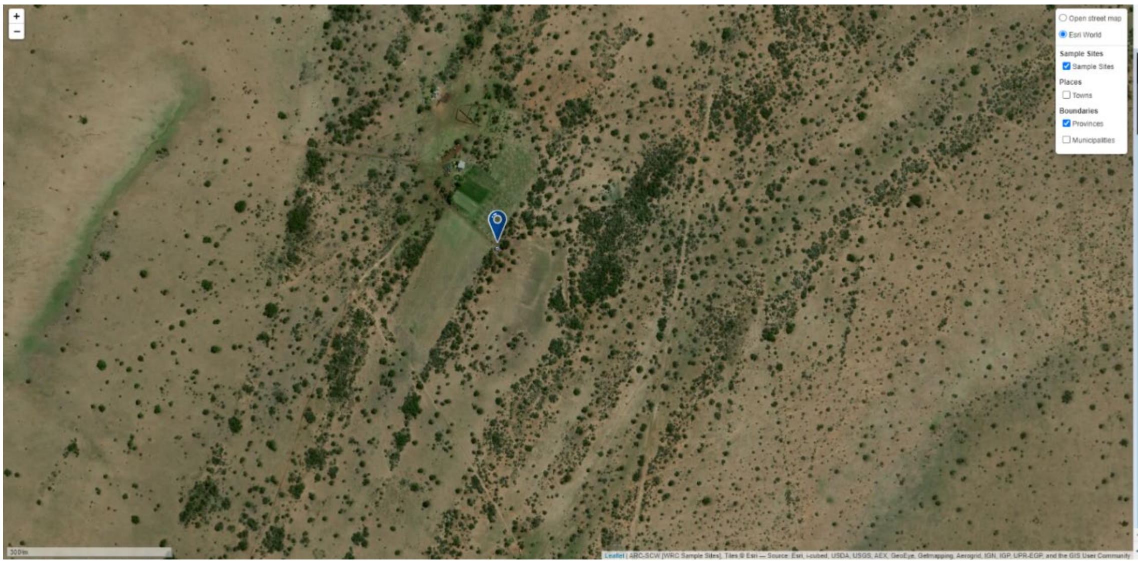


Figure 22: Zoom into a point to get context

CHAPTER 3: DATA MINING

Data input spreadsheets were developed by the Research Team. The spreadsheets were developed in two sections as presented in Table 1 (i) Contaminant information table which inputs all available information relating to each contaminant per group – this would include common names, official IUPAC naming as well as it's metabolites. Furthermore, it includes basic breakdown and solubility information (ii). The Environmental information table, which includes information mined from published manuscripts – this included site information (co-ordinates or catchment), concentration detected, methods used for extraction and quantification as well as the Digital Object Identifier (DOI) per method used as well as the manuscript link itself. The data input sheets were used to extract data from published manuscripts and will be used to develop the input sheets required on the front-end website design. The CEC table exports can be found in Supplementary information (Supplementary Table 2).

Table 1: The contaminant information per selected contaminant within each group as extracted from accredited online sources.

Contaminant information	
	E.g.
Knowledge Hub ID	Unique identifier (To be confirmed)
Name of contaminant	Dichlorodiphenyltrichloroethane
Commonly known as	DDT
Metabolites	DDE, DDD, p,p'-DDT, o,p'-DDT, o,o'-DDT
IUPAC Name	1,1'-(2,2,2-Trichloroethane-1,1-diyl)bis(4-chlorobenzene)
Synonym	
Formula	$C_{14}H_9Cl_5$
Molar mass	354.48 g·mol^{-1}
Density	0.99 g/cm^3
Melting point	108.5°C (227.3°F; 381.6 K)
Boiling point	260°C (500°F; 533 K) (decomposes)
Solubility in water	25 µg/L (25°C)
Environmental information	
	E.g.
Sampling site	ZWARTKOPJES

Feature at sampling site	Collected at dam wall
Point_latitude	-26.3797
Point_longitude	28.0711
Origin of co-ordinate	Exact co-ordinate/Catchment site
Sample collection notes	Collected by boat/edge of the bank/using a sample grabber
Instrument used	GC-MS/GC/Q-TOF
Concentration detected in sample/Detection limit of machine	<0.001 ng/L
Reference for analysis method	doi: 10.3390/ijerph14050456
Replicates collected	n=3
Unit of measure	mg/L
Unit of measure full name	MILLIGRAM PER LITRE
Data Reference/DOI	DOI of article used

3.1 SELECTION OF CECS

The selection of CECs was based on current information in literature as well as international databases as outlined below. The following CECs were selected as the primary contaminants within the CEC-KH: Perfluoroctane Sulfonate (PFOS), Alkylphenols (AP) and Alkylphenol Ethoxylates (APE), Polybrominated Diphenyl Ethers (PBDEs) or Flame Retardants, Polychlorinated Biphenyls (PCB), Polycyclic Aromatic Hydrocarbon (PAHs), Current Use Pesticides, Pyrethroid, Cypermethrin, Chlorinated Paraffins, Pharmaceuticals and Personal Care Products (PPCP), Microbiological CECs, Triclosan, Microplastics, Engineered Nanomaterials (ENM) and Heavy metals.

3.2. CHEMICAL CLASSING

3.2.1. Globally Harmonized System of Classification and Labelling of Chemicals

The Globally Harmonized System of Classification and Labelling of Chemicals (GHS) aims to classify chemicals by their hazard potential and propose a harmonized system to be used which would be globally recognizable. Since chemicals pose a risk during all phases of the lifecycle (production, transport, product usage and release) they could pose a danger to both humans and the environment. If chemicals are classed into this system they become internationally applicable which would be useful as the Knowledge Hub can be expanded upon to the rest of Africa.
The GHS system uses three classes of classification (i) *Physical hazards group*: These risks are classified according to their physical or chemical features. Anyone who comes into contact with these dangers may suffer physical injury. Examples include Flammable Liquids and Solids, Radioactive Materials, and Corrosives. (ii) *Health hazards group*: Exposure to these dangers can result in negative

health impacts in users. Examples include acute toxicity, carcinogenicity and respiratory sensitization. (iii) *Environmental hazards group*: When released into air, water or land this group of hazards can have a negative impact on biota. Examples include acute aquatic toxicity and rapid bioaccumulation potential. Because it is not recognized or enforced as a hazard in the United States and Canada, this is the hazard group that is most often overlooked. A challenge would be that manufactures would be required to classify the products they manufacture which could lead to further issues with intellectual property protection. There are already various classification systems in place and each are not without their challenges.

3.2.2. Classification and categorization of emerging contaminants

Emerging contaminants are unregulated contaminants found in the environment and it is becoming apparent that the vast majority of contaminants being produced are unregulated while a small amount is regulated by governing bodies worldwide. As our detection tools have improved over the last 10-15 years we have begun to realize that there is a large chemical universe which is still unidentified (Stefanakis and Becker, 2020). One of the major issues with classifying CECs is that their potential risks on the aquatic environment and biota within it remains largely unknown.

Dey et al. (2019) make mention of the NORMAN list of classification, but this is still under development as only the complete list of CECs is currently available (https://www.norman-network.net/sites/default/files/files/Emerging_substances_list_Feb_16/NORMAN%20list_2016_FINAL.XLSX). An example of the prioritized list of CEC classification can be seen outlined in Figure 23.

Stefanakis and Becker (2020) propose a three tier category system as follows: i) chemicals that have only lately entered the environment (e.g. industrial additives), ii) substances that may have been present in the environment for many years in the past, but whose presence was only recently discovered and whose relevance began to pique curiosity (e.g. pharmaceuticals) and iii) chemicals that have been known for a long time but whose potential for harm to humans and the environment has only lately been discovered (e.g. hormones). An example of a pharmaceutical classification can be found in Figure 24.

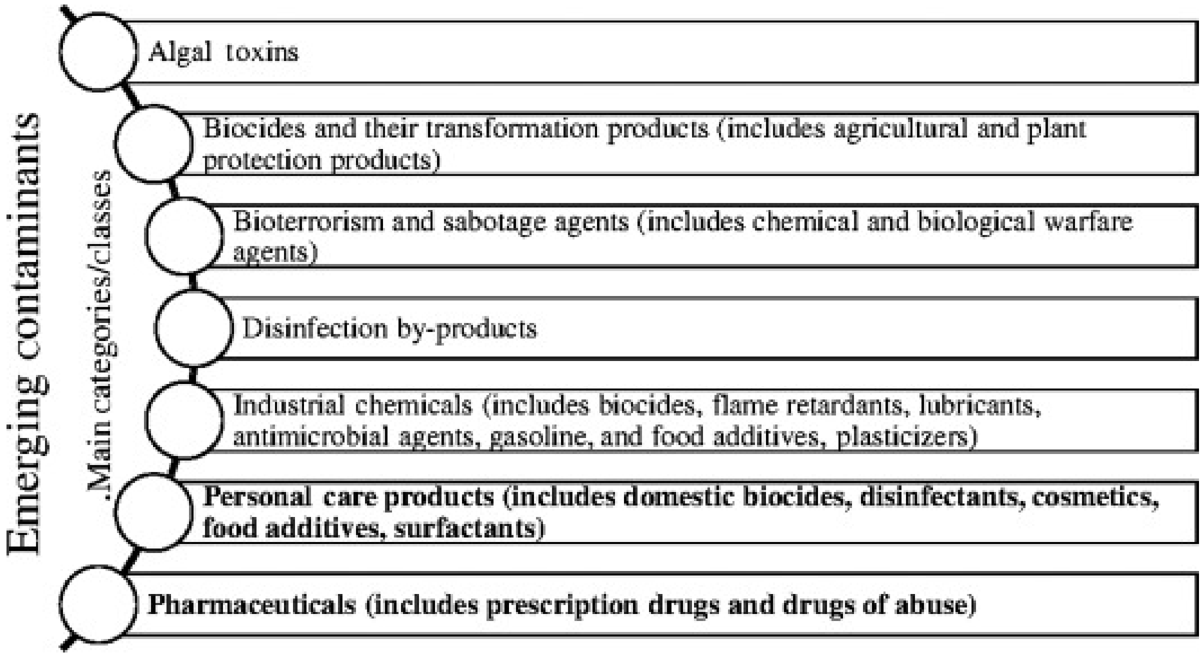


Figure 23: Classification and categorization of emerging contaminants as outlined by Dey et al. (2019)

Emerging Contaminant groups	Examples
Pharmaceuticals	
Human antibiotics and veterinary	Trimethoprim, erytromycine, amoxicillin, lincomycin, sulfamethaxozole, chloramphenicol
Analgesics, anti-inflammatory drugs	Ibuprofene, diclofenac, paracetamol, codein, acetaminophen, acetylsalicilyc acid, fenoprofen
Psychiatric drugs	Diazepam, carbamazepine, primidone, salbutamol
β-blockers	Metoprolol, propanolol, timolol, atenolol, sotalol
Lipid regulators	Bezafibrate, clofibric acid, fenofibric acid, etofibrate, gemfibrozil
X-ray contrasts	Iopromide, iopamidol, diatrizoate
Personal care products (PCPs)	
Fragrances	Nitro, polycyclic and macrocyclic musks, phthalates
Sun-screen agents	Benzophenone, methylbenzylidene camphor
Insect repellents	N,N-diethyltoluamide
Endocrine Disrupting Chemicals (EDCs)	Octylphenols, nonylphenols, Di(2-ethylhexyl)phthalate (DEHP)
Hormones and steroids	Estradiol, estrone, estriol, diethylstilbestrol (DES)
Perfluoronated compounds	Perfluorotoctane sulfonates (PFOs), perfluoroctanoic acid (PFOA)
Surfactants and surfactant metabolites	Alkylphenol ethoxylates, 4-nonylphnol, 4-octylphenol, alkylphenol carboxylates
Flame retardants	Polybrominated diphenyl ethers (PBDEs): polybromonated biphenyls (PBBs) – polybromonated dibenzo-*p*-dioxins (PBDDs) – polybromonated dibenzofurans (PBDFs), Tetrabromo bisphenol A, C10-C13 chloroalkanes, Tris (2-chloroethyl)phosphate, Hexabromocyclododecanes (HBCDs)
Industrial additives and agents	Chelating agents (EDTA), aromatic sulfonates
Gasoline additives	Dialkyl ethers, Methyl-t-butyl ether (MTBE)
Antiseptics	Triclosan, chlorophene

Figure 24: Classification and categorization of emerging contaminants as outlined by Stefanakis and Becker (2020)

3.3 DATA INPUT

The CEC Knowledge Hub currently has four main contaminant classes namely organic contaminants, inorganic contaminants, particulate contaminants, and microbiological contaminants. Of these inputs there are currently (December 2022) 590 data points present within the hub where the majority are PPCPs followed by microplastics (Figure 25).

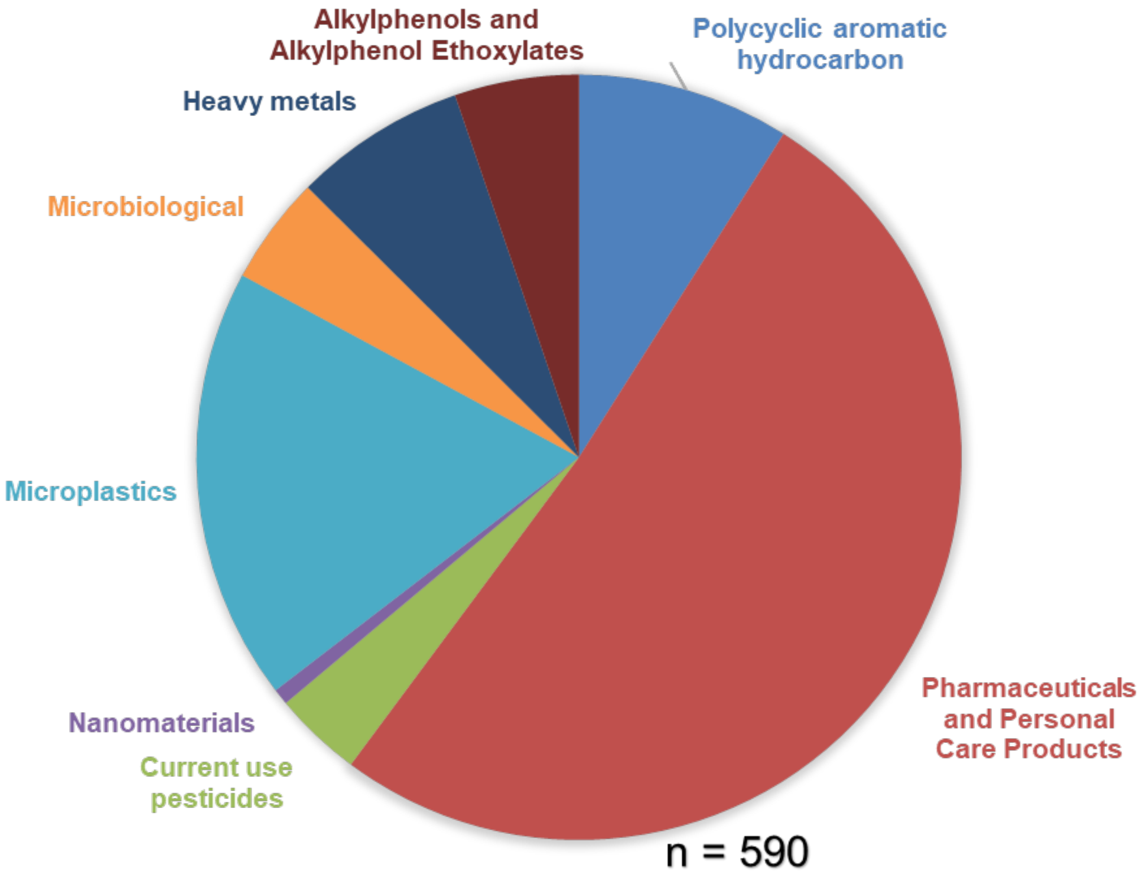


Figure 25: The frequency of terms of all Contaminants currently listed in the CEC Knowledge Hub

3.3.1. Organic contaminants

Alkylphenols and Alkylphenol Ethoxylates (APEs)

Since the 1940s, a series of synthetic compounds known as alkylphenols and their precursors, or APEs, have mostly been employed as surfactants in detergents and cleaning solutions for home and industrial purposes (Klosterhaus, Allen and Davis, 2012). APEs are also used as "inert ingredients" in pesticide formulations as additives to enhance efficiency, in the manufacture of paper, leather and textiles, metalworking, as chemicals in oil fields and for the cleanup of oil spills, and as components of paints, adhesives, personal care products, and spermicidal lubricants. APEs are categorized as high production volume (HPV) chemicals due to their global production volume of over a million tons. When APs and ethylene oxide react, a molecule made up of the AP and the ethoxylate moiety is produced, which is used to make APEs. APEs are water soluble owing to it structure, which also aids in removing grease and debris from dirty surfaces. Nonylphenol ethoxylates (NPEs) the most common APEs are produced in the U.S. and make up 80 to 85 percent of all APEs manufactured commercially (Acir and Guenther, 2018).

Very few studies conducted in South Africa report on the levels of APEs in surface waters (Figure 26). The reported concentration range of the metabolites of APEs were as follows: Nonylphenol (NP) 0.38-9.35 µg/L (Sibali, Okonkwo and McCrindle, 2010); NPEs 0.08-0.31 µg/L (Chokwe et al., 2015; Sibali, Okonkwo and McCrindle, 2010), nonylphenol monoethoxylate (NP-1EO) 0.044-0.73 µg/L (Chokwe et al., 2015), nonylphenol di-ethoxylates (NP-2EO) 0.13-0.94 µg/L (Chokwe et al., 2015), octylphenol penta ethoxylates (OPPEs) 0.31-6.01 µg/L (Chokwe et al., 2015; Sibali, Okonkwo and McCrindle, 2010) and octyl phenol ethoxylates (OPnEO3) 60.1-92.7 µg/L (Sibali, Okonkwo and McCrindle, 2010). The two sites studied are the Vaal River and Jukskei River catchment areas, both in the Gauteng Province of South Africa. Farounbi and Ngqwala (2020) reported NPs and octylphenol (OP) in the range of 0.031-2.55 µg/L and 0.0097-2.72 µg/L, respectively, in four major rivers of the Eastern Cape (Bloukrans, Buffalo, Swartkops and Tyume). There is a pressing need for such investigations in the other provinces around South Africa as evidenced by the paucity of published studies on the freshwater levels of APEs and their metabolites in other provinces.

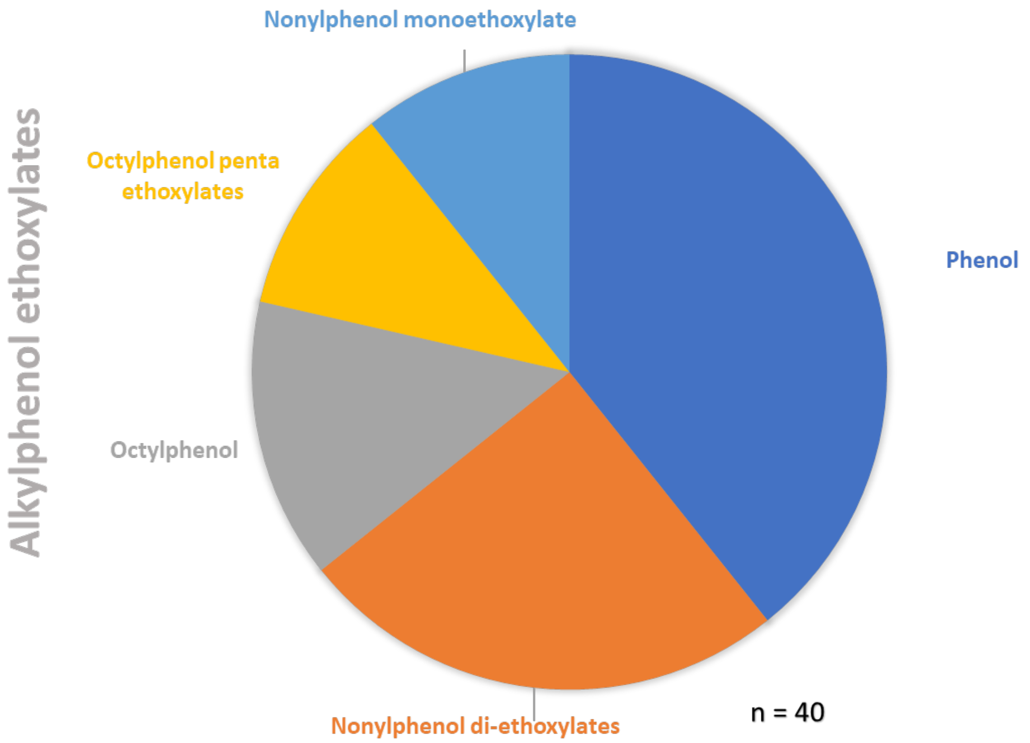


Figure 26: The frequency of terms of all Alkylphenol ethoxylates currently listed in the CEC Knowledge Hub

Polychlorinated Biphenyls (PCB)

Polychlorinated biphenyls are not a single chemical, rather a group of related chemicals, belonging to broad family of human-made organic chemicals known as chlorinated organic chemicals that have been developed for a variety of industrial and commercial purposes. These chemicals were manufactured worldwide from 1929 until the United States of America banned their manufacture in 1979. The ban on PCBs was primarily due to mounting scientific evidence that PCBs accumulate in the environment and at high, enough concentrations adversely affect humans and other biota – the ban took place under the Toxic Substances Control Act (Piramoon et al., 2017). Although the ban stopped production, lipophilic PCBs are able to bioaccumulate in lipid tissue of higher organisms including humans, and are still present within the environment and remain an emerging concern at waste sites.

Due to the chemical stability, ability to avoid inflammation, insulating properties and high boiling points PCBs have been used to hundreds if not thousands of commercial products. Some of these products include transformers and capacitors, oils used hydraulic equipment; as plasticizers in paints, rubber products; in pigments, dyes, and carbonless copy paper and electrical equipment including voltage regulators, switches, re-closers, bushings, and electromagnets (Bjurlid at al., 2017). Due to their wide use and persistence in the environment they can be released and accumulate further by waste disposal, vaporization from unenclosed uses, volatilization and runoff from landfills containing PCB waste, accidental release of PCBs during the industrial process and as well as incineration of waste containing PCBs (Kampire et al., 2017).

Current Use Pesticides

The term “pesticides” includes all insecticides, herbicides, fungicides, rodenticides, and antimicrobials. Based on the literature reviewed with papers obtained from the key words “Current use of pesticides AND South Africa AND water”, it can be concluded that the South African waterways are greatly threatened by agrochemicals such as fertilizers and pesticides. While some pesticides are already subject to regulation throughout the country, many more are not regulated nor monitored in our waterways. For example, there is still a gap in studies that focus on interaction points in water systems such as estuaries that are a link between fresh and saline water bodies. Furthermore, majority of the surface studies are on WWTPs mainly in big cities such as Johannesburg but there is little focus on rural communities and other provinces in the country. There is a great disproportionality between the number of permitted-for-use pesticides and regulated pesticides in South African surface water sources. Evidently, there are specific pesticide characteristics gaining increasing attention such as toxicity and susceptibility tests of certain pesticides in various animals especially fish. There is undoubtedly a sizable knowledge gap that has to be addressed and targeted for further study, but many pesticides also lack regulatory guidelines. There should be more focus on first establishing standard limits as there still are pesticides that have been permitted to be used for decades yet are not regulated even though they are detected.

Pyrethroid, commonly known as PYR or Pyrethrin, is produced using pyrethrums flowers (*Chrysanthemum cinerariaefolium* and *C. coccineum*) (Chrustek et al., 2018). It has been in use or manufacturing since 1977 for uses in the commercial agricultural market, where it is frequently used as a pesticide (Ensley, 2018). These substances are well known for targeting the voltage-gated calcium and voltage-gated chloride channels in insects' nervous systems, which results in "hyperexcitation" (Ensley, 2018). These pollutants are discharged into our water systems via irrigation runoff, storm-related soil erosion, and airborne spraying (Mi et al., 2019). Since they normally do not enter the groundwater table, once present, they can partially dissolve and bind to soil particles at shallow depths (Zhu et al., 2020). Acute toxicity to aquatic life, such as fish and various invertebrates, is among the dangers of exposure (Zhan et al., 2020).

A total of four studies – of which five sites were chosen – have been carried out based on the literature. The ranges detected were between 0.00006 and 132.878 µg/L with majority of the studies focusing only on water and its impact on human health but also included information on concentrations in human breast milk (0.072 µg/L). Few studies have been published on PYR in water in South Africa.

Cypermethrin is commonly known as CP or Alpha-cypermethrin and is a synthetic pyrethroid known for being fast-acting neurotoxin in pests but generally regarded as a moderately toxic pesticide that is very toxic to fish and other aquatic organisms (Yılmaz and Erbaşlı, 2004). CP has been in use/production since 1974 for application in large scale agriculture initially in the cotton farms but later gained popularity in fruit and vegetable pest control as well (World Health Organization, 1992). Once present, these pollutants can rapidly breakdown in soil but remain "fairly immobile" in water due to low solubility. They are introduced into our water systems through runoff during rainstorms and air drift during spraying (World Health Organisation, 2014). High fish toxicity, immobilization, and potential death of unintended insects and terrestrial animals are some of the risks linked with exposure (Ylmaz and Erbaşl, 2004).

According to the literature, three locations were chosen for a total of two CP studies that were conducted in South Africa (Figure 27). The ranges detected were between 0.000 and 0.028 µg/L. Data found prioritized the detection as well as impact of Cypermethrin persistence in humans with insufficient data on the environmental and ecological impact.

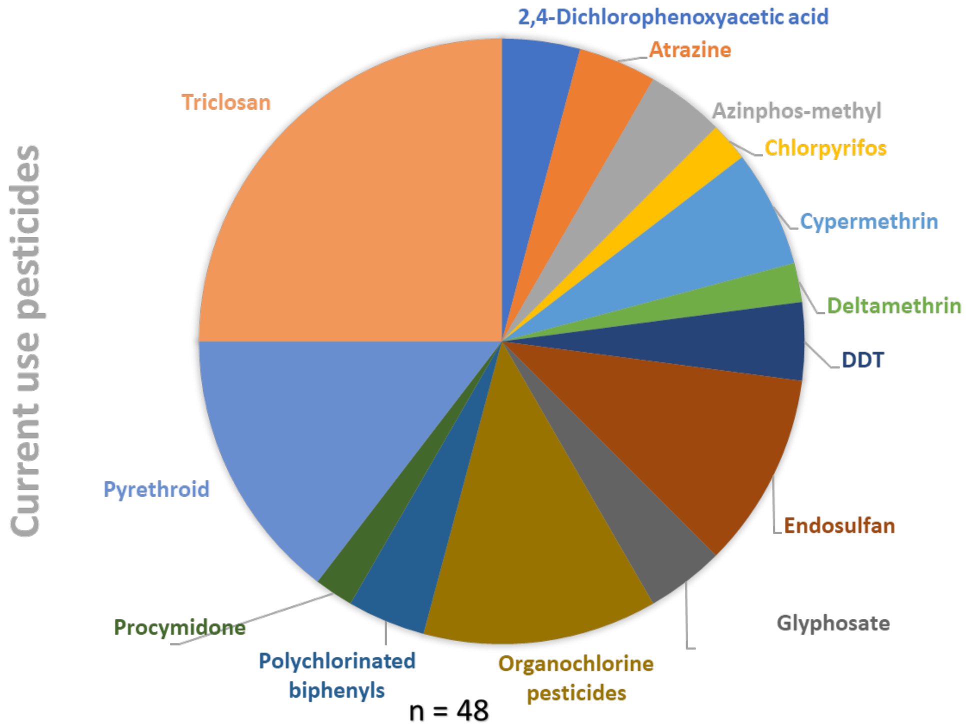


Figure 27: The frequency of terms of all Current use pesticides currently listed in the CEC Knowledge Hub

Chlorinated Paraffins

Since the 1930s, chlorinated straight-chain hydrocarbons, known as chlorinated paraffins (CPs), have been synthesized in high quantities. CPs are often employed as additives in cutting fluids, lubricants, as well as flame retardants in sealants, leather, and plastics because of their thermal and chemical resilience (Chen et al., 2011; Bayen et al., 2006). As a result, CPs have been found in trace amounts in a variety of environmental compartments, including freshwater, ocean, air, freshwater sediments, aquatic and terrestrial biota, marine mammals, human tissues, and breast milk. Its widespread distribution is likely caused by both the variety of applications and the incorrect disposal of products containing CP (Bayen et al., 2006). Studies have suggested that CPs may be carcinogenic to humans and have identified target organs for toxicity, including the kidneys, liver, the parathyroid and thyroid glands, despite the lack of information on the biological effects, fate, and concentrations of CPs in the environment (Ali and Legler, 2010). When coupled to mammalian toxicity there have been hypotheses that CPs are biomagnified and bioaccumulated in food webs in addition to mammalian toxicity (Chen et al., 2011). This warrants further investigation into the mechanisms underlying CP toxicity as well as environmental monitoring and management. Due to the CPs' propensity to persist in the environment and their potential for long-range environmental transport, more emphasis on legislation to manage CPs is also necessary (Ali and Legler, 2010).

Pharmaceuticals and Personal Care Products (PPCP)

Pharmaceuticals and personal care products are essential to human daily existence. With global population increase and lifestyle adaptations pharmaceuticals are being used and discarded more often by people and in animal husbandry. Pharmaceuticals are created specifically to treat or eradicate infection or disease by influencing the physiology of the species (human or animal) (Arnold et al., 2014). However, they may well become potentially hazardous pollutants in environmental matrices. However, there has been an increase in research into the environmental impact of pharmaceuticals over the past decade. Their abundance and fate in the environment are still largely unknown. The extent of PPCP pollution of environmental matrixes has been highlighted by this increasing study interest and advancements in analytical equipment which can detect these contaminants, even at extremely low levels. Policy makers would need information and data from the multiple research efforts in order to establish regulation of PPCPs (Agunbiade and Moodley, 2015).

Considering the large range of potential contaminants in the category, research on the pollution of environmental matrices by PPCPs and their degradation products is scarce in South Africa. According to Wood et al. (2015), RSA is the country that uses the most antiretroviral drugs per capita globally in the effort to combat HIV/AIDS, which is projected to result in an increase in the concentration of these medications released through the sewage system. Waterways in RSA have a substantial amount of pharmaceutical pollution, according to research conducted there over the last decade. Considering the large range of potential contaminants in the category, research on the pollution of environmental matrices by PPCPs and their degradation products is scarce in South Africa. According to Wood et al. (2015), RSA is the country that uses the most antiretroviral drugs per capita globally in the effort to combat HIV/AIDS, which is projected to result in an increase in the concentration of these medications released through the sewage system. Waterways in RSA have a substantial amount of pharmaceutical pollution, according to research conducted there over the last decade. These include nonsteroidal anti-inflammatory drugs (NSAIDs) along Mgeni and Msunduzi river sediments in KwaZulu-Natal (Gumbi et al., 2017), antiretroviral medications in surface water sources throughout RSA (Wood et al., 2015), antibiotics and analgesics in river and sediment samples from the Umgeni river/sediments, and Hartbeespoort Dam (Rimayi et al., 2018). Others include analgesics/anti-inflammatory medications in wastewater treatment plant (WWTP) sludge, antipyretics and antibiotics in the Msunduzi river in KZN (Agunbiade and Moodley, 2015; Matongo et al., 2014), and more (Ademoyegun et al., 2020). Antibiotics, NSAIDs, antihistamines, stimulants, anti-epileptics, anti-depressants, analgesics, medications for diabetics and hypertension, drug precursors, plasticizers, UV filters, parabens, x-ray contrast media, and beta blockers were among the 40 pharmaceuticals and PPCPs that Archer et al. (2017) found in a surface water source in Gauteng. A targeted analysis of samples taken from the Buffalo, Bloukrans, Swartkops, and Tyhume rivers in the Eastern Cape found high levels of antibiotic, antiepileptic, and anti-inflammatory drug residues (Vumazonke et al., 2020) (Figure 28).

The reality that these chemicals are present in South African surface waters suggests that WWTPs are ineffective at eliminating them throughout the sewage treatment process (Ademoyegun et al., 2020; Hlengwa and Mahlambi, 2020). To reduce the levels in the environment, regulations for the disposal of PPCPs must be put in place.

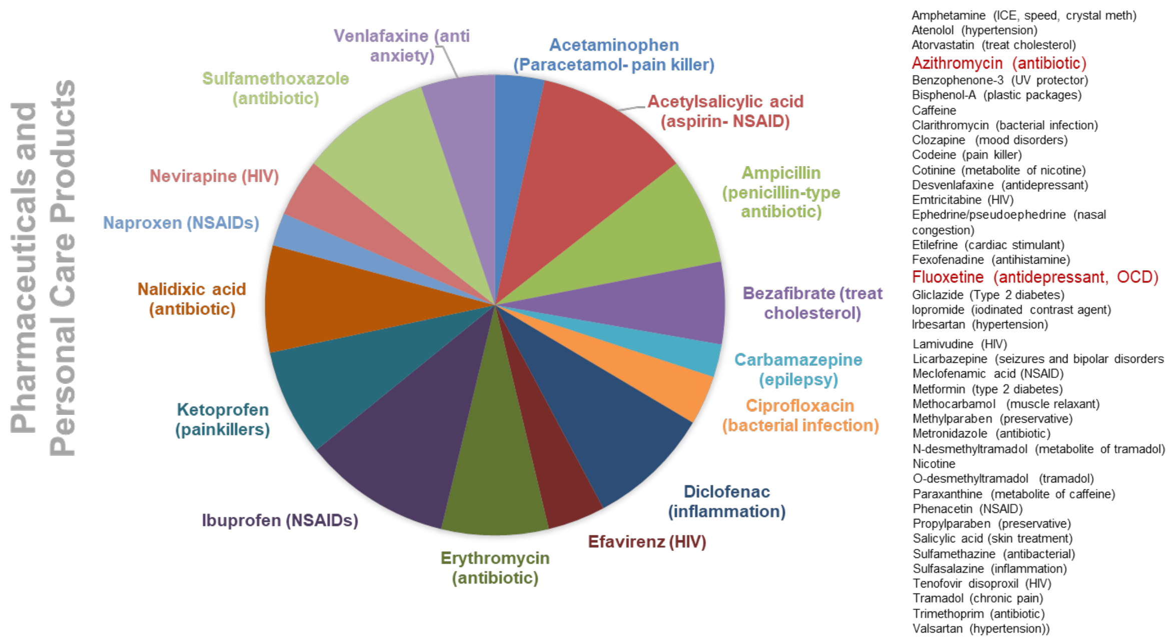


Figure 28: The frequency of terms of all Pharmaceuticals and personal care products currently listed in the CEC Knowledge Hub

Perfluoroctane Sulfonate (PFOS)

The most studied class of polyfluoroalkyl compounds is perfluorooctane sulfonate (PFOS). For application in the manufacturing of fabrics, these substances are mostly utilized as surfactants as well as in oil- and water-repellent coatings. Additionally, they are utilized chemically in products like firefighting foams and pesticides. They are therefore dispersed into the environment through industrial uses and have become pollutants of rising concern (Ssebugere et al., 2020). Their entry into the market was approved in the 1940s (Renner, 2001), and they eventually found their way into the environment where they may potentially expose people, domestic animals, and wildlife all over the world. Despite their rapid rate of environmental contamination, little is known about how widespread PFASs are globally due to the severe lack of PFAS studies, particularly in Africa when compared to Asian, European, and North American countries (Bangma et al., 2017). Since these compounds are continuously released into the environment, in-depth analyses are required to fully understand the implications that these substances may have. PFOA and PFOS levels in drinking water in Africa have only been the subject of a few studies, and in certain cases, the levels were higher than those recommended in EPA drinking water guidelines (Ssebugere et al., 2020).

Polybrominated Diphenyl Ethers (PBDEs)/Flame Retardants

Since the 1970s, when polychlorinated biphenyls (PCBs), the first flame retardants, were gradually phased out due to their toxicity, polybrominated diphenyl ethers have been used to replace them. A flame retardant made of bromine is called polybrominated diphenyl ethers (PBDEs). A functional class of chemical compounds known as "flame retardants" is added to some manufactured products to lessen the likelihood of fire occurring or to delay the spread of fire. These products include upholstery carpets, drapes, wire insulation, foam padding for furniture, and plastic enclosures for televisions, laptops, and other small appliances. The chemical components of flame retardants, such as whether they contain boron, bromine, phosphorus, nitrogen, metals, or chlorine, are frequently used to categorize them. The most widely used flame retardants are PBDEs. Due to their inability to chemically bond with the items they are added to, polybrominated diphenyl ethers can be released from these products into the air, water, and soil during production, use, and disposal. Therefore, fresh streams that are close to highly industrialized areas or that are contaminated by home and industrial trash are more likely to encounter PBDEs. Although information is limited about the production of PBDEs in African countries, many export products contain PBDEs (Olisah et al., 2020). The usage of PBDEs is currently under investigation, and nations like the US and EU have banned or restricted certain of their use and environmental discharge (Chokwe et al., 2019).

Polycyclic aromatic hydrocarbons (PAHs)

Polycyclic aromatic hydrocarbons are a class of ubiquitously distributed toxic organic compounds possessing two or more fused aromatic rings and they are persistent in the environment because of their hydrophobicity, low aqueous solubility, and stability of their aromatic ring structure. PAHs are categorized as either low molecular weight (LMW), which have two or three aromatic rings, or high molecular weight (HMW), which have four or more rings. Due to their greater environmental persistence and resistance to biodegradation, HMW PAHs (Rimayi et al., 2018, Awe et al., 2020). Despite being formed via the incomplete combustion of coal, coal tar, diesel exhaust, asphalt, and other fossil fuels as well as occurring naturally in those fuels. While tobacco smoke contains a considerable amount of PAHs, they are also typically created by the burning of organic substances including wood, waste, smoked and barbecue foods (Mojiri et al., 2019; Adeniji et al., 2019).

They are usually introduced into freshwater systems by anthropogenic activities which include leakage (run off) of mine wastewaters, industrial discharges, and domestic wastes (Rimayi et al., 2018; Adeniji et al., 2019). Nitrated and oxygenated PAHs are created when PAHs combine with oxidants such NOx, O3, and OH. These compounds are drawn to air particulate matter and then enter aquatic habitats as rain fallout (Mojiri et al., 2019). Once in the water system, the PAHs associate with dissolved organic matter through several means of binding and adsorption, paving way for their subsequent deposition and accumulation in water and its sediments (Adeniji et al., 2019A). In freshwater, PAHs pose risks such as mutagenicity, teratogenicity, carcinogenicity, and disruption to the endocrine system. Their reactive metabolites, such as epoxides and dihydrodiols are considered to have greater deleterious effects, given their ease of binding to cellular proteins and DNA (Adeniji et al.. 2019B). As a result of these toxicities, sixteen of the PAHs are prioritized and included in the European Union (EU) and United States Environmental Protection Agency (US EPA) priority list of pollutants.

Although not enough data is available for PAHs in our water bodies, currently reported are findings from six study sites in South Africa, spanning 4 provinces – Eastern Cape, Western Cape, Limpopo and Mpumalanga provinces. Adeniji et al. (2019a and 2019b) determined PAH values in the Algoa Bay and Buffalo River estuary, respectively, both in the Eastern Cape province. The concentrations detected for individual PAHs ranged from no detection (below detection level, bdl) to a high of 24.91 μg/L (Adeniji et al., 2019a and 2019b) while total for all 16 priority PAHs was up to 206 μg/L. In the Algoa Bay, samples collected at bottom levels were found to contain higher concentrations of PAHs than the surface level water samples (Adeniji et al., 2019A). Seasonal variations in concentrations were observed at both sites, with summer concentrations generally greater. Some individual PAHs, such as Naphthalene, Chrysene and Benzo(a)pyrene exceeded maximum allowable concentrations in fresh and marine waters as per British Columbia report (1993) and mean total PAHs exceeded limit of 30 μg/L allowable limit for marine water as per the Western Australia Department of Environment regulations (Adeniji et al., 2019A and 2019B).

In the Western Cape province, Awe et al. (2020) reported on the levels of PAHs in the Diep River. They detected concentrations for each individual PAHs ranging from below detection level to a high of 72.38 μg/L with Chrysene being consistently high. Total for all 16 PAHs reported was up to 310.52 μg/L at a single sampling point (Awe et al., 2020) (Figure 29). Concentrations were also found to be season-dependent with higher concentrations in summer and probable carcinogenic PAHs such as

Benzo(a)antharcene, Chrysene, Benzo(b)fluoranthene, Benzo(k)fluoranthene, Benzo(a)pyrene, and dibenzo(ah)anthracene were prevalent. The levels of some PAHs exceeded the threshold range stipulated by the Canadian Council of Ministers of the Environment water quality guideline recommended for the protection of aquatic life (CCME, 1999). The Diep River was therefore considered highly polluted with PAHs capable of adversely impacting aquatic lives.

Two separate reports from the Limpopo province detected PAHs in the Nandoni dam (Nthunya et al., 2019) and in both Blood and Mokolo rivers (Mogashane et al., 2022). In the three water bodies, individual PAHs concentration ranged from 0.0001 µg/L in the Nandoni dam to 1.53 µg/L in the Mokolo river. The Nandoni dam serves to provide a sustainable water-supply for domestic, irrigation as well as forestry purposes and concentrations of individual PAHs (naphthalene, acenaphthene, pyrene, benz(a)anthracene and benzo(a)pyrene) fell within the threshold limits which were typically less than 0.1 µg/L Concentrations varied per PAH, many of which were below regulatory bodies' threshold values such the USEPA, SANS 241, and WHO, but the total of the 16 priority PAHs was concerning (Nthunya et al., 2019). As for the two rivers, they are close to anthropogenic sources of pollution such as mining and industrial effluents which could have contributed pollution into the rivers. Low molecular weight PAHs were mostly not detected, and benzo(a)anthracene had the highest concentration at several sampling points. Comparing the two rivers, Mokolo has higher PAH concentrations than Blood River and this could be attributed to the coal mining and industries in proximity.

Seopela et al. (2022) reported on PAHs from Loskop dam in Mpumalanga Province. The dam is situated in a nature reserve and serves important functions associated with food security, wildlife conservation and tourism. The dam receives water from the much-polluted Olifants River. Total average concentration of PAHs across three years of sampling ranged from 0.15 to 49.8 µg/L. Compared to some other water bodies, this concentration is lower, but it tended to increase across the three years. Current contamination level was therefore deemed low to average but environmental monitoring is warranted.

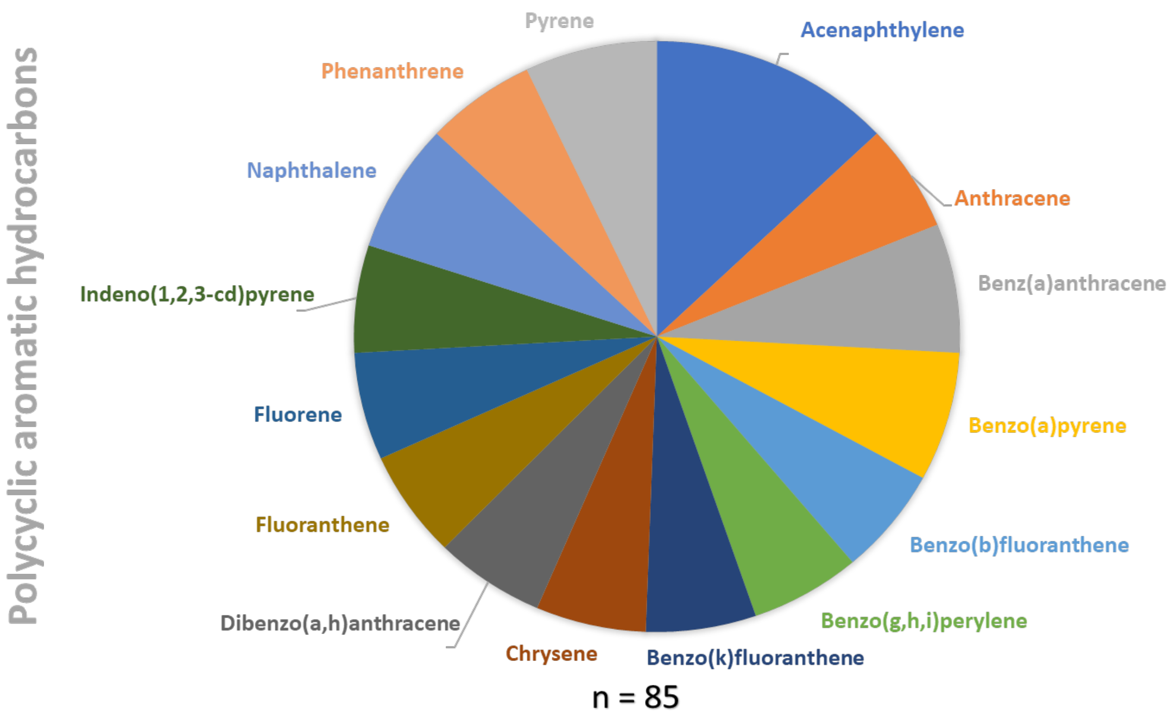


Figure 29: The frequency of terms of all Polycyclic aromatic hydrocarbons currently listed in the CEC Knowledge Hub

Triclosan

Triclosan, also referred to as TCS, is typically found in agricultural and domestic antibacterial and antifungal products (Glazer, 2004). Since 1972, it has been used or produced for use in hospitals and other medical institutions, but it is currently used in a variety of consumer goods, including soap, toothpaste, detergents, and insecticides (Alfhili and Lee, 2019). Triclosan is dispersed into our water systems by runoff, domestic disposal, and wastewater treatment plant outflow (Kaur et al., 2019). Triclosan can partially breakdown and produce hazardous metabolites and compounds. The dangers of exposure include the potential for hormone disruption and the activation of genes related to antimicrobial resistance (Marques et al., 2017).

Six studies – of which six sites were chosen – have been carried out overall based on the literature. The ranges detected were between 0,00 and 1264.2 mg/L. Most of the studies focused on wastewater treatment plants outputs in cities, with only a few on rural settlements and hospitals. Also, there is little or no date for provinces such as Mpumalanga, Eastern Cape and Free State.

3.3.2. Inorganic contaminants

Heavy metals

Metallic substances known as heavy metals often have a higher density than water. Cadmium (Cd), chromium (Cr), lead (Pb), and mercury (Hg) are a few examples of heavy metals that are regarded as emerging contaminants of concern. The majority of these are located in polluted areas such water bodies, agro-ecosystems, and industrial effluents (Iloms et al., 2020). Certain metals are highly soluble in salt form in aquatic environments, making them easily absorbed by living things and transferable to people through food consumption. They may have negative consequences, including harm to the brain, kidneys, and growing fetuses, and in rare situations, they may even be cancerous. Nonetheless, there are permissible amounts of heavy metals that are accepted in water, as per DWAF and WHO recommendations in Table 2, and these levels are associated with low health risks in humans (Kinuthia et al., 2020). The allowable standard limits for some metals of concern in water are as follows:

Table 2: Standard limit for drinking water quality (Edkopayi et al., 2018)

Metals	**DWAF guidelines (mg/L)**	**WHO guidelines (mg/kg dry mass)**
Cadmium	0-0.005	3
Chromium	0-0.005	350
Lead	0-0.1	100
Zinc	0-3	200
Copper	0-1	120

In the majority of South Africa's water study sites undergoing research, several of these metals are present in excess of permitted limits. This necessitates more concern to the detection and measurement of heavy metals in SA water sources. The sequence of selected metals' human toxicity levels, according to Kinuthia et al. (2020), is Co Al Cr Pb Ni Zn Cu Cd Hg. However, over the past ten years, Cd, Hg, Cr, and Pb have attracted the most attention (Figure 30).

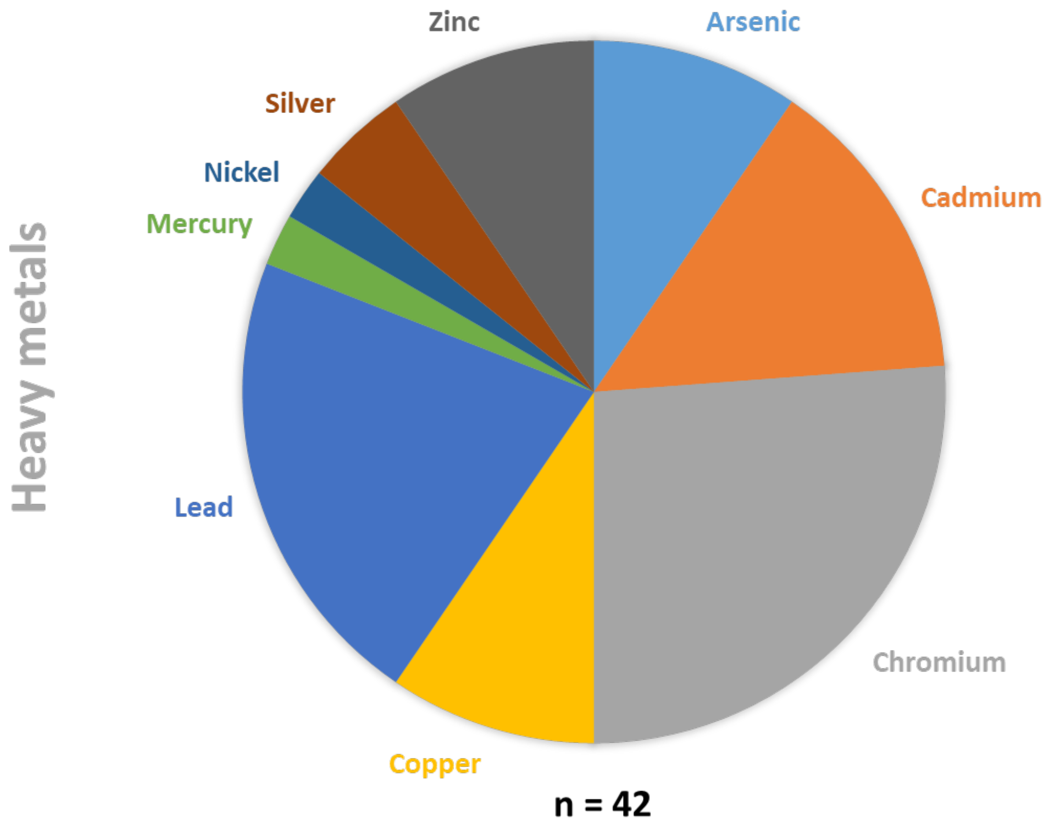


Figure 30: The frequency of terms of all Heavy metals currently listed in the CEC Knowledge Hub

3.3.3. Particulate contaminants

Microplastics

Plastic particles smaller than 5 mm are referred to as microplastics. Some of these particles are produced by the breakdown of bigger plastic particles, some are released into the environment as a result of the negligent disposal of plastic trash (nurdles), and some may develop originate as microbeads (Nel et al., 2017). According to Auta et al. (2017), land-based activities are to blame for the marine environment's microplastic contamination. Microplastics have entered the marine environment by leaching from landfills, sewage leaks, and effluents from wastewater treatment plants due to inefficient waste management systems, poor infrastructure, and ineffective legislative laws (Wang et al., 2020). Due to their non-biodegradable nature, plastic particles linger in marine bodies for decades once introduced into that environment. Since marine animals select the food range that microplastics fall into, it is inevitable that fish, mollusks, invertebrates, and plankton will consume microplastics (Mao et al., 2020; Wang et al., 2018). Given that they can act as adsorbents for other contaminants, such as pesticides, polyaromatic compounds, and heavy metals, microplastics' large surface areas make them more hazardous since they expose organisms to a range of contaminations in a single intake (Li et al., 2020). According to Mao et al. (2020), marine species' consumption of microplastics has detrimental effects on their health since it results in inflammation and mineral deficiencies, interferes with reproduction, and causes them to consume less food.

The literature reports 15 investigations on microplastics in South African water. Five of them concentrated on the eastern coast sites, two on the Orange and Vaal River sites, two on the Cape Town coast sites, two on the Braamfonteinspruit sites, one on the Plankenburg River site, one published dissertation on the Algoa Bay sites, one WRC report on rivers in Gauteng and the Northwest provinces, and the other centred on all of South Africa's coast lines. In general, a commonly used method for water sampling in South Africa was the use of manta trawl fitted with nylon mesh, followed by the use of sieves together with metal buckets. The advantage of using manta trawl is that microplastics are filtered through a huge amount of water sample as such giving a better representation of microplastics distribution in water. However, the pore size of the mesh is 300 μm thus disregarding microplastics that are smaller than that. Whereas in using sieves, mesh sizes of up to 5 μm can be used to trap microplastics of smaller diameter. The classification of microplastics rather than identifying the type of polymer used for production was the primary focus of the studies that were analysed (Figure 31). Only three out of 15 studies went on to identify the type of polymer the discovered microplastics were made of. Although other studies were conducted focusing on South African water bodies, majority of them focused on testing microplastics in sediments and invertebrates rather than surface water.

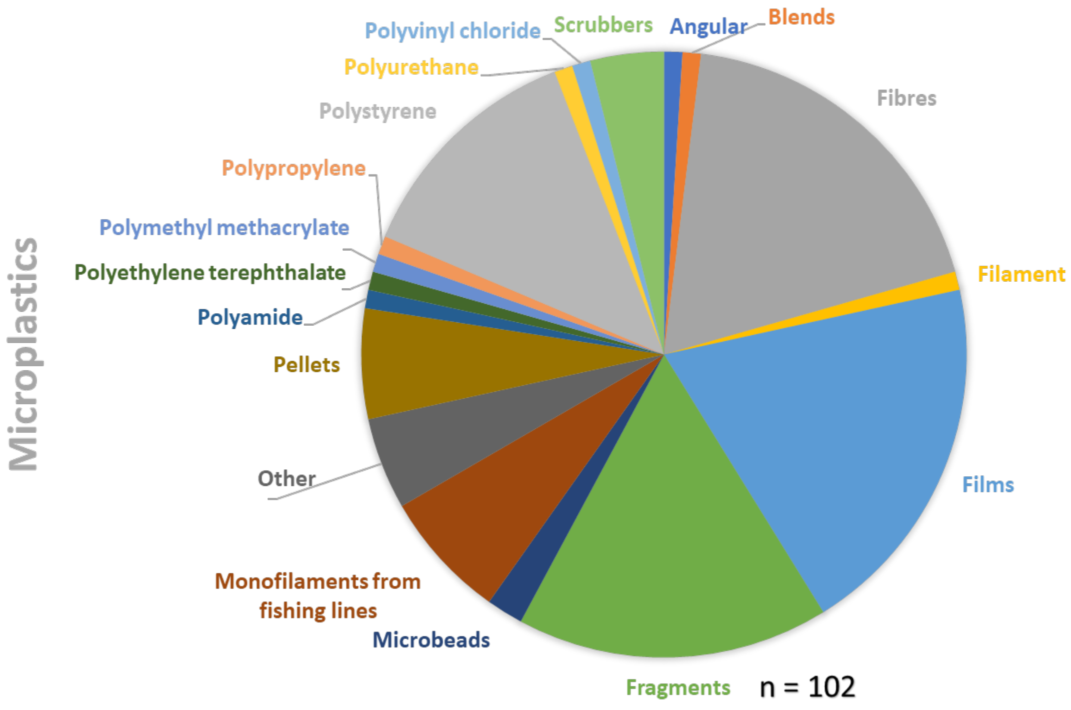


Figure 31: The frequency of terms of all Microplastics currently listed in the CEC Knowledge Hub

Engineered Nanomaterials (ENM)

Materials with at least one exterior dimension between 1 and 100 nm are referred to as nanomaterials. According to the criteria provided by the European Commission, at least half of the particles in the number size distribution must have a particle size of 100 nm or less (2011/696/EU). Nanomaterials can be produced for a specific use in industry, occur naturally, or be produced as combustion reaction byproducts. When compared to their bulk counterparts, nanomaterials typically have unique physical and chemical properties (metals or carbon based).

The production of nanomaterials can be done as very thin surface coatings (one dimension), nanowires and nanotubes (two dimensions), or nanoparticles (three dimensions) (Mansoori & Soelaiman, 2005). By advancing nanotechnology, ENMs can be used to create durable and more effective materials that take use of the unique properties found at the nanoscale. Nanomaterials are used in medicine for in vivo drug administration, optical image enhancement, and diagnostic products (Klaine et al., 2008).

Nanomaterials have the potential to release into the environment at any or all stages of the production process, from release during synthesis to release at the end of product life, due to their wide variety of applications. These ENMs can interact with environmental media to agglomerate, weakly bind to suspended solids or sediment, become ingested or accumulated by organisms and enter drinking water and food sources after they are discharged into the environment (Boxall et al., 2007). The fate of ENMs is determined by both their own properties and those of the ecosystem they are discharged into. Size, surface charge, functional groups, and particle make up are characteristics that may have an impact on how ENMs (metal or an organic) behave. Therefore, they can react differently in the environment and have a varied level of toxicity by changing one component of the ENM. Exposure to ENMs in the environment and in humans is increasing as ENM production develops. Scientific experts agree that assessing the risks associated with nanotechnology is challenging due to the difficulty in tracking the production of different ENMs and their effects (Nanoionics, 2016). The overall volume of industrial nanomaterials is predicted to rise from 1000 to 58000 tons by the year 2020. This raises serious concerns about the release of nanomaterials during manufacture (Cornelis, 2015). The Department of Science and Innovation (DSI) of South Africa launched a research platform in 2016 to look into the environmental, safety, and health implications of nanotechnology.

In South Africa, of the 45 manuscripts identified with the selected terms in Scopus, 54% of the studies were based on nanomaterial synthesis and applications. While 13.3% used modelling data to review the expected concentrations to be released into the environment. However only one of the three manuscripts of environmental data was found suitable (Maiga et al., 2020) which determined the concentration of titanium dioxide ENMs, found in sunscreen products, in five dams in South Africa. The concentrations of titanium ions determined by acid digesting the nanomaterials ranged between 14.87-43.94 µg/L while the agglomerates ranged between a means size of 102.91-158.92 nm. The highest concentration and agglomerates were found in North West while the smallest and lowest were found in two sites in the Western Cape.

Even though lab-based studies on ecotoxicological effects of ENMs have been reported for a number of aquatic organisms there is still the majority that is unknown. Scientific data on ENMs in the environment is scarce and further research is needed, specifically towards ENMs characterization and detection in different media as well as their biological and environmental fate (Klaine et al., 2008).

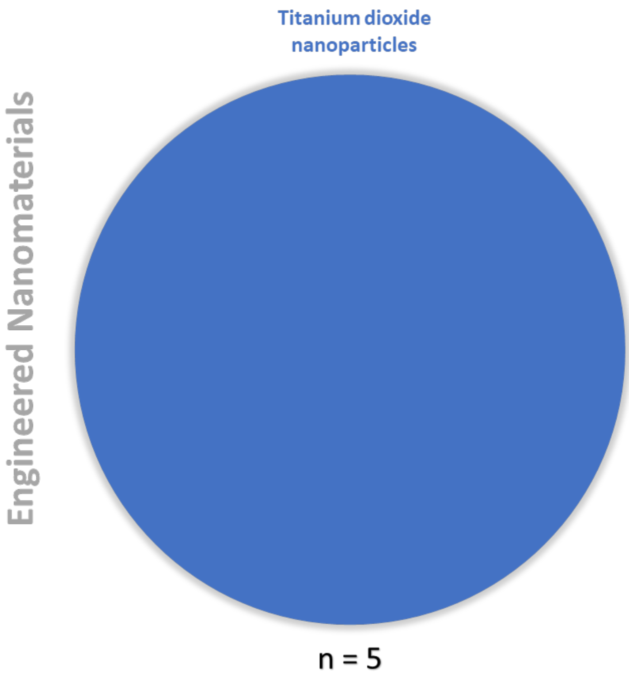


Figure 32: The frequency of terms of all Engineered nanomaterials currently listed in the CEC Knowledge Hub

3.3.4. Biological contaminants

Microbiological CECs

Concerning microbial contaminants in environmental water bodies include cyanobacteria, helminths, pathogenic bacteria, viruses, and protozoa (Ahmed et al., 2019). According to Masters et al. (2011), microbial contaminants can enter rivers from a variety of sources, including residential, veterinary, and industrial ones. Once there, they have the ability to infect both humans and animals and to cause epidemics of waterborne diseases. Waterborne microbiological pollutants must be carefully monitored and controlled due to their potential to pose serious health concerns (Alegbeleye et al., 2016). A thorough literature survey on microbial contaminants in South African waterways revealed that research focus on aquatic microbial contaminants has predominantly centred on indicators of faecal contamination such as *Escherichia coli* and coliforms (Enitan-Folami et al., 2020; Makhadi et al., 2020; Ololade et al., 2019). The criteria for contaminants of rising concern are not sufficiently met by such indicator species, which have typically been used to evaluate faecal contamination of rivers. Instead of limiting their findings to cultivable microorganisms, recent South African studies have reported on the use of cutting-edge molecular techniques such as Next Generation Sequencing (NGS) to uncover the abundance of potentially harmful microbes in a number of streams (Jordaan et al., 2019; Maguvu et al., 2020). These techniques allow for the detection of new microbial pollutants, such as pathogenic bacteria from the genus *Acinetobacter*, *Clostridium*, *Legionella*, *Pseudomonas* and *Serratia Tatlockia* as revealed in a study by Maguvu et al. (2020). Regarding whether aquatic contaminants influence microbial community structure, diversity, and ecological function, there is currently a substantial study deficit in South Africa. For instance, a number of research conducted outside of SA have shown a favourable relationship between heavy metal pollution of aquatic environments and the selection of genes for antibiotic resistance (Chen et al., 2019; Di Cesare et al., 2016; Dickinson et al., 2019). This is of particular concern due to the possibility of heavy metal pollution to indirectly induce pathogen outbreaks of multiple antibiotic resistant microbes. This also reiterates the need for aquatic CECs to be assessed in totality, not in isolation, as contaminants interact with each other and influence biotic parameters.

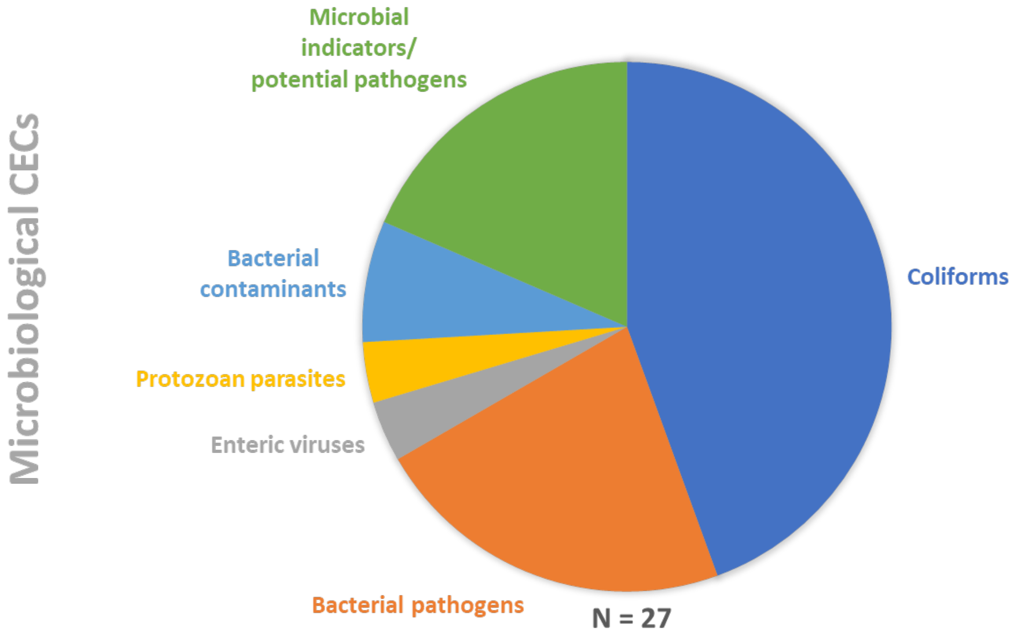


Figure 33: The frequency of terms of all Microbiological contaminants currently listed in the CEC Knowledge Hub

3.4. TOXICITY CATEGORIZATION

CECs cover tens of thousands of chemicals, making it impossible to review them all in depth in one document. By using key classes focused on significant types of CECs (alkylphenols and alkylphenol ethoxylates, bisphenols, organophosphate esters, phthalates, and PFAS), which can be classified either by function or societal use (current-use pesticides [and degradates] with urban applications; pharmaceuticals; personal care and cleaning product ingredients), the data becomes more manageable. It must be reiterated that this would not make the toxicology categorization absolute leaving large margins for error. The various metabolites biotransformation products of CECs could each have a different toxicological response. Another challenge is nanomaterials where the shape, composition, functional group, and dissolution play a significant role in the toxic potential of a compound. For example, citrate capped spherical shape nanogold has low toxicity while CTAB capped rod-shaped nanogold has high toxicity (Carnovale et al., 2019). Therefore, various factors are at play while toxicity is directly related to human health and environmental risk and caution should be taken in drawing conclusions.

Anderson et al. (2012) proposed a chemical-by-chemical risk-based approach for screening CECs to determine those most likely to be a threat to ecological receptors or public health. The establishment of monitoring trigger levels (MTLs), which can be used as a technique to conservatively identify particular CECs that might be considered for further monitoring in different types of ecosystems, is a step in the risk-based screening process. This risk assessment comprises of four steps. (i) Develop MTLs for CECs that, based on reported effects concentrations, pose the highest potential harm to aquatic systems. (ii) Compile measured or predicted environmental concentrations for CECs for which MTLs could be estimated. (iii) Identify those CECs that have the greatest potential to pose a risk by determining a

CECs monitoring trigger quotient; calculated by dividing the measure/predicted value by the MTL and where this value is greater than "1" are then identified for further monitoring. (iv) Apply the approach to representative scenarios that capture the key types of exposure (sources and fate) to water systems receiving CECs (Maruya et al., 2013).

Sutton et al. (2022) have followed this approach using a three-tiered categorization model based on risk quotients. A risk quotient (RQ) is the ratio between a point estimate of exposure (likelihood of exposure) and a point estimate of effects (once exposed how the organism responds). The RQ is highly dependent on the type of environmental matrix as well as the physicochemical parameters of water, the approach is to determine each compound's 90th percentile concentration to its appropriate ecological risk threshold. Each tier is then assigned according to the following categories:

- *High Concern*

RQs between 10 and 100. Examples with this category are: imidacloprid, pyrethroids, and specific pharmaceuticals (ibuprofen, fluoxetine, and azithromycin).

- *Moderate Concern*

RQs between 1 and 10. Examples with this category are: Bisphenols and some additional pharmaceuticals (metoprolol, gemfibrozil, ciprofloxacin, clarithromycin, and erythromycin).

- *Low Concern*

RQs less than 1. Examples with this category are: Antimicrobial-triclosan and the synthetic musk galaxolide.

CHAPTER 4: CONCLUSIONS & RECOMMENDATIONS

4.1 CONCLUSIONS

The creation of a CEC Knowledge Hub with a basis in South Africa has been essential in establishing a digital specimen bank of collected pollution data. The strength of the data will increase as additional information is submitted to the Hub, even though it already indicates where the majority of research has been conducted and areas of concern have been identified in South Africa. In the future, as the Hub becomes more populated, we expect it's usage to become more routine in any sciences related to CECs in the environment. Due to seasonal fluctuations in data and potential limitations in the detection methods utilized, responsible scientific communication is essential, and skilled researchers are needed to analyse and understand the material extracted from the hub. The toxicological assessment is a vast undertaking and requires various stakeholders to work together in order to build a categorization that is trusted and based on a high level of science.

4.2 RECOMMENDATIONS

The development and the establishment of a knowledge hub was limited to contaminants of emerging concern characterised in surface waters (rivers, lakes, springs, dams) in South Africa. There are gaps in the CECs reported in different provinces and this could be potentially addressed by including unpublished data that is collected by the custodian government departments as part of national, provincial and municipal monitoring of water quality in resources programmes. The recent spate of beaches in the eastern and western coasts of South Africa closing due to major sewage pollution, highlights the need to expand the knowledge hub to include other water resources such as marine water and estuaries. According to an article published in The Conversation (2022), in 2013, 29% of SA wastewater treatment plants were in a critical state. In 2022, the number has risen to 39% (Winter and Carden, 2022), this warrants the scope of the knowledge hub to be potentially expanded to include wastewater treatment plants.

To our knowledge there is no interactive knowledge hub for CECs that exists in South Africa or in SADC. Expanding and establishing a regional knowledge hub within the SADC is recommended to improve the regional data output and environmental monitoring campaigns that would benefit the SADC region, which in some instances share aquatic ecosystems.

REFERENCES

- ABU-KHASAN, M. AND EGOROV, V., 2020, February. The Influence of Different Types of Reinforcement on the Deformation Characteristics of Clay Soil in the Conditions of Seasonal Freezing and Thawing. In IOP conference series: materials science and engineering (Vol. 753, No. 4, p. 042083). IOP Publishing.
- ACIR I.H., GUENTHER K. (2018) Endocrine-disrupting metabolites of alkylphenol ethoxylates – a critical review of analytical methods, environmental occurrences, toxicity, and regulation. Sci Total Environ 635:1530-1546. https://doi.org/10.1016/j.scitotenv.2018.04.079
- ADENIJI, A. O., OKOH, O. O., & OKOH, A. I. (2019). Distribution pattern and health risk assessment of polycyclic aromatic hydrocarbons in the water and sediment of Algoa Bay, South Africa. Environmental geochemistry and health, 41(3), 1303-1320. https://doi.org/10.1007/s10653-018-0213-x(0123456789().,-volV)(0123456789().,-volV)
- ADENIJI, A. O., OKOH, O. O., & OKOH, A. I. (2019). Levels of polycyclic aromatic hydrocarbons in the water and sediment of Buffalo River Estuary, South Africa and their health risk assessment. Archives of environmental contamination and toxicology, 76(4), 657-669. https://doi.org/10.1007/s00244-019-00617-w
- AGUNBIADE, F.O., MOODLEY, B. (2016). Occurrence and distribution pattern of acidic pharmaceuticals in surface water, wastewater, and sediment of the Msunduzi River, KwaZulu-Natal, South Africa. Environmental Toxicology and Chemistry, 35(1), pp.36-46.
- AHMED, W., HAMILTON, K., TOZE, S., COOK, S., & PAGE, D. (2019). A review on microbial contaminants in stormwater runoff and outfalls: Potential health risks and mitigation strategies. Science of the Total Environment, 692, 1304-1321.
- ALEGBELEYE, O. O., OPEOLU, B. O., JACKSON, V. A. (2016). Investigation into the bacterial pollution levels at various sites along the Diep and Plankenburg river systems, 3 Western Cape, South Africa. Water Science and Technology, 73(11), 2590-2599.
- ALI, T.ES. AND LEGLER, J. (2010). Overview of the Mammalian and Environmental Toxicity of Chlorinated Paraffins. In: Boer, J. (eds) Chlorinated Paraffins. The Handbook of Environmental Chemistry, vol 10. Springer, Berlin, Heidelberg. https://doi.org/10.1007/698_2010_56.
- AMIN, M.T., ALAZBA, A.A. & MANZOOR, U. 2014. A Review of Removal of Pollutants from Water/Wastewater Using Different Types of Nanomaterials. Advances in Materials Science and Engineering, 2014.
- ANDERSON P.D., DENSLOW N.D., DREWES J.E., OLIVIERI A.W., SCHLENK D., SCOTT G.I., SNYDER S.A. 2012. Monitoring strategies for chemicals of emerging concern (CECs) in California's aquatic ecosystems. Recommendations of a Science Advisory Panel. Final Report. Costa Mesa (CA), USA: Southern California Coastal Water Research. Project Authority. Technical Report 692.
- ARNOLD, K.E., BROWN, A.R., ANKLEY, G.T. AND SUMPTER, J.P. 2014. Medicating the environment: assessing risks of pharmaceuticals to wildlife and ecosystems. Philos Trans R Soc Lond B Biol Sci. 2014 Nov 19;369(1656):20130569. doi: 10.1098/rstb.2013.0569. PMID: 25405959; PMCID: PMC4213582.
- AUTA, H.S., EMENIKE, C.U., FAUZIAH, S.H. (2017). Distribution and importance of microplastics in the marine environment: A review of the sources, fate, effects, and potential solutions. Environment International, 102, pp. 165-176.
- AWAN, S., IPPOLITO, J.A., ULLMAN, J.L., ANSARI, K., CUI, L. AND SIYAL, A.A., 2021. Biochars reduce irrigation water sodium adsorption ratio. Biochar, 3(1), pp.77-87.
- AWE, A. A., OPEOLU, B. O., OLATUNJI, O. S., FATOKI, O. S., JACKSON, V. A., & SNYMAN, R. G. (2020). Occurrence of PAHs in water samples of the Diep River, South Africa. Water SA, 46(1), 80-93. https://doi.org/10.17159/wsa/2020.v46.i1.7888

- BAYEN, S., OBBARD J.P. AND THOMAS G.O. 2006. Chlorinated paraffins: a review of analysis and environmental occurrence. Environ Int. 2006 Sep;32(7):915-29. doi: 10.1016/j.envint.2006.05.009. Epub 2006 Jun 30. PMID: 16814386.
- BJURLID F., ROOS A., ERICSON JOGSTEN I., HAGBERG J. 2017. Temporal trends of PBDD/Fs, PCDD/Fs, PBDEs and PCBs in ringed seals from the Baltic Sea (Pusa hispida botnica) between 1974 and 2015. Sci Total Environ. 2018 Mar;616-617:1374-1383. doi: 10.1016/j.scitotenv.2017.10.178. Epub 2017 Oct 21. PMID: 29066193.
- BRITISH COLUMBIA (1993) Water quality. Ambient water quality criteria for polycyclic aromatic hydrocarbons (PAHs): Overview Report. Ministry of Environment, Lands and Parks, p 9
- BUNDSCHUH, M., FILSER, J., LÜDERWALD, S., MCKEE, M.S., METREVELI, G, SCHAUMANN, G.E., SCHULZ, R. & WAGNER, S. 2018. Nanoparticles in the environment: where do we come from, where do we go to? Environmental Sciences Europe, 30, pp. 6.
- CANADIAN COUNCIL OF MINISTERS OF THE ENVIRONMENT. 1999. Canadian water quality guidelines for the protection of aquatic life: Polycyclic aromatic hydrocarbons (PAHs). In: Canadian environmental quality guidelines, 1999, Canadian Council of Ministers of the Environment, Winnipeg.
- CARNOVALE, C., BRYANT, G., SHUKLA, R. AND BANSAL, V. 2019. Identifying Trends in Gold Nanoparticle Toxicity and Uptake: Size, Shape, Capping Ligand, and Biological Corona. ACS Omega 2019 4 (1), 242-256. DOI: 10.1021/acsomega.8b03227
- CARVALHO, R.N. CERIANI, L. IPPOLITO, A. LETTIERI, T. 2015. Development of the First Watch List under the Environmental Quality Standards Directive. JRC Science Hub (2015)
- CHAUKURA, N., GWENZI, W., TAVENGWA, N. AND MANYUCHI, M.M., 2016. Biosorbents for the removal of synthetic organics and emerging pollutants: opportunities and challenges for developing countries. Environmental Development, 19, pp.84-89.
- CHEN M.Y., LUO X.J., ZHANG X.L., HE M.J., CHEN S.J. AND MAI B.X. 2011. Chlorinated paraffins in sediments from the Pearl River Delta, South China: spatial and temporal distributions and implication for processes. Environ Sci Technol. 2011 Dec 1;45(23):9936-43. doi: 10.1021/es202891a. Epub 2011 Nov 4. PMID: 22014313.
- CHRUSTEK A., HOŁYŃSKA-IWAN I., DZIEMBOWSKA I., BOGUSIEWICZ J., WRÓBLEWSKI M., CWYNAR A., OLSZEWSKA-SŁONINA D. 2018. Current Research on the Safety of Pyrethroids Used as Insecticides. Medicina (Kaunas). 2018 Aug 28;54(4):61. doi: 10.3390/medicina54040061. PMID: 30344292; PMCID: PMC6174339.
- CHEN, H., JIA, Q., ZHAO, X., LI, L., NIE, Y., LIU, H. & YE, J. 2020. The occurrence of microplastics in water bodies in urban agglomerations: Impacts of drainage system overflow in wet weather, catchment land-uses, and environmental management practices. Water Research, 183, pp. 116073.
- CHOWDARY, V.M., RAO, N.H. AND SARMA, P.B.S., 2005. Decision support framework for assessment of non-point-source pollution of groundwater in large irrigation projects. Agricultural Water Management, 75(3), pp.194-225.
- CORWIN, D.L. AND YEMOTO, K., 2020. Salinity: Electrical conductivity and total dissolved solids. Soil Science Society of America Journal, 84(5), pp.1442-1461.
- DAUGHTON, C.G. 2004. Non-regulated water contaminants: emerging research. Environmental Impact Assessment Review. Volume 24, Issues 7-8. pp 711-732. ISSN 0195-9255,https://doi.org/10.1016/j.eiar.2004.06.003.
- DE VILLIERS, M.C., ELOFF, J.F., BARNARD, R.O., MULIBANA, E., MKHIZE, S. AND MSOMI, B., 2004. Land and water management: South Africa situation analysis. In Regional Situational Analysis: Land and Water Management in the SADC Region. SADC Workshop Proceedings (Vol. 1, pp. 93-112).
- DEPARTMENT OF HEALTH. 2010. Environmental health practitioner manual: a resource manual for environmental health practitioners working with aboriginal and torres strait islander

communities. Available from https://www1.health.gov.au/internet/publications/publishing.nsf/Content/ohp-enhealth-manual-atsi-cnt-l~ohp-enhealth-manual-atsi-cnt-l-ch6~ohp-enhealth-manual-atsi-cnt-l-ch6.1. [Accessed on 25/11/2020].

- DEPARTMENT OF ENVIRONMENT (2003) Assessment levels for soil, sediment and water. Contaminated sites management series, Western Australia. Version 3, p 21
- DEPARTMENT OF WATER AFFAIRS AND FORESTRY, AND WATER RESEARCH COMMISSION (1996). The Philosophy and Practice of Integrated Catchment Management – Implications for Water Resource Management in South Africa. WRC REPORT NO. TT 81/96.Water Research Commission, PRETORIADOS SANTOS, S., ADAMS, E.A., NEVILLE, G., WADA, Y., DE SHERBININ, A., BERNHARDT, E.M. AND ADAMO, S.B., 2017. Urban growth and water access in sub-Saharan Africa: Progress, challenges, and emerging research directions. Science of the Total Environment, 607, pp.497-508.
- DEPARTMENT OF WATER AND SANITATION. Green drop report 2022. https://ws.dws.gov.za/iris/releases/Report_DPW_Rev02_29Mar22_MN%20web.pdf
- DI CESARE A, ECKERT EM, D'URSO S, BERTONI R, GILLAN DC, WATTIEZ R, CORNO G. 2016. Co-occurrence of integrase 1, antibiotic and heavy metal resistance genes in municipal wastewater treatment plants. Water Res. 2016 May 1;94:208-214. doi: 10.1016/j.watres.2016.02.049. Epub 2016 Feb 23. PMID: 26945964.
- DICKINSON, A. W., POWER, A., HANSEN, M. G., BRANDT, K. K., PILIPOSIAN, G., APPLEBY, P., ... & VOS, M. (2019). Heavy metal pollution and co-selection for antibiotic resistance: A microbial palaeontology approach. Environment international, 132, 105117.
- EDOKPAYI JN, ODIYO JO, POPOOLA EO, MSAGATI TAM. 2018. Evaluation of Microbiological and Physicochemical Parameters of Alternative Source of Drinking Water: A Case Study of Nzhelele River, South Africa. Open Microbiol J. 2018 Feb 28;12:18-27. doi: 10.2174/1874285801812010018. PMID: 29541268; PMCID: PMC5842400.
- ENSLEY, S. M. 2018. Chapter 39 – Pyrethrins and Pyrethroids. Veterinary Toxicology (Third Edition). Academic Press, 2018. pp 515-520. ISBN 9780128114100. https://doi.org/10.1016/B978-0-12-811410-0.00039-8.
- ENITAN-FOLAMI, A. M., MUTILENI, N., ODIYO, J. O., SWALAHA, F. M., EDOKPAYI, J. N. (2020). Hadrochemical, bacteriological assessment, and classification of groundwater quality in Thulamela Municipality, South Africa: potential health risk. Human and Ecological Risk Assessment: An International Journal, 26(8), 2044-2058.
- FERNANDO, W.A.M., ILANKOON, I.M.S.K., SYED, T.H. AND YELLISHETTY, M., 2018. Challenges and opportunities in the removal of sulphate ions in contaminated mine water: A review. Minerals Engineering, 117, pp.74-90.
- FEY, M.V., 2010, August. A short guide to the soils of South Africa, their distribution and correlation with World Reference Base soil groups. In Proceedings (Vol. 19, pp. 32-35).
- FOROUDI, P. & MELEWAR, T. & GUPTA, SURAKSHA. (2017). Corporate Logo: History, Definition, and Components. International Studies of Management & Organization. 47. 176-196. 10.1080/00208825.2017.1256166
- GAVRILESCU M, DEMNEROVÁ K, AAMAND J, AGATHOS S, FAVA F. 2015. merging pollutants in the environment: present and future challenges in biomonitoring, ecological risks and bioremediation. N Biotechnol. 2015 Jan 25;32(1):147-56. doi: 10.1016/j.nbt.2014.01.001. Epub 2014 Jan 21. PMID: 24462777.
- GRABICOVA, K., GRABIC, R., FEDOROVA, G., FICK, J., CERVENY, D., KOLAROVA, J., TUREK, J., ZLABEK, V. AND RANDAK, T., 2017. Bioaccumulation of psychoactive pharmaceuticals in fish in an effluent dominated stream. Water research, 124, pp.654-662.
- GUMBI, B.P., MOODLEY, B., BIRUNGI, G. AND NDUNGU, P.G. (2017). Assessment of nonsteroidal anti-inflammatory drugs by ultrasonic-assisted extraction and GC-MS in Mgeni

and Msunduzi river sediments, KwaZulu-Natal, South Africa. Environmental Science and Pollution Research, 24(24), pp.20015-20028. DOI 10.1007/s11356-017-9653-6
- HALDEN, R. U. 2015. Epistemology of contaminants of emerging concern and literature meta-analysis. Journal of Hazardous Materials, 282, pp. 2-9.
- HONDA, R.J., KEENE, V., DANIELS, L. & WALKER, S.L. 2014. Removal of TiO2 Nanoparticles During Primary Water Treatment: Role of Coagulant Type, Dose, and Nanoparticle Concentration. Environmental Engineering Science, 31, pp. 127-134.
- ILOMS, E., OLOLADE, O.O., OGOLA, H.J. AND SELVARAJAN, R. 2020. Investigating industrial effluent impact on municipal wastewater treatment plant in Vaal, South Africa. International Journal of Environmental Research and Public Health, 17(3), p.1096.
- JAMBECK, J.R., GEYER, R. WILCOX, C. SIEGLER, T.R., PERRYMAN, M. ANDRADY, M., NARAYAN, R., & LAW, K.L. 2015. Plastic waste inputs from land into the ocean. Science, 347, pp. 768-771.
- JIANG, L., HE, S., WANG, D., LI, C., ZHOU, X. & YAN, B. 2020. Polyvinylidene fluoride micropore membrane for removal of the released nanoparticles during the application of nanoparticle-loaded water treatment materials. Journal of Cleaner Production, 261, pp. 121246.
- JOERGENSEN, R.G. AND EMMERLING, C., 2006. Methods for evaluating human impact on soil microorganisms based on their activity, biomass, and diversity in agricultural soils. Journal of Plant Nutrition and Soil Science, 169(3), pp.295-309.
- JORDAAN, K., COMEAU, A. M., KHASA, D. P., & BEZUIDENHOUT, C. C. (2019). An integrated insight into the response of bacterial communities to anthropogenic contaminants in a river: A case study of the Wonderfonteinspruit catchment area, South Africa. PloS one, 14(5), e0216758.
- JURADO, A., VÀZQUEZ-SUÑÉ, E., CARRERA, J., DE ALDA, M.L., PUJADES, E. AND BARCELÓ, D., 2012. Emerging organic contaminants in groundwater in Spain: a review of sources, recent occurrence and fate in a European context. Science of the total environment, 440, pp.82-94.
- KAMPIRE, E., RUBIDGE, G. AND ADAMS, J.B. 2017. Characterization of polychlorinated biphenyls in surface sediments of the North End Lake, Port Elizabeth, South Africa. Water SA. DOI: 10.4314/wsa.v43i4.12.
- KHURANA, P., THATAI, S., SAPNAC & KUMAR, D. 2019. Destruction of recalcitrant nanomaterials contaminants in industrial wastewater. Emerging and Nanomaterial Contaminants in Wastewater, Elsevier, pp. 137-158.
- KINUTHIA, G.K., NGURE, V., BETI, D., LUGALIA, R., WANGILA, A. AND KAMAU, L. (2020). Levels of heavy metals in wastewater and soil samples from open drainage channels in Nairobi, Kenya: Community health implication. Scientific Reports, 10(1), pp.1-13.
- KLAINE, S.J., EDGINGTON, A., SEDA, B. (2013). Nanomaterials in the Environment. Encyclopedia of Aquatic Ecotoxicology. Springer, New York, NY.
- KLAINE, S.J., ALVAREZ, P.J.J., BATLEY, G.E., FERNANDES, T.F., HANDY, R.D., DELINE, L.Y., MAHENDRA, S., MCLAUGHLIN, M.J., LEAD, J.R. (2009). Nanomaterials in the Environment: Behaviour, Fate, Bioavailability and Effects. Environmental Toxicology and Chemistry, 27 (9): 1825-1851
- KLOSTERHAUS, S., R.M. ALLEN, AND J. DAVIS. 2012. Contaminants of Emerging Concern in the San Francisco Estuary: Alkylphenol Ethoxylates. A Report of the Regional Monitoring Program for Water Quality in the San Francisco Estuary. SFEI Contribution #657. Final Report. San Francisco Estuary Institute, Richmond, CA.
- LE ROUX, P.A.L., DU PREEZ, C., STRYDOM, M., VAN RENSBURG, L. AND BENNIE, A., 2007. Effect of irrigation on soil salinity profiles along the Lower Vaal River, South Africa. Water Sa, 33(4).

- LI, P., ZOU, X., WANG, X., SU, M., CHEN, C., SUN, X. & ZHANG, H. 2020. A preliminary study of the interactions between microplastics and citrate coated silver nanoparticles in aquatic environments. Journal of Hazardous Materials, 385, pp. 121601.
- MADKOUR, L.H. 2020. Metal nanoparticles (MNPs) and particulate matter (PM) induce toxicity. Reactive Oxygen Species (ROS) Nanoparticles, and Endoplasmic Reticulum (ER) Stress-Induced Cell Death Mechanism, Academic Press, pp. 397-419.
- MAGUVU TE, BEZUIDENHOUT CC, KRITZINGER R, TSHOLO K, PLAATJIE M, MOLALE-TOM LG, MIENIE CM, COERTZE RD. 2020. Combining physicochemical properties and microbiome data to evaluate the water quality of South African drinking water production plants. PLoS One. 2020 Aug 13;15(8):e0237335. doi: 10.1371/journal.pone.0237335. PMID: 32790793; PMCID: PMC7425920.
- MAKHADI, R., OKE, S. A., & OLOLADE, O. O. (2020). The Influence of Non-Engineered Municipal Landfills on Groundwater Chemistry and Quality in Bloemfontein, South Africa. Molecules, 25(23), 5599.
- MAIGA, D.T., MAMBA, B.B., MSAGATI, T.A.M. (2020). Distribution profile of titanium dioxide nanoparticles in South African aquatic systems. Water Supply, 20 (2): 516-528. doi: https://doi.org/10.2166/ws.2019.185.
- MAO, R., HU, Y., ZHANG, S., WU, R., GUO, X. 2020. Microplastics in the surface water of Wuliangsuhai Lake, northern China. Science of The Total Environment, 723, pp. 137820.
- MANSOORI, G.A., AND SOELAIMAN, T.A. (2005). Nanotechnology — An Introduction for the Standards Community. Journal of Astm International, 2, 1-22.
- MARUYA, K. A., SCHLENK, D., ANDERSON, P. D., DENSLOW, N. D., DREWES, J. E., OLIVIERI, A. W., … SNYDER, S. A. (2013). An Adaptive, Comprehensive Monitoring Strategy for Chemicals of Emerging Concern (CECs) in California's Aquatic Ecosystems. Integrated Environmental Assessment and Management, 10(1), 69-77. doi:10.1002/ieam.1483
- MASTERS, N., WIEGAND, A., AHMED, W. & KATOULI, M. (2011). Escherichia coli virulence gene profile of surface waters as an indicator of water quality. Water Research 45 (19), 6321-6333.
- MASUBELELE, M.L., HOFFMAN, M.T. AND BOND, W.J., 2015. Biome stability and long-term vegetation change in the semi-arid, south-eastern interior of South Africa: A synthesis of repeat photo-monitoring studies. South African Journal of Botany, 101, pp.139-147.
- MOGASHANE, T. M., MUJURU, M., & AMBUSHE, A. A. (2022). Determination and distribution of 16 polycyclic aromatic hydrocarbons in water samples from Blood and Mokolo Rivers in Limpopo Province, South Africa. Physics and Chemistry of the Earth, Parts A/B/C, 103165. https://doi.org/10.1016/j.pce.2022.103165
- MOJIRI, A., ZHOU, J. L., OHASHI, A., OZAKI, N., KINDAICHI, T. (2019). Comprehensive review of polycyclic aromatic hydrocarbons in water sources, their effects and treatments. Science of the Total Environment, 696, 133971.
- MOODLEY, B., BIRUNGI, G. & NDUNGU, P. 2016. Detection and Quantification of Emerging Organic Pollutants in the Umgeni and Msunduzi Rivers. Water Research Counsil Report No. 2215/1/16. Available from: http://www.wrc.org.za/wp-content/uploads/mdocs/2215-1-16.pdf. [Accessed on: 25/11/2020].
- MORI, T., ISHIZUKA, S., KONDA, R., GENROKU, T., NAKAMURA, R., KAJINO, H., WICAKSONO, A., HERIYANTO, J., HARDJONO, A. AND OHTA, S., 2018. Potassium and magnesium in leaf and top soil affected by triple superphosphate fertilisation in an Acacia mangium plantation. Journal of Tropical Forest Science, pp.1-8.
- NATIONAL WATER ACT 36 OF 1998 | SOUTH AFRICAN GOVERNMENT. https://www.gov.za/documents/national-water-act

- NECIBI, M.C.; DHIBA, D.; EL HAJJAJI, S. 2021. Contaminants of Emerging Concern in African Wastewater Effluents: Occurrence, Impact and Removal Technologies. Sustainability 2021, 13, 1125. https://doi.org/10.3390/su13031125
- NEL, H.A., HEAN, J.W., NOUNDOU, X.S., FRONEMNA, P.W. (2017). Do microplastic loads reflect the population demographics along the southern African coastline? Marine Pollution Bulletin, 115, pp. 115-119.
- NELL, J.P. AND VAN HUYSSTEEN, C.W., 2018. Prediction of primary salinity, sodicity and alkalinity in South African soils. South African Journal of Plant and Soil, 35(3), pp.173-178.
- NOGUERA-OVIEDO, K. AND AGA, D.S., 2016. Lessons learned from more than two decades of research on emerging contaminants in the environment. Journal of Hazardous Materials, 316, pp.242-251.
- NTHUNYA, L N. KHUMALO, N P. VERLIEFDE, A R. MAMBA, B B. MHLANGA S D.2019. Quantitative analysis of phenols and PAHs in the Nandoni Dam in Limpopo Province, South Africa: A preliminary study for dam water quality management. Physics and Chemistry of the Earth, Parts A/B/C, Volume 112, 2019, Pages 228-236, ISSN 1474-7065, https://doi.org/10.1016/j.pce.2019.02.003
- ODENDAAL, C., SEAMAN, M.T., KEMP, G., PATTERTON, H.E. & PATTERTON, H.G. 2015. An LC-MS/MS based survey of contaminants of emerging concern in drinking water in South Africa. South African Journal of Science, 111, pp. 6.
- OLOLADE, O. O., MAVIMBELA, S., OKE, S. A., & MAKHADI, R. (2019). Impact of leachate from northern landfill site in Bloemfontein on water and soil quality: Implications for water and food security. Sustainability, 11(15), 4238.
- OWUSU-SEKYERE, E., SCHEEPERS, M.E. AND JORDAAN, H., 2016. Water footprint of milk produced and processed in South Africa: Implications for policy-makers and stakeholders along the dairy value chain. Water, 8(8), p.322.
- PACHECO-BLANDINO, I., VANNER, R. & BUZEA, C. 2012. Toxicity of nanoparticles. Toxicity of Building Materials, Woodhead Publishing, pp. 427-475.
- PANDEY, V.C. & SINGH, V. 2019. Exploring the Potential and Opportunities of Current Tools for Removal of Hazardous Materials From Environments. Phytomanagement of Polluted Sites, pp. 501-516.
- PARK, J. AND SANTAMARINA, J.C., 2017. Revised soil classification system for coarse-fine mixtures. Journal of Geotechnical and Geoenvironmental Engineering, 143(8), p.04017039.
- PETRIE, B., BARDEN, R. & KASPRZYK-HORDERN, B. 2015. A review on emerging contaminants in wastewaters and the environment: current knowledge, understudied areas and recommendations for future monitoring. Water Research, 72, pp. 3-27.
- PIRAMOON, S., ABEROOMAND P., SABER A.M., SIRWAN T., TAVASSOLI, A.M. 2017. Solid-phase nanoextraction of polychlorinated biphenyls in water and their determination by gas chromatography with electron capture detector. Journal of Separation Science. https://doi.org/10.1002/jssc.201600720
- POSCHENRIEDER, C., FERNÁNDEZ, J.A., RUBIO, L., PÉREZ, L., TERÉS, J. AND BARCELÓ, J., 2018. Transport and use of bicarbonate in plants: current knowledge and challenges ahead. International Journal of Molecular Sciences, 19(5), p.1352.
- POYNTON, H.C. AND VULPE, C.D., 2009. Ecotoxicogenomics: emerging technologies for emerging contaminants 1. JAWRA Journal of the American Water Resources Association, 45(1), pp.83-96.
- QUATRINI, R. AND JOHNSON, D.B., 2018. Microbiomes in extremely acidic environments: functionalities and interactions that allow survival and growth of prokaryotes at low pH. Current opinion in microbiology, 43, pp.139-147.

- RASA, K., HEIKKINEN, J., HANNULA, M., ARSTILA, K., KULJU, S. AND HYVÄLUOMA, J., 2018. How and why does willow biochar increase a clay soil water retention capacity?. Biomass and Bioenergy, 119, pp.346-353.
- RASHEED, T., BILAL, M., NABEEL, F., ADEEL, M. & IQBAL, H. M. N. 2019. Environmentally-related contaminants of high concern: Potential sources and analytical modalities for detection, quantification, and treatment. Environment International, 122, pp. 52-66.
- RIMAYI, C., CHIMUKA, L., GRAVELL, A., FONES, G.R. & MILLS, G.A. 2019. Use of the Chemcatcher® passive sampler and time-of-flight mass spectrometry to screen for emerging pollutants in rivers in Gauteng Province of South Africa. Environmental Monitoring and Assessment, 191, pp. 388-402 .
- RIMAYI, C., ODUSANYA, D., WEISS, J.M., DE BOER, J. AND CHIMUKA, L. (2018). Contaminants of emerging concern in the Hartbeespoort Dam catchment and the uMngeni River estuary 2016 pollution incident, South Africa. Science of the Total Environment, 627, pp.1008-689 1017. DOI: 10.1016/j.scitotenv.2018.01.263
- SAHIN, O., GUNES, A., TASKIN, M.B. AND INAL, A., 2017. Investigation of responses of some apple (Mallus x domestica Borkh.) cultivars grafted on MM106 and M9 rootstocks to lime-induced chlorosis and oxidative stress. Scientia Horticulturae, 219, pp.79-89.
- SAUVÉ S, DESROSIERS M. 2014. A review of what is an emerging contaminant. Chem Cent J. 2014 Feb 26;8(1):15. doi: 10.1186/1752-153X-8-15. PMID: 24572188; PMCID: PMC3938815.
- SAIDI, T. & DOUGLAS, T.S. 2017. Nanotechnology in South Africa – Challenges in evaluating the impact on development. South African Journal of Science, 113, pp. 7-8.
- SEOPELA, M. P., MCCRINDLE, R. I., COMBRINCK, S., & AUGUSTYN, W. (2020). Occurrence, distribution, spatio-temporal variability and source identification of n-alkanes and polycyclic aromatic hydrocarbons in water and sediment from Loskop dam, South Africa. Water Research, 186, 116350. https://doi.org/10.1016/j.watres.2020.116350.
- SEOPELA, M.P., MCCRINDLE, R.I., COMBRINCK, S., AUGUSTYN, W. 2022. Temporal and spatial variations of organochlorine pesticides (OCPs) and phthalates affecting the quality of water and sediment from Loskop Dam, South Africa. Water SA. http://dx.doi.org/10.17159/wsa/2021.v47.i2.10918
- SHEN, M., SONG, B., ZHU, Y., ZENG, G., ZHANG, Y., YANG, Y., WEN, X., CHEN, M. & YI, H. 2020. Removal of microplastics via drinking water treatment: Current knowledge and future directions. Chemosphere, 251, pp. 126612.
- SHEN, M., SONG, B., ZHU, Y., ZENG, G., ZHANG, Y., YANG, Y., WEN, X., CHEN, M. & YI, H. 2020. Removal of microplastics via drinking water treatment: Current knowledge and future directions. Chemosphere, 251, pp. 126612.
- SIBALI, L.L., OKONKWO, J.O. AND MCCRINDLE, R.I. (2010) Levels of Selected Alkylphenol Ethoxylates (APEs) in Water and Sediment Samples from Jukskei River Catchment Area in Gauteng, South Africa. Water SA, 36, 229-238.
- STEFANAKIS, A. I. & BECKER, J. A. (2020). A Review of Emerging Contaminants in Water: Classification, Sources, and Potential Risks. In I. Management Association (Ed.), Waste Management: Concepts, Methodologies, Tools, and Applications (pp. 177-202). IGI Global. https://doi.org/10.4018/978-1-7998-1210-4.ch008
- SUTTON, R; MILLER, E; WONG, A; MENDEZ, M; LIN, D. 2022. CECs in California’s Ambient Aquatic Ecosystems: Occurrence and Risk Screening of Key Classes. ASC Technical Report: Contribution #1066. Aquatic Science Center, Richmond, CA.
- TAYLOR, A.T., IRAGANJE, E. & LAI, EP.C. 2020. A method for the separation of TiO2 nanoparticles from Water through encapsulation with lecithin liposomes followed by adsorption onto poly(Llysine) coated glass surfaces. Colloids and Surfaces B: Biointerfaces, 187, pp. 110732.

- THIEBAULT, T., GUÉGAN, R. AND BOUSSAFIR, M. 2015. Adsorption mechanisms of emerging micro-pollutants with a clay mineral: Case of tramadol and doxepine pharmaceutical products. Journal of Colloid and Interface Science, 453, pp. 1-8.
- TIEN, C. J., WANG, Z. X. & CHEN, C. S. 2020. Microplastics in water, sediment and fish from the Fengshan River system: Relationship to aquatic factors and accumulation of polycyclic aromatic hydrocarbons by fish. Environmental Pollution, 265(Pt B), pp. 114962
- TURTON AR. 2000. Precipitation, People, Pipelines and Power in Southern Africa: Towards a 'Virtual Water'-based Political Ecology Discourse. In Stott P & Sullivan S. Eds. Political Ecology: Science, Myth and Power. London: Arnold & New York: Oxford University Press.
- US EPA. 2014. Priority Pollutant List. https://www.epa.gov/sites/default/files/2015-09/documents/priority-pollutant-list-epa.pdf
- VAN AVERBEKE, W., DENISON, J. AND MNKENI, P.N.S., 2011. Smallholder irrigation schemes in South Africa: A review of knowledge generated by the Water Research Commission. Water SA, 37(5), pp.797-808.
- VERLICCHI, P. AND GRILLINI, V., 2020. Surface water and groundwater quality in South Africa and Mozambique – Analysis of the Most critical pollutants for drinking purposes and challenges in water treatment selection. Water, 12(1), p.305.
- WANG, Z., SEDIGHI, M. AND LEA-LANGTON, A. 2020. Filtration of microplastic spheres by biochar: removal efficiency and immobilisation mechanisms. Water Research, 184, pp. 116165.
- WANG, W., YUAN, W., CHEN, Y. & WANG, J. 2018. Microplastics in surface waters of Dongting Lake and Hong Lake, China. Science of The Total Environment, 633, pp. 539-545.
- WEINSTEIN, J. E., DEKLE, J. L., LEADS, R. R. & HUNTER, R. A. 2020. Degradation of bio-based and biodegradable plastics in a salt marsh habitat: Another potential source of microplastics in coastal waters. Marine Pollution Bulletin, 160, pp. 111518.
- WHO recommended classification of pesticides by hazard and guidelines to classification, 2019 edition. Geneva: World Health Organization; 2020. Licence: CC BY-NC-SA 3.0 IGO
- WILLIAMS-WYNN, M. D. & NAIDOO, P. 2020. A review of the treatment options for marine plastic waste in South Africa. Marine Pollution Bulletin, 161, pp. 111785.
- WINTER, K., CARDEN, K. 2022. South Africa's ability to manage wastewater is collapsing: what's at risk. Available at https://theconversation.com/south-africas-ability-to-manage-wastewater-is-collapsing-whats-at-risk-181608. Accessed on 29 January 2023
- WOOD, T.P., DUVENAGE, C.S. AND ROHWER, E., 2015. The occurrence of anti-retroviral compounds used for HIV treatment in South African surface water. Environmental Pollution, 199, pp.235-243.
- XIAO, B., WANG, X., YANG, J., WANG, K., ZHANG, Y., SUN, B., ZHANG, T. & ZHU, L. 2020. Bioaccumulation kinetics and tissue distribution of silver nanoparticles in zebrafish: The mechanisms and influence of natural organic matter. Ecotoxicology and Environmental Safety, 194, pp. 110454.
- YADAV, A.N., 2017. Beneficial role of extremophilic microbes for plant health and soil fertility. J Agric Sci, 1(1), p.30.
- YERMIYAHU, U., TAL, A., BEN-GAL, A., BAR-TAL, A., TARCHITZKY, J. AND LAHAV, O., 2007. Rethinking desalinated water quality and agriculture. Science, 318(5852), pp.920-921.
- YILMAZ M., GÜL A., AND ERBAŞLI K. (2004) Acute toxicity of alpha-cypermethrin to guppy (Poecilia reticulata Pallas, 1859). Chemosphere 56:381-385.
- ZHAN H, HUANG Y, LIN Z, BHATT P, CHEN S. 2020. New insights into the microbial degradation and catalytic mechanism of synthetic pyrethroids. Environ Res. 2020 Mar;182:109138. doi: 10.1016/j.envres.2020.109138. Epub 2020 Jan 14. PMID: 32069744.
- ZHANG, C., WANG, S., SUN, D., PAN, Z., ZHOU, A., XIE, S., WANG, J. & ZOU, J. 2020. Microplastic pollution in surface water from east coastal areas of Guangdong, South China and

preliminary study on microplastics biomonitoring using two marine fish. Chemosphere, 256, pp. 127202.
- ZHANG, Y., SHEN, H., HE, X., THOMAS, B.W., LUPWAYI, N.Z., HAO, X., THOMAS, M.C. AND SHI, X., 2017. Fertilization shapes bacterial community structure by alteration of soil pH. Frontiers in Microbiology, 8, p.1325.

APPENDIX A: KNOWLEDGE HUB MANUAL

APPENDIX B: CONTAMINANT OF EMERGING CONCERN KNOWLEDGE HUB CODE

Knowledge Hub Manual

Ashira Roopnarain

4-3-2023

Contents

1. Introduction

Contaminants of Emerging Concern are unregulated pollutants that have previously been at levels below detection limits, which are now being detected by water professionals in our water bodies. These can include *Nanomaterials*, *Flame Retardants*, *Microplastics*, *Agricultural Waste*, *Microbial Contaminants*, *Heavy Metals*, *Pharmaceuticals* and *Personal Care Products*, which may cause ecological and human health impacts.

This **CEC Knowledge Hub** was developed with the aim to collate all published information of CECs in South Africa Water bodies.

2. How The System Works:

The system is web based and can be accessed via the following web browsers:

- Google Chrome
- Microsoft Edge
- Firefox

Unfortunately, based on some of the technologies used in developing this system, the other popular web browsers will not work.

The system can be accessed from the following URL: https://www.ceckh.agric.za

Clicking on the above supplied **URL**, will present the user with the **MAIN PAGE** of the **CEC KNOWLEDGE HUB:**

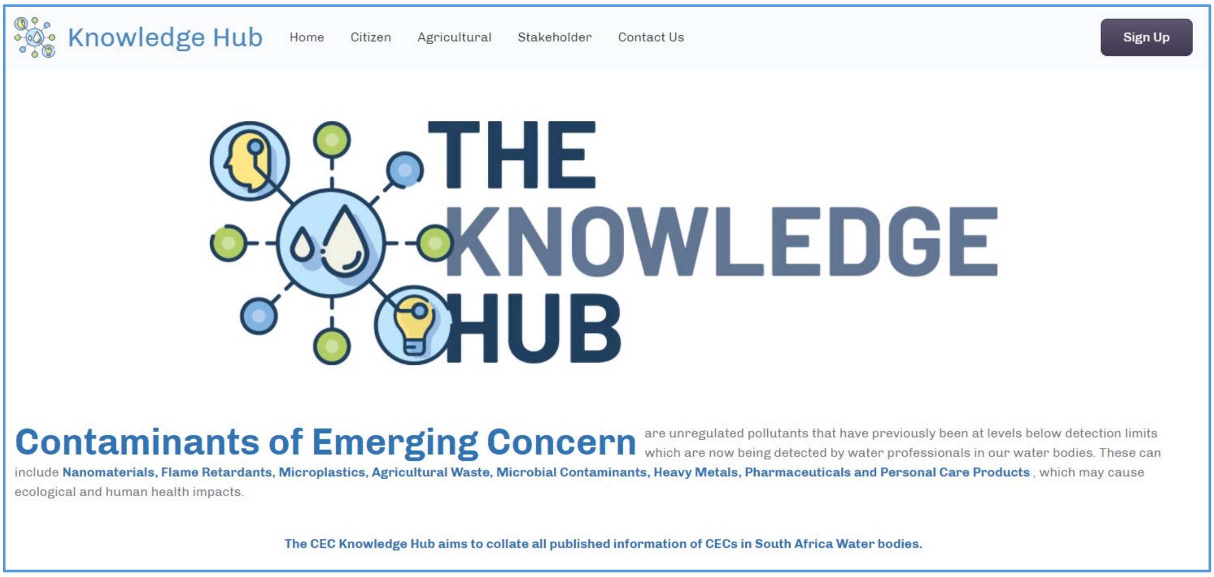


Figure 1: Home Page

From the **MAIN PAGE**, the user is presented with the following options, as can be seen in the menu ribbon at the top of the page:

- **CLICKABLE KNOWLEDGE HUB LOGO**
  - Takes the user back to the main page of the system

- **HOME**
  - Takes the user back to the main page of the system

- **CITIZEN**
  - Page containing profiles of various CEC's
  - Profiles for listed CEC's can be downloaded as a one-pager PDF document
  - Users can also view a short informative video expanding on the said CEC profile

- **AGRICULTURAL**
  - Page containing interactive image
  - Displaying the effects of additions of CEC's in our water bodies from various agricultural activities

- **STAKEHOLDER**
  - Restricted area of the system
  - Available to registered users only
  - Available options:
    - View CEC data spatially
    - Input CEC data (single record)
    - Bulk import of CEC data
    - Export CEC data to MS Excel format
    - Verification of captured CEC data (only for **System Admin** users)

- **CONTACT US**
  - Page showing the various partners / stakeholders / contributors to the project
  - Contact information, part of clickable logos

- Ability to send Comments or Suggestions

- **SIGN UP**
    - Page where users can register on the system

3. Different Options Explained:

3.1. Citizen:

Clicking this option, the user will be presented with the following page:

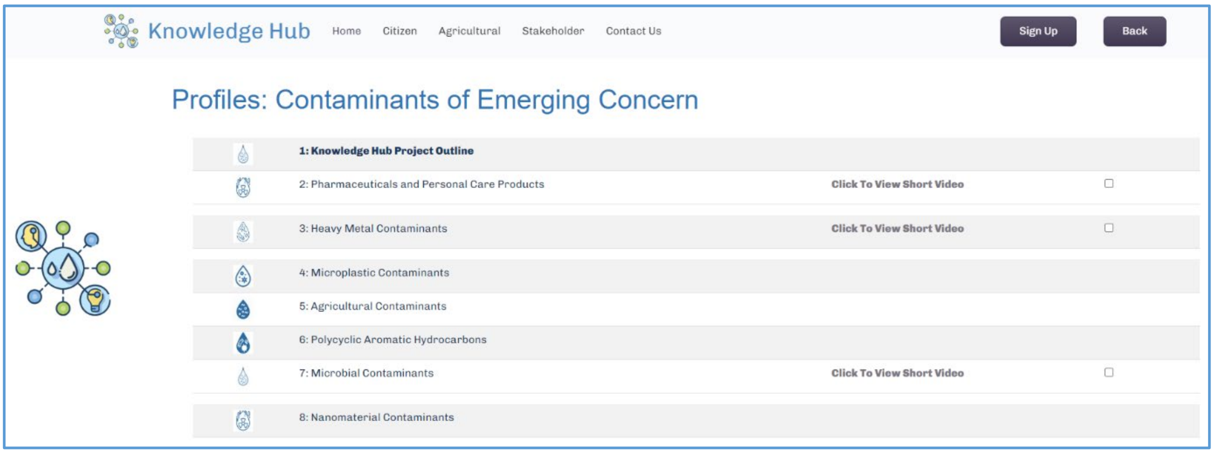


Figure 2: Citizen Page

The *CITIZEN Page* contains links to various **CEC Profiles**. These profiles can be downloaded as one-pager PDF documents by clicking on desired link of the relevant CEC profile.

Users also have the option to view short informative videos expanding on the selected CEC. These videos can be viewed by selecting or deselecting the corresponding check box, as shown in the image below:

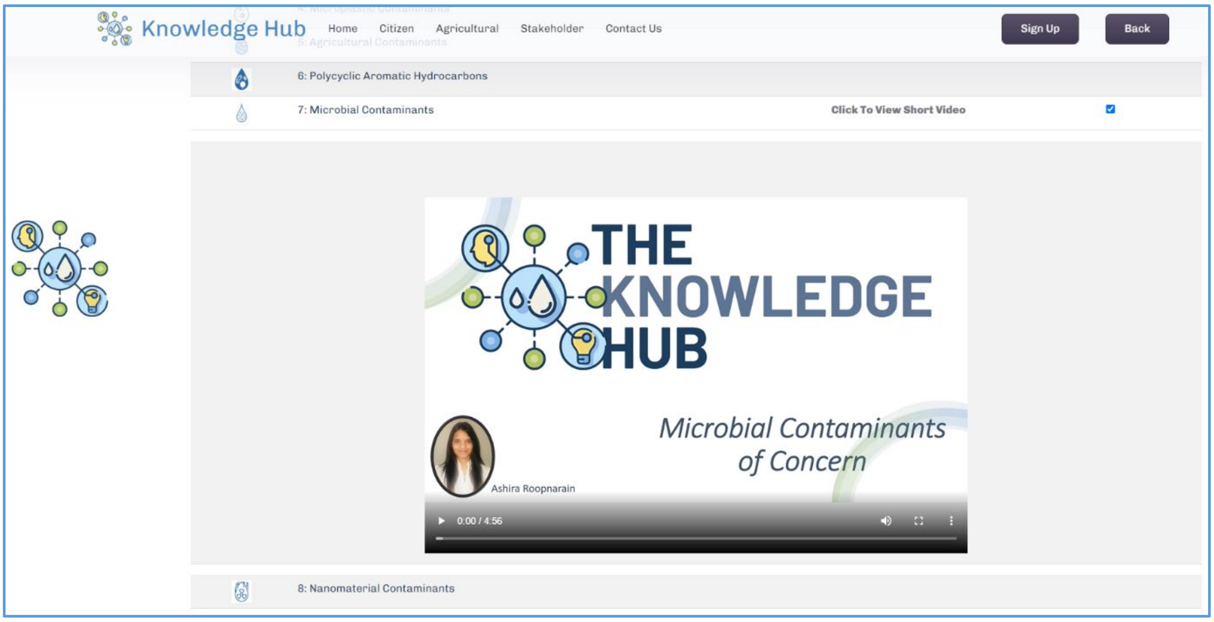
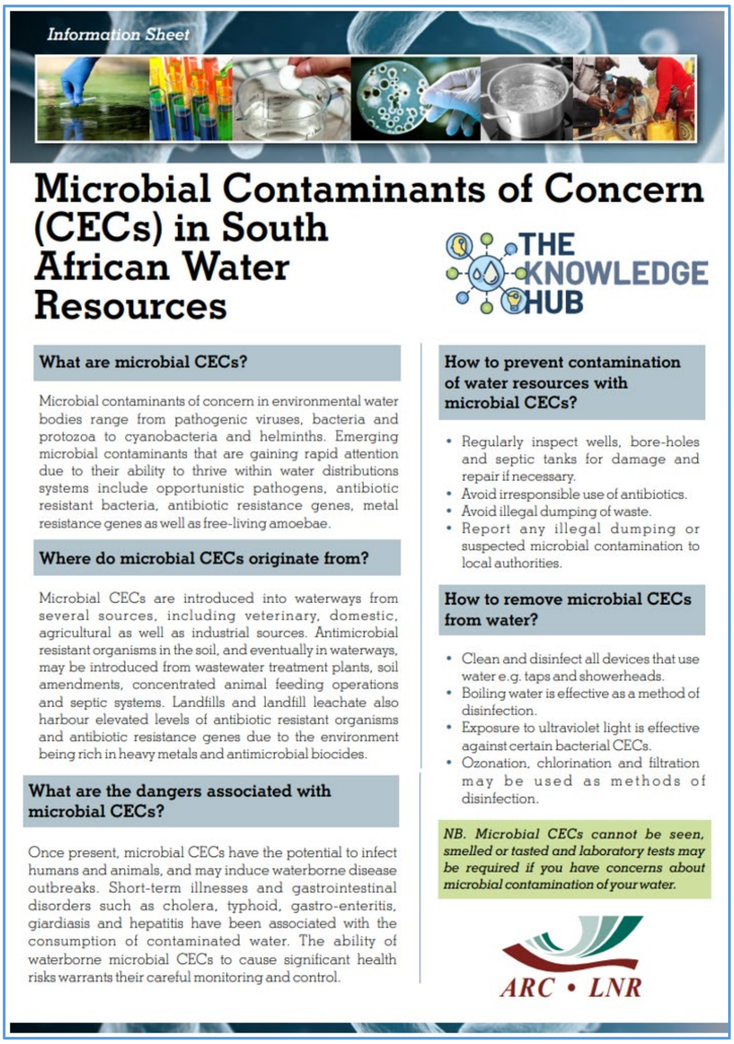


Figure 3: Videos

Below is an example of such a *CEC Profile Document*:



Information Sheet

Microbial Contaminants of Concern (CECs) in South African Water Resources

THE KNOWLEDGE HUB

What are microbial CECs?

Microbial contaminants of concern in environmental water bodies range from pathogenic viruses, bacteria and protozoa to cyanobacteria and helminths. Emerging microbial contaminants that are gaining rapid attention due to their ability to thrive within water distributions systems include opportunistic pathogens, antibiotic resistant bacteria, antibiotic resistance genes, metal resistance genes as well as free-living amoebae.

Where do microbial CECs originate from?

Microbial CECs are introduced into waterways from several sources, including veterinary, domestic, agricultural as well as industrial sources. Antimicrobial resistant organisms in the soil, and eventually in waterways, may be introduced from wastewater treatment plants, soil amendments, concentrated animal feeding operations and septic systems. Landfills and landfill leachate also harbour elevated levels of antibiotic resistant organisms and antibiotic resistance genes due to the environment being rich in heavy metals and antimicrobial biocides.

What are the dangers associated with microbial CECs?

Once present, microbial CECs have the potential to infect humans and animals, and may induce waterborne disease outbreaks. Short-term illnesses and gastrointestinal disorders such as cholera, typhoid, gastro-enteritis, giardiasis and hepatitis have been associated with the consumption of contaminated water. The ability of waterborne microbial CECs to cause significant health risks warrants their careful monitoring and control.

How to prevent contamination of water resources with microbial CECs?

- Regularly inspect wells, bore-holes and septic tanks for damage and repair if necessary.
- Avoid irresponsible use of antibiotics.
- Avoid illegal dumping of waste.
- Report any illegal dumping or suspected microbial contamination to local authorities.

How to remove microbial CECs from water?

- Clean and disinfect all devices that use water e.g. taps and showerheads.
- Boiling water is effective as a method of disinfection.
- Exposure to ultraviolet light is effective against certain bacterial CECs.
- Ozonation, chlorination and filtration may be used as methods of disinfection.

NB. Microbial CECs cannot be seen, smelled or tasted and laboratory tests may be required if you have concerns about microbial contamination of your water.

ARC • LNR

Figure 4: CEC Profile Document

Figure 4: CEC Profile Document

3.2. Agricultural:

Clicking this option, the user will be presented with the following page:

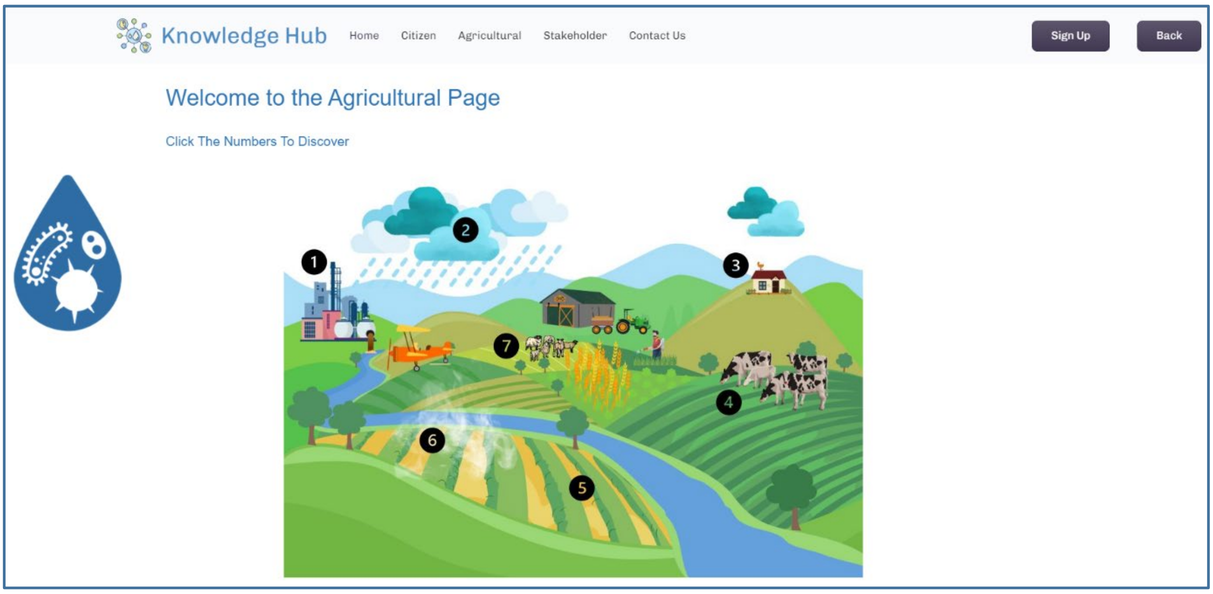


Figure 5: Agricultural Page

The *AGRICULTURAL Page* is an interactive representation of the effects of using certain practices in Agriculture which in turn adds to CEC's in water bodies.

By clicking on the black numbered circles, the image will change accordingly to display the associated effects.
The seven Agricultural practices / products indicated is:

1. Industrial upstream waste with Precision Agriculture
2. Acid Rain
3. Cleaning products
4. Pathogens
5. Fertilizers runoff
6. Spray drift pesticides
7. Pharmaceuticals

The image below shows **Number One** selected:

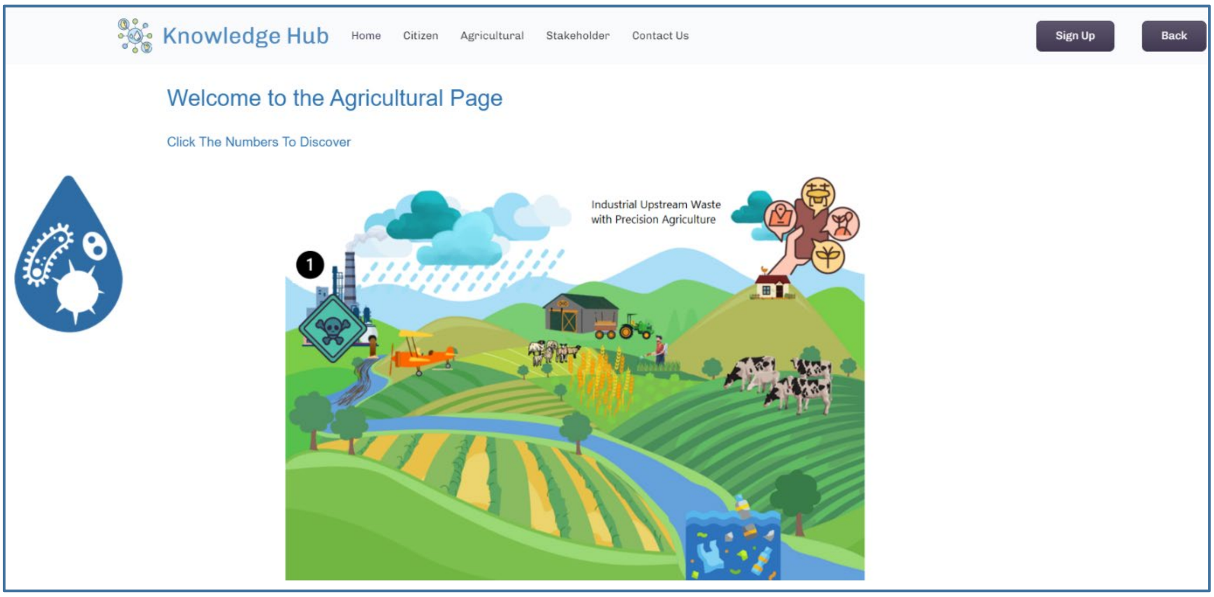


Figure 6: Number 1 selected

3.3. Stakeholder:

Clicking this option, the user will be presented with the following page used to log in to the **STAKEHOLDER** Section of the *CEC Knowledge Hub*:

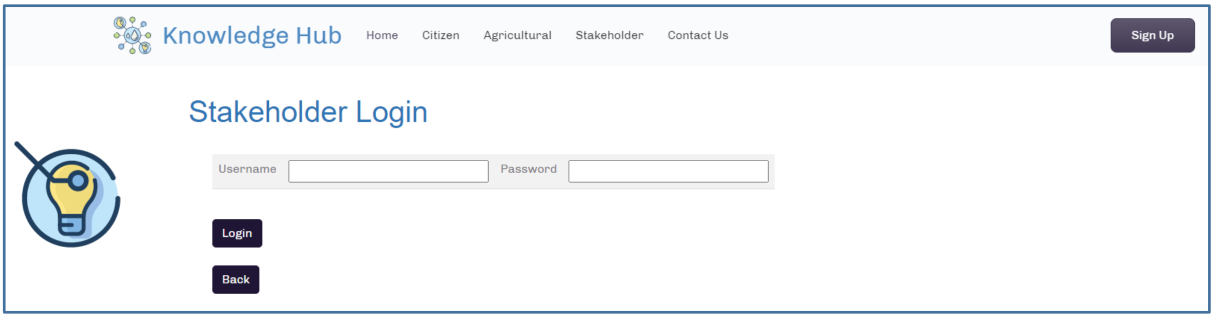


Figure 7: Stakeholder Login Page

After supplying your email address and password, click **LOGIN** to access the ***STAKEHOLDER Options***.

Alternatively, click on **SIGN UP** should you wish to register and access the **STAKEHOLDER Options**.

The **STAKEHOLDER Options Page** after a successful login:

Figure 8:Stakeholder Page

The following options are available to the user:

- **VIEW DATA**
  - View CEC Data spatially on a map

- **INPUT DATA**
  - Capture CEC Data in the system
  - Done record by record

- **BULK IMPORT DATA**
    - Bulk import of CEC data in MS-Excel format
    - MS-Excel file template should be used with this option
    - Can be downloaded from the *BULK IMPORT DATA* Page

- **EXPORT DATA**
    - Export CEC data in PDF Format
    - Grouped by ***CONTAMINANT TYPE***

If the current user is a **SYSTEM ADMIN User**, the **STAKEHOLDER Options Page** offers an added option, namely: **VERIFY CAPTURED DATA** as seen in the image below:

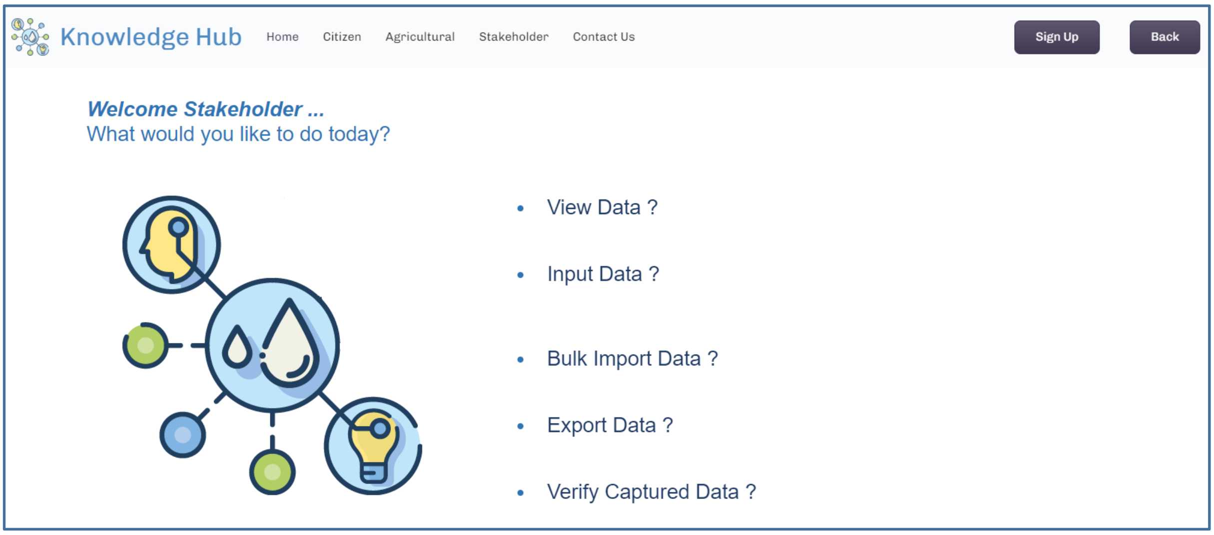


Figure 9: System Admin User Login Options

If an incorrect username and or password is supplied, the user will be presented with the following page:

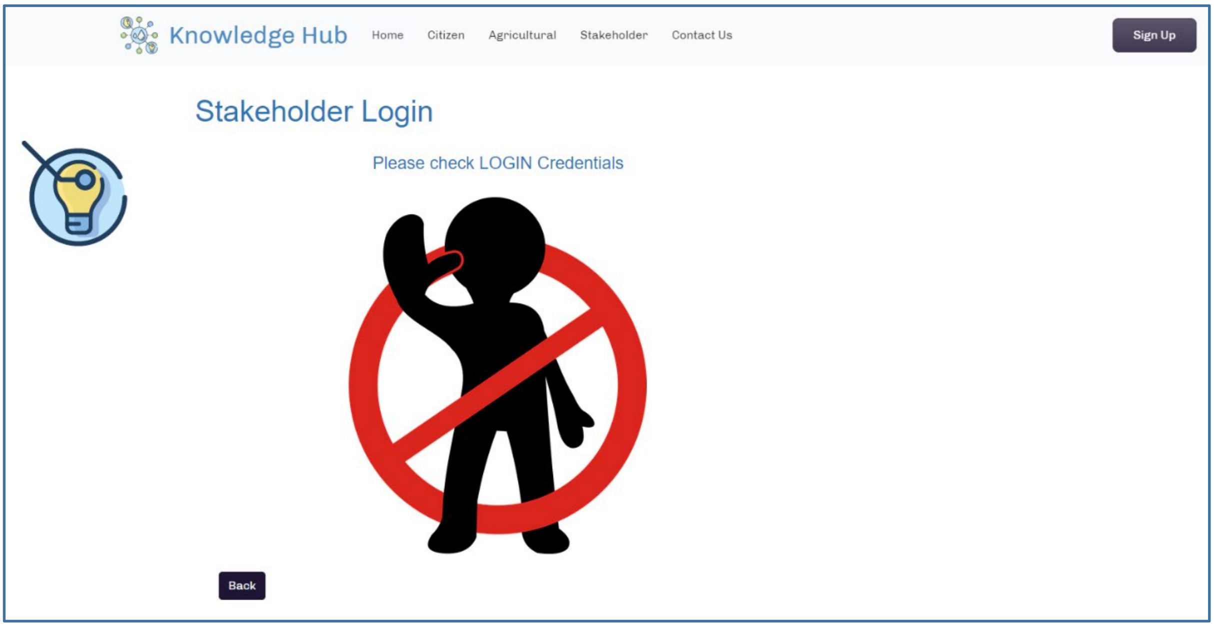


Figure 10: Login Error

Click the **BACK** button to supply the *Username* and *Password* again.

3.3.1. View Data

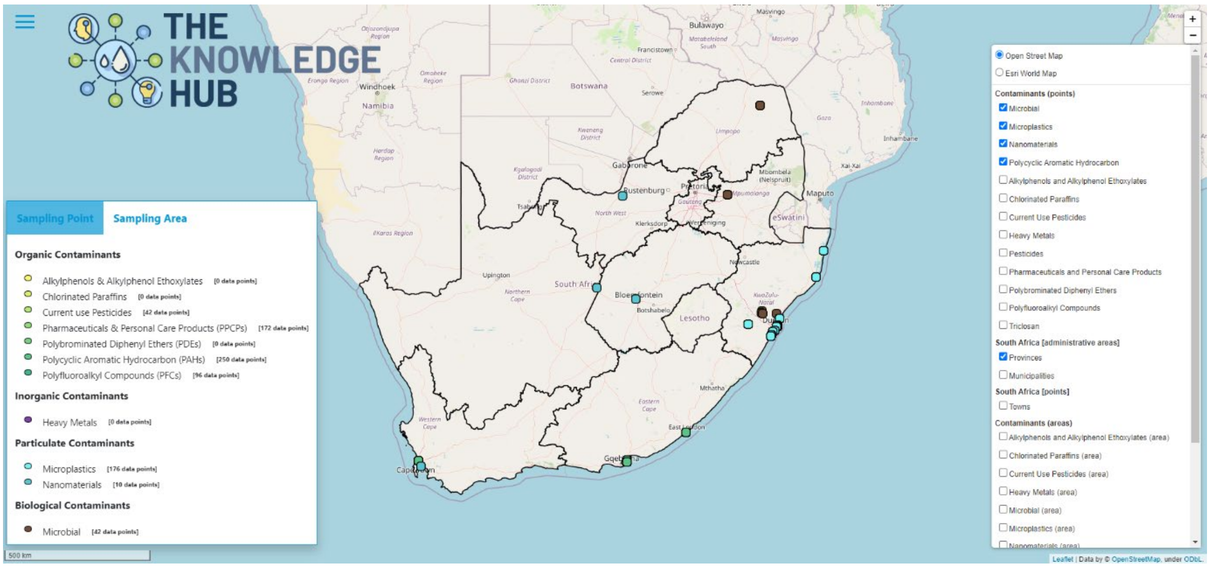


Figure 11: Spatial Viewer

The spatial viewer (figure 11) is used to view the collected sample point data on a map. To use it one must be familiar with online maps. This part of the document gives uses pointers on how to use this part of the Knowledge Hub.

3.3.1.1. Welcome Screen

On opening the spatial.html page one is greeted by the welcome screen (figure 12).

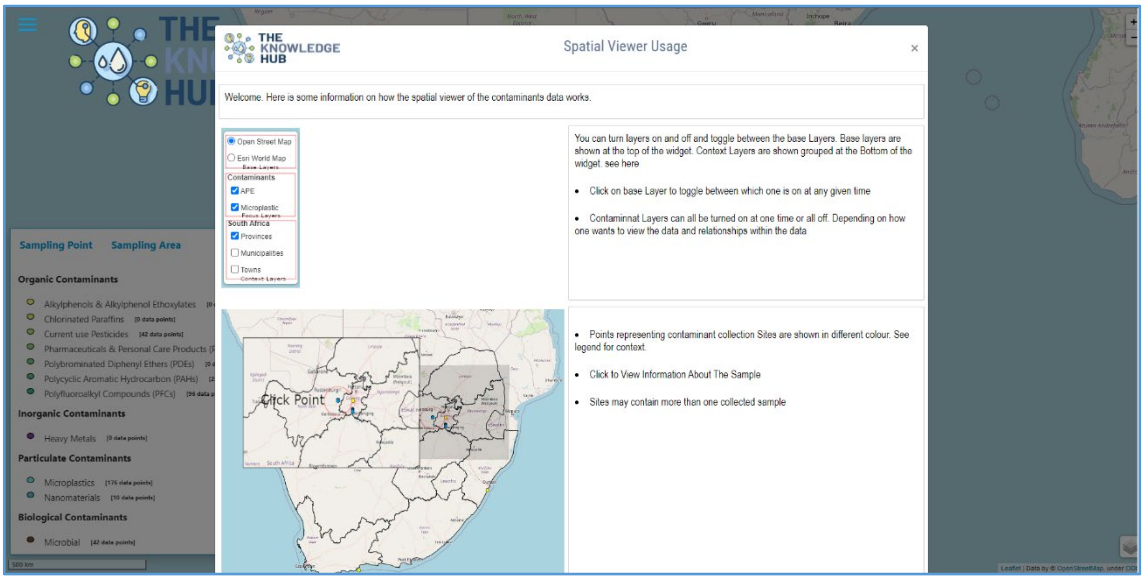


Figure 12: Welcome Screen

The welcome screen gives a quick overview of how to use this page.

3.3.1.2. Spatial Viewer

The spatial viewer (see Figure 11) is composed of multiple objects.

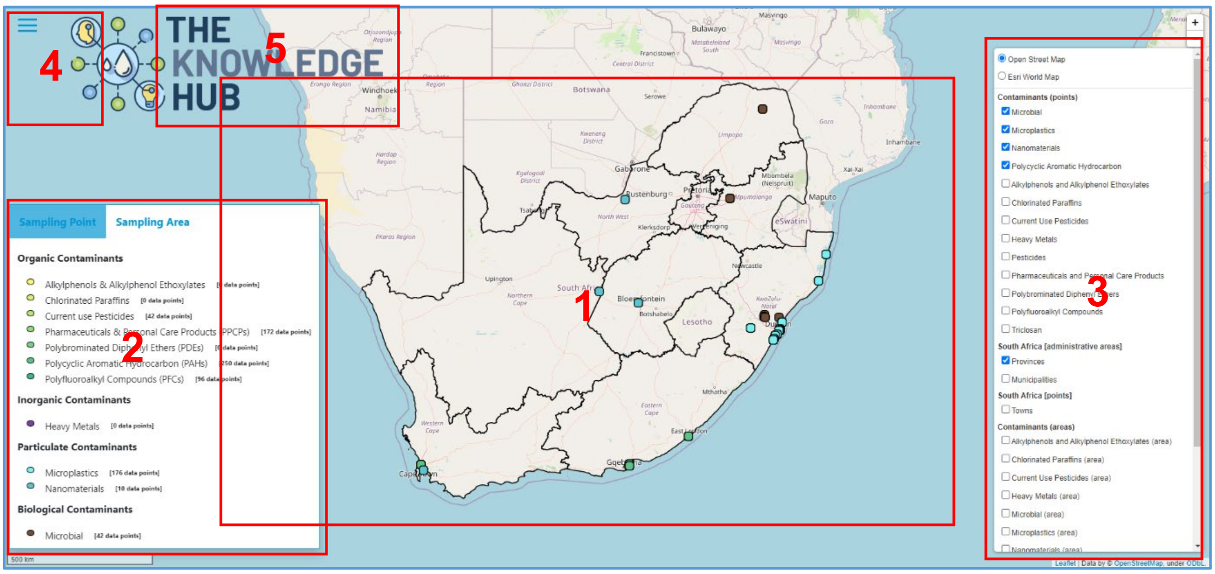


Figure 13: Objects that make up the spatial viewer

It is comprised of

1. The main map viewer (Figure 13-1) – this is where the points and areas of sampling for contamination are shown.
2. The Legend (13-2) – this is used to identify the different contaminants identified on the map. This has two tabs one for the points and the other for the area these are very similar they are both included for the sake of representing the fact that point and areas are displayed differently within the map.

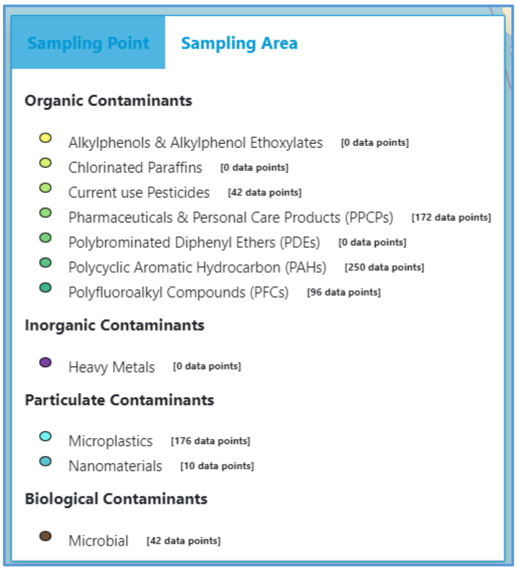


Figure 14: Legend

3. Layer toggle on/off (Figure 13-3) – This is used to toggle layers on or off. As well as select, which base map will be used. You can turn layers on and off and toggle between the base Layers.

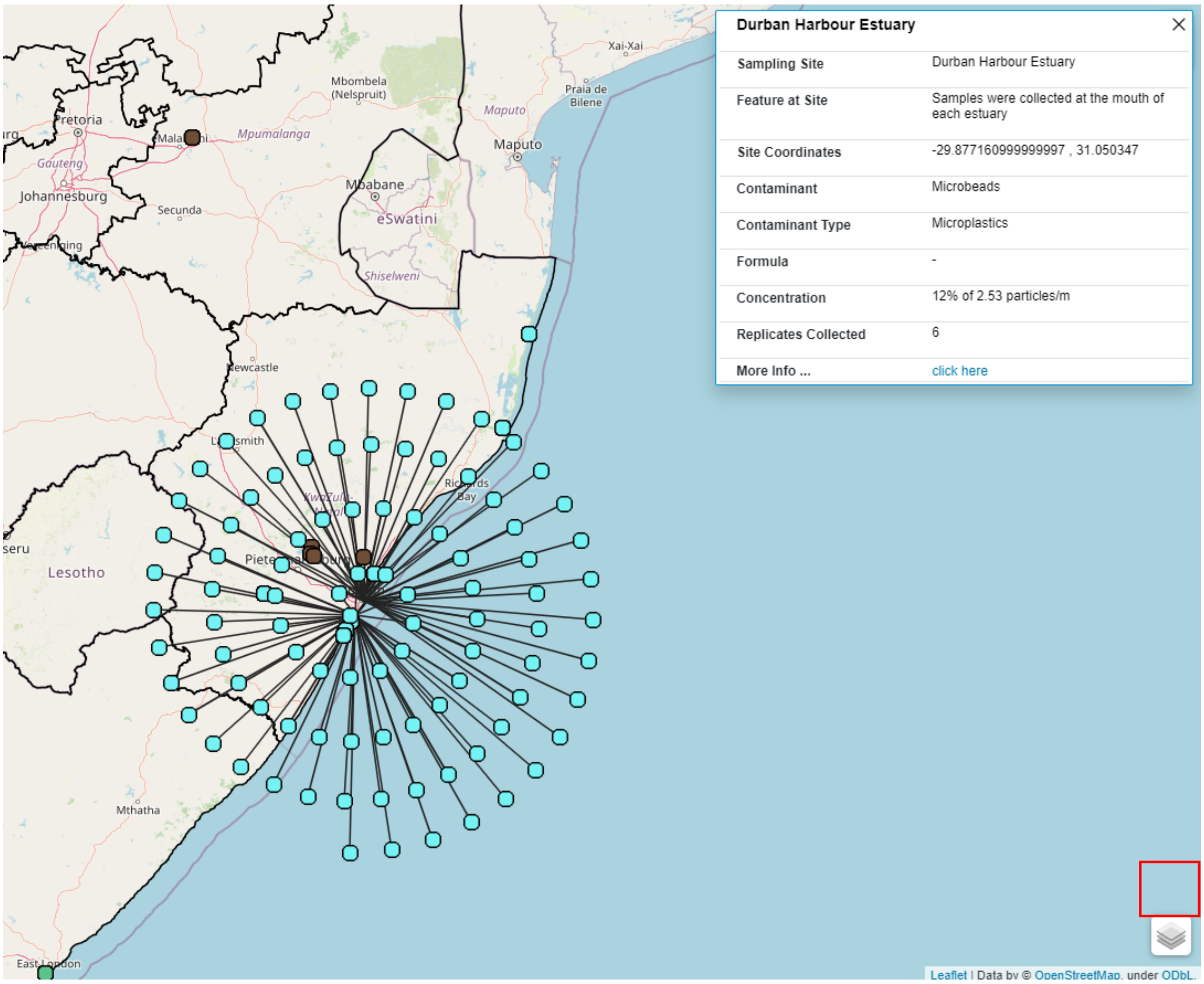


Figure 15: layer toggle on/off widget button location on map

To access this layer toggle, click on the layer toggle on/off widget button at the bottom right of the map viewer.

Figure 16: layer toggle on/off widget button

Base layers are shown at the top of this widget. Context Layers are shown grouped under the heading South Africa (administrative areas).

- Click on base Layer to toggle between which one is on at any given time
- Contaminant Layers can all be turned on at one time or all off. Depending on how one wants to view the data and relationships within the data

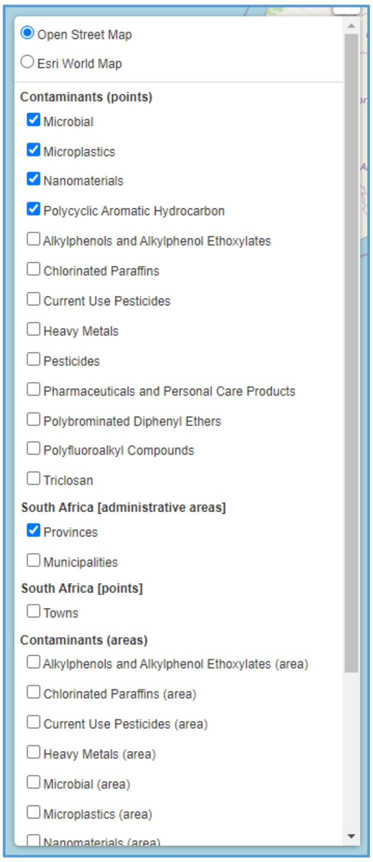


Figure 17: Layers toggle on/off

3.1.1. Navigational Menu (figure 18) – this is used to navigate to other pages in the knowledge hub.

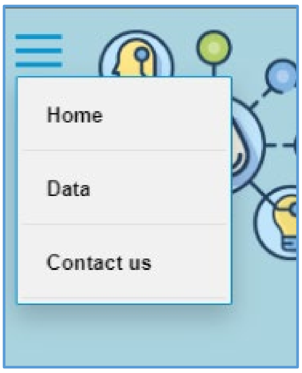


Figure 18: Navigational Menu

4. Branding – This is simply the knowledge hub full logo (Figure 199).

Figure 19: The knowledge hub full logo

3.3.1.3. Map Usage

Points representing contaminant collection sites are shown in different colors as either points or areas (see figure 20). See legend for context. To view Information about the sample collected at a point or site. Click the point or rectangle at that site. Sites may contain more than one collected sample.

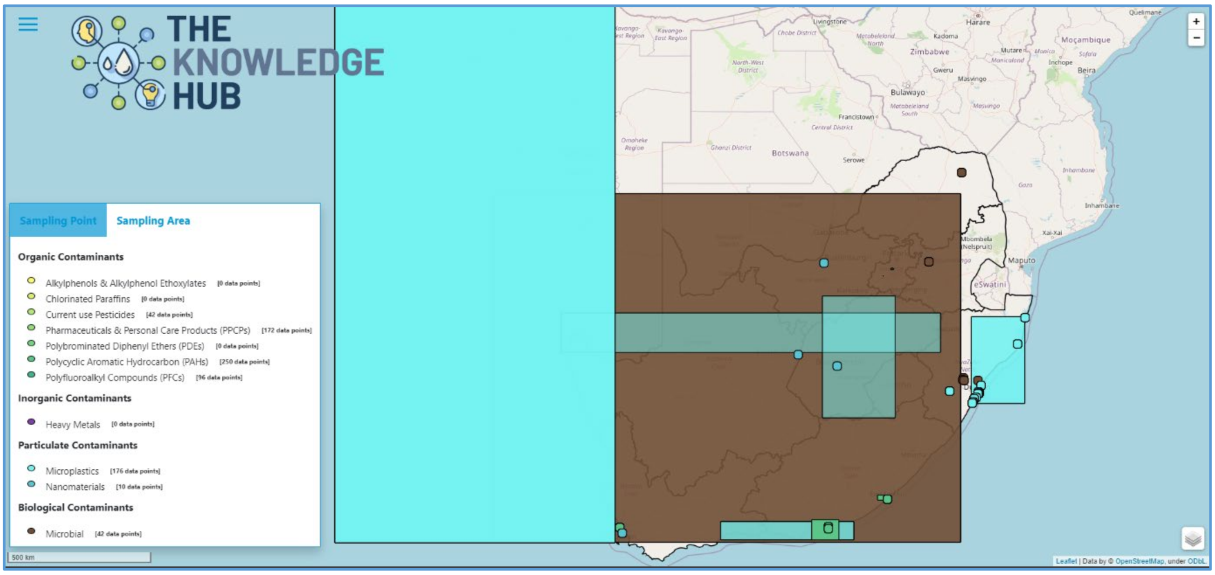


Figure 20: Sample collections sites represented as areas with point sites in the background

Sites may contain more than one collected sample. Click points to view other possible samples collected. If other samples have been collected, points will firstly spider out (figure 21) from under that point and then secondly spiral out in an anticlockwise direction so users can move orderly through the expanded points. Click these Individual points or areas to view their information (Figure 22)

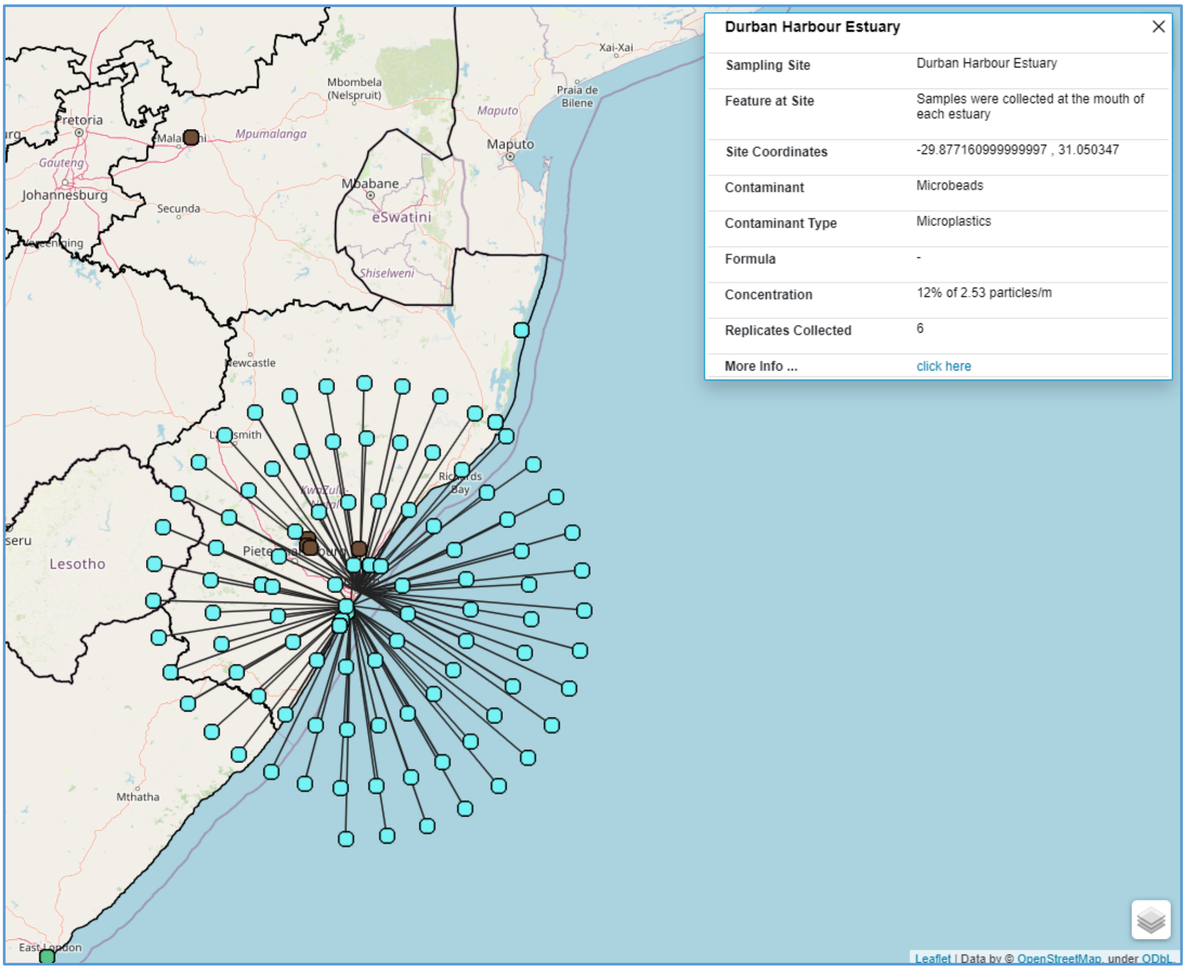


Figure 21: Points firstly spiderfy then spiral outwards

On the info bar (Figure 23) one can click more info (click here …) to view all the information about a particular point or area. This will open a new window with a table display information about that point (Figure 244).

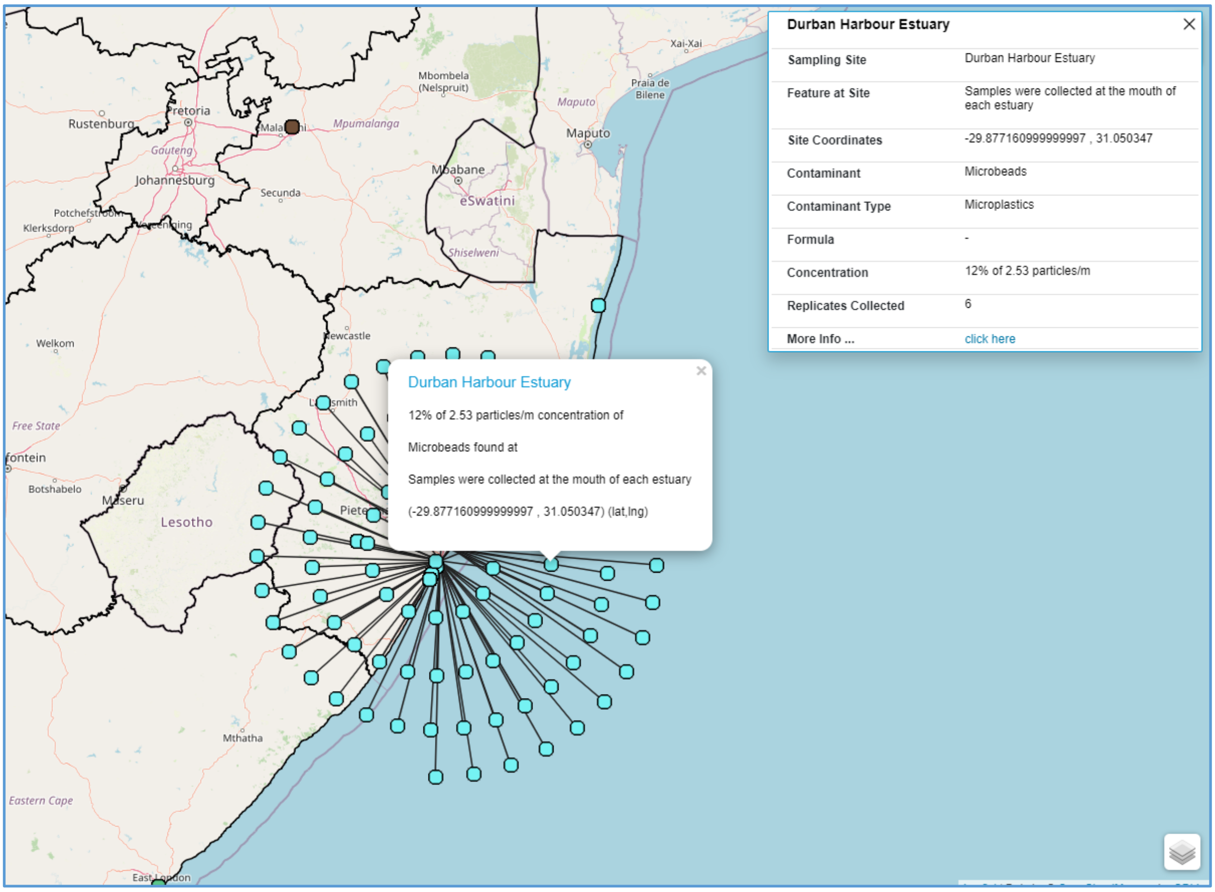


Figure 22: Info Box and Info Bar showing context information about a point

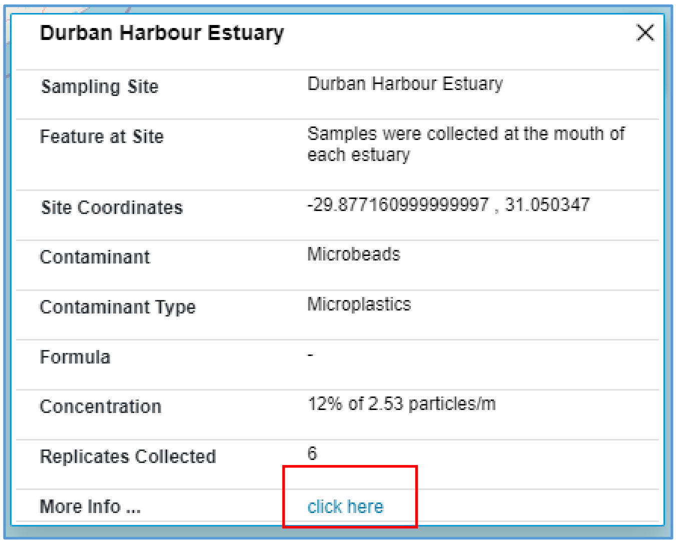


Figure 23: Info Bar

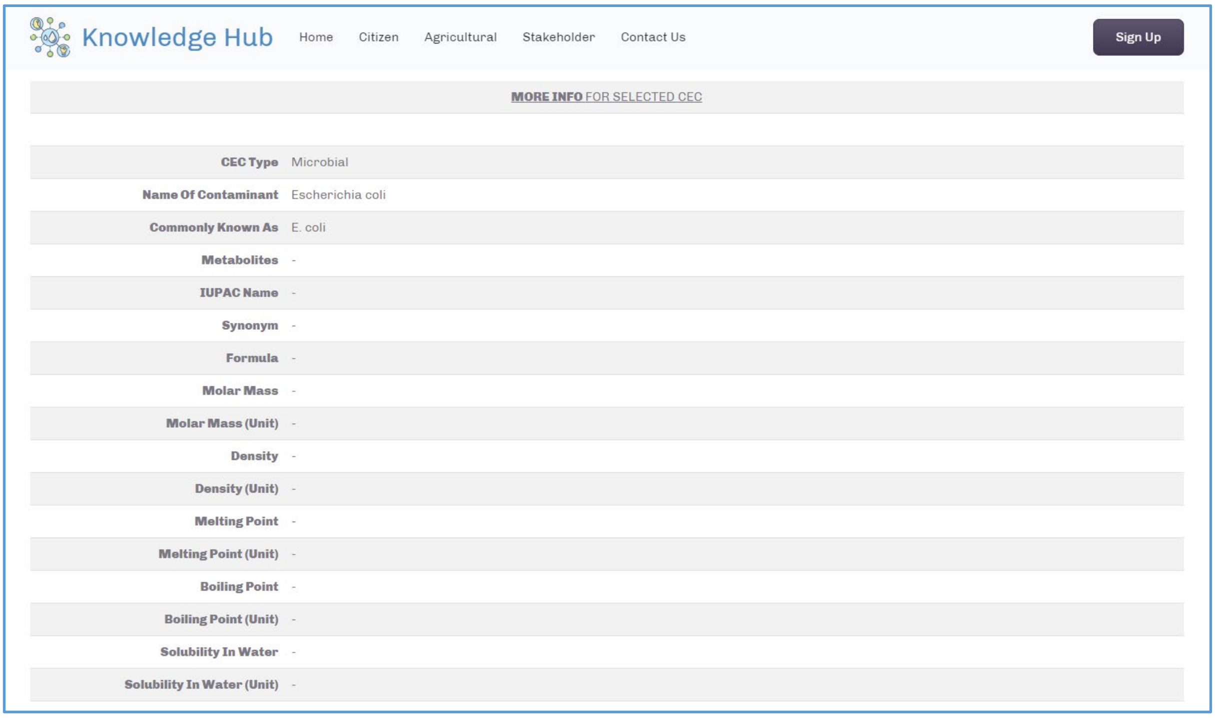


Figure 24: Full information about a sample

3.3.2. Input Data

Clicking this option, the user will be presented with the following page:

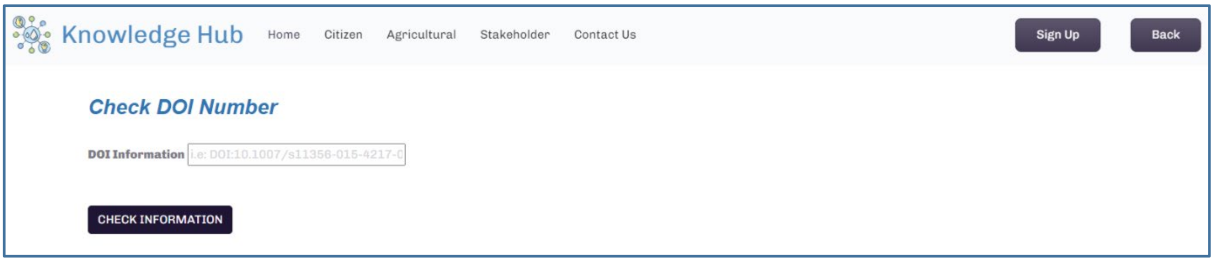


Figure 25: Check DOI Reference Number

Here the user can check if CLC data with the same DOI Reference number has already been loaded onto the Knowledge Hub.
The user can enter the complete DOI Ref number of only parts of it. These parts can either be at the start, middle or end of the DOI number.
It is recommended that the user enter only part of the DOI Ref number to ensure better search results.

<u>Supplying part of the DOI Ref number:</u>

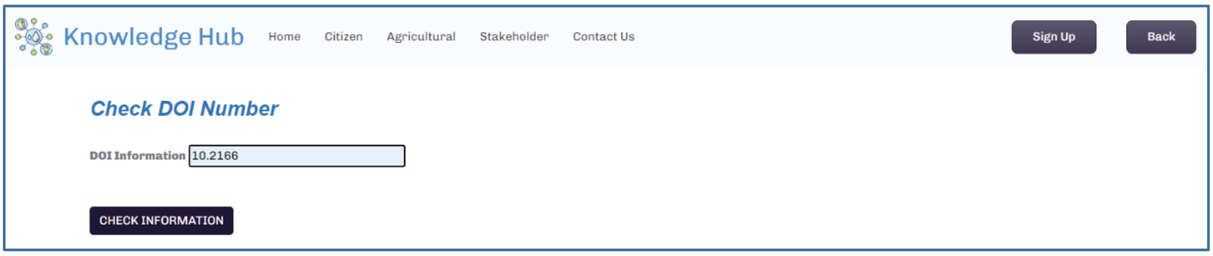
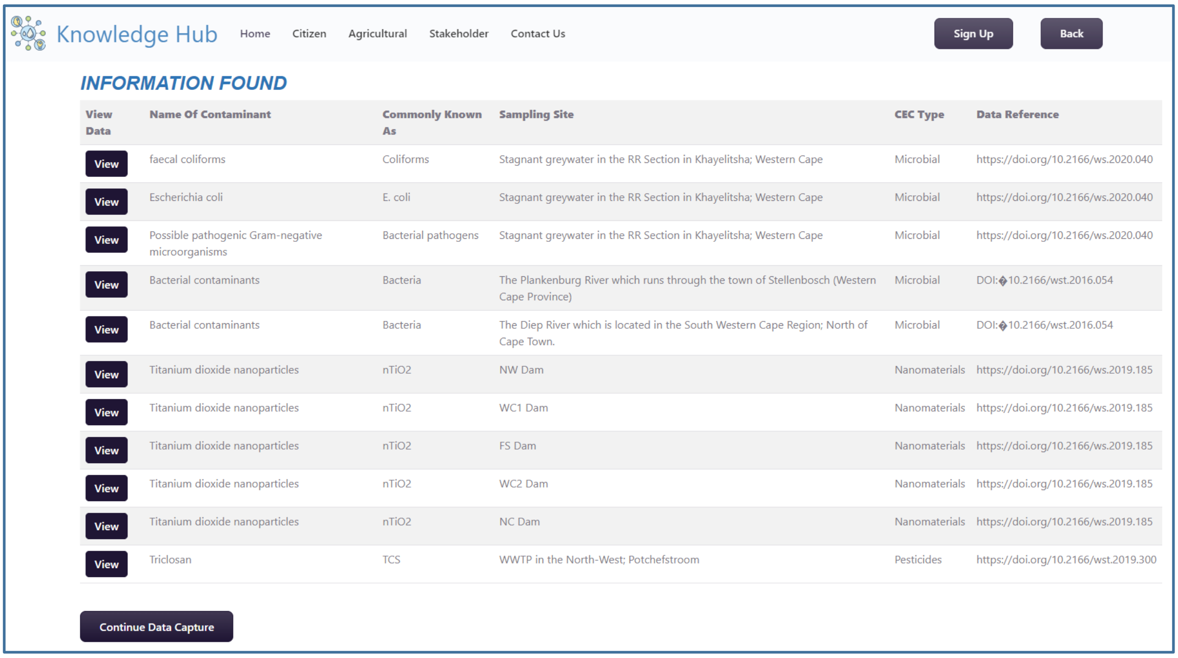


Figure 26: Check DOI Reference Number

Click on **CHECK INFORMATION** to start the search.

Search results, if any, will be displayed as in the image shown below:



View Data	Name Of Contaminant	Commonly Known As	Sampling Site	CEC Type	Data Reference
View	faecal coliforms	Coliforms	Stagnant greywater in the RR Section in Khayelitsha; Western Cape	Microbial	https://doi.org/10.2166/ws.2020.040
View	Escherichia coli	E. coli	Stagnant greywater in the RR Section in Khayelitsha; Western Cape	Microbial	https://doi.org/10.2166/ws.2020.040
View	Possible pathogenic Gram-negative microorganisms	Bacterial pathogens	Stagnant greywater in the RR Section in Khayelitsha; Western Cape	Microbial	https://doi.org/10.2166/ws.2020.040
View	Bacterial contaminants	Bacteria	The Plankenburg River which runs through the town of Stellenbosch (Western Cape Province)	Microbial	DOI:�10.2166/wst.2016.054
View	Bacterial contaminants	Bacteria	The Diep River which is located in the South Western Cape Region; North of Cape Town.	Microbial	DOI:�10.2166/wst.2016.054
View	Titanium dioxide nanoparticles	nTiO2	NW Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Titanium dioxide nanoparticles	nTiO2	WC1 Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Titanium dioxide nanoparticles	nTiO2	FS Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Titanium dioxide nanoparticles	nTiO2	WC2 Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Titanium dioxide nanoparticles	nTiO2	NC Dam	Nanomaterials	https://doi.org/10.2166/ws.2019.185
View	Triclosan	TCS	WWTP in the North-West; Potchefstroom	Pesticides	https://doi.org/10.2166/wst.2019.300

Figure 27: DOI Reference Number Search Results

From these search results, the user can click on **VIEW** to see the full record. Should the user wish to capture the data anyhow, they can do so by clicking **CONTINUE DATA CAPTURE.**

This will open the **DATA CAPTURE PAGE** as shown below:

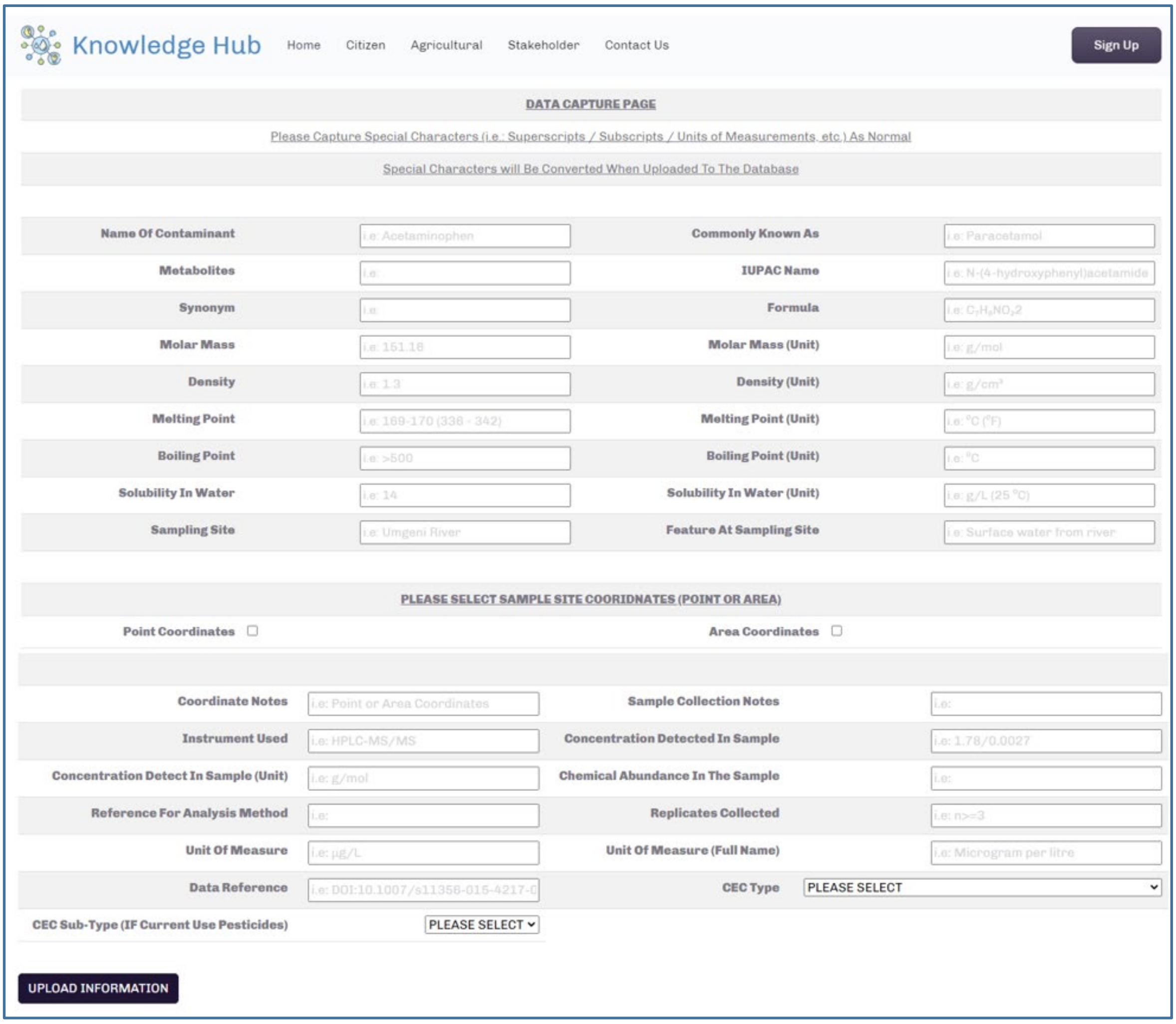


Figure 28: Data Capture Page

On this page, the user can capture **CEC Data** one record at a time.

The user also has the option to choose between *POINT COORDINATES* as well as *AREA COORDINATES*.
When selecting *POINT COORDINATES*, the user will be presented with the following to input a single **LATITUDE** and **LONGITUDE** value:

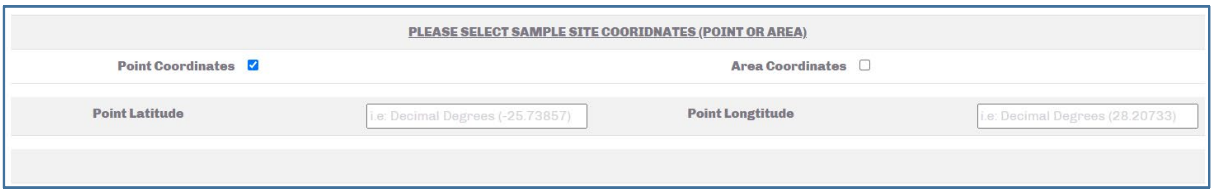


Figure 29: Insert Point Coordinates

When selecting the *AREA COORDINATES*, the user will be presented with the following to input two sets of **LATITUDE** and **LONGITUDE** values.
The **TOP LEFT LATITUDE** and **LONGITUDE** set as well as the **BOTTOM RIGHT LATITUDE** and **LONGITUDE** set:

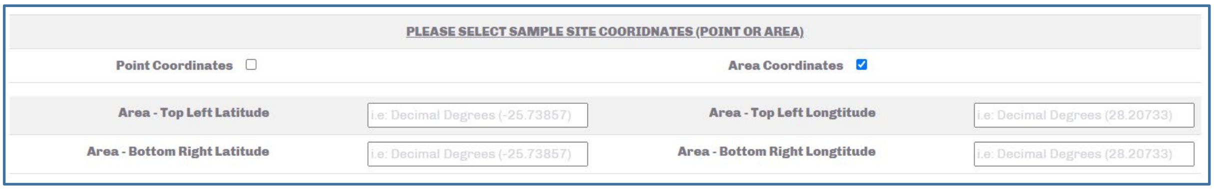


Figure 30: Insert Area Coordinates

After supplying all the relevant information, click **UPLOAD INFORMATION** to commit this CEC data set to the database.

3.3.3. Bulk Import Data:

Clicking this option, the user will be presented with the following page:

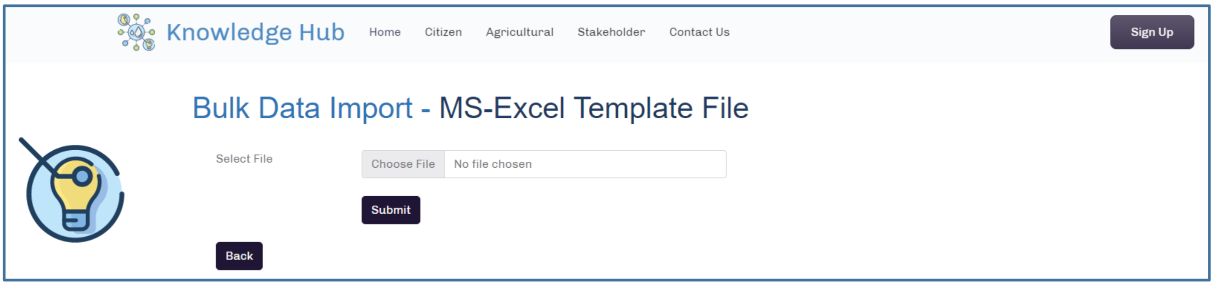


Figure 31: Bulk Import

Users can download the MS-Excel Template file by clicking on the dark blue '**MS-Excel Template File**' text, as shown in the image below. A tooltip hint will also be displayed when the mouse icon hovers over the highlighted text.

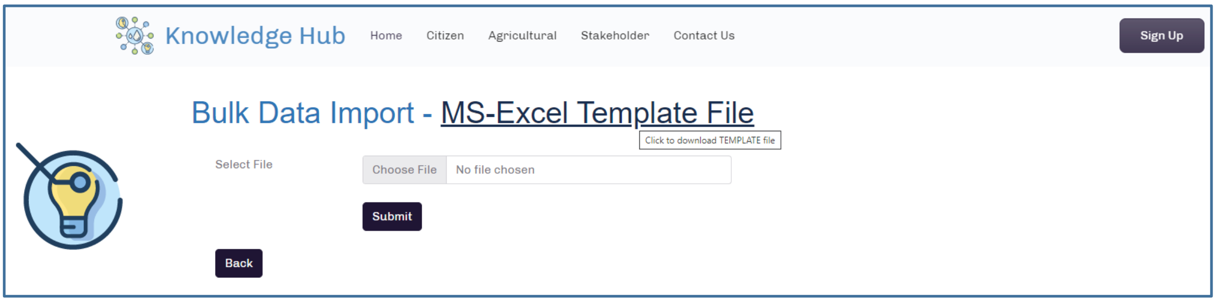


Figure 32: Bulk Import Tooltip

Clicking **CHOOSE FILE**, the user will be presented with the *FILE OPEN / SEARCH* dialog box:

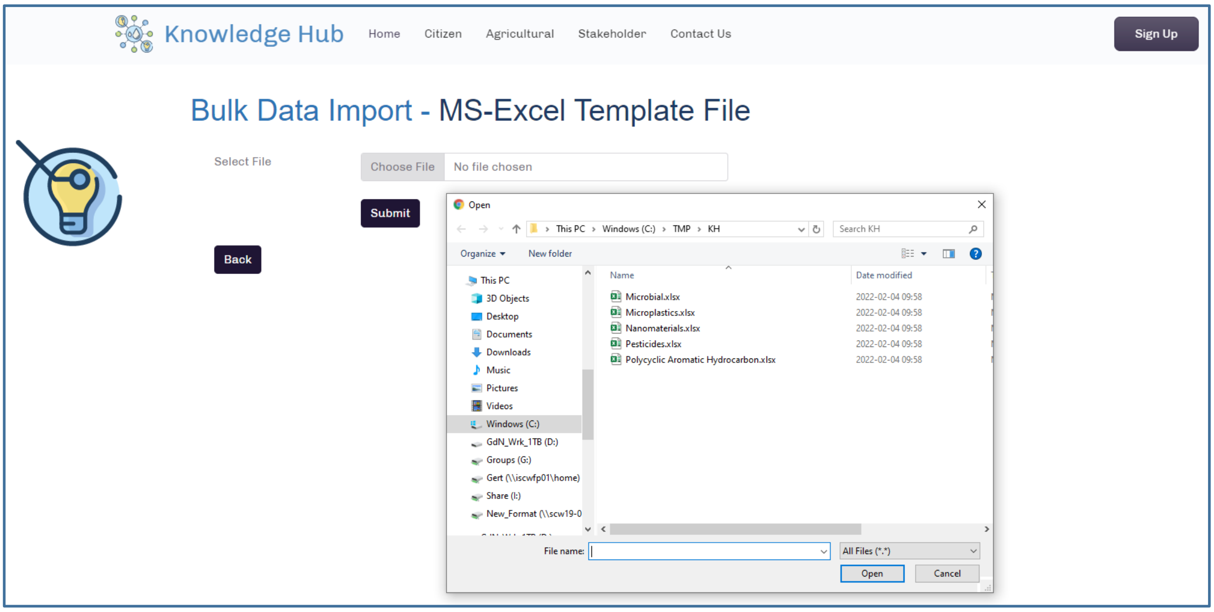


Figure 33: Bulk Import Navigate to file

Navigate to where the file is stored on the PC, click once on it and then on **OPEN**. The file name plus path will be displayed on the page. Click **SUBMIT** to upload the file to the database.

3.3.4. Export Data:

Clicking this option, the user will be presented with the following page:

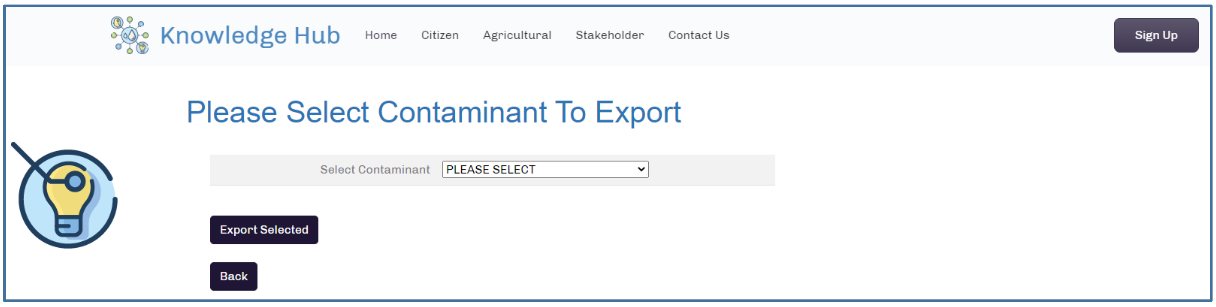


Figure 34: Export Data

Select the contaminant type to export from the drop-down options:

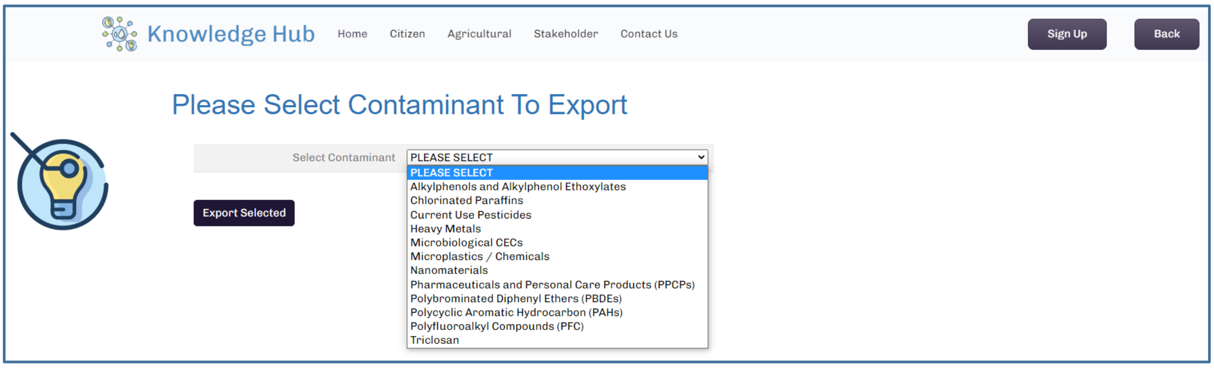
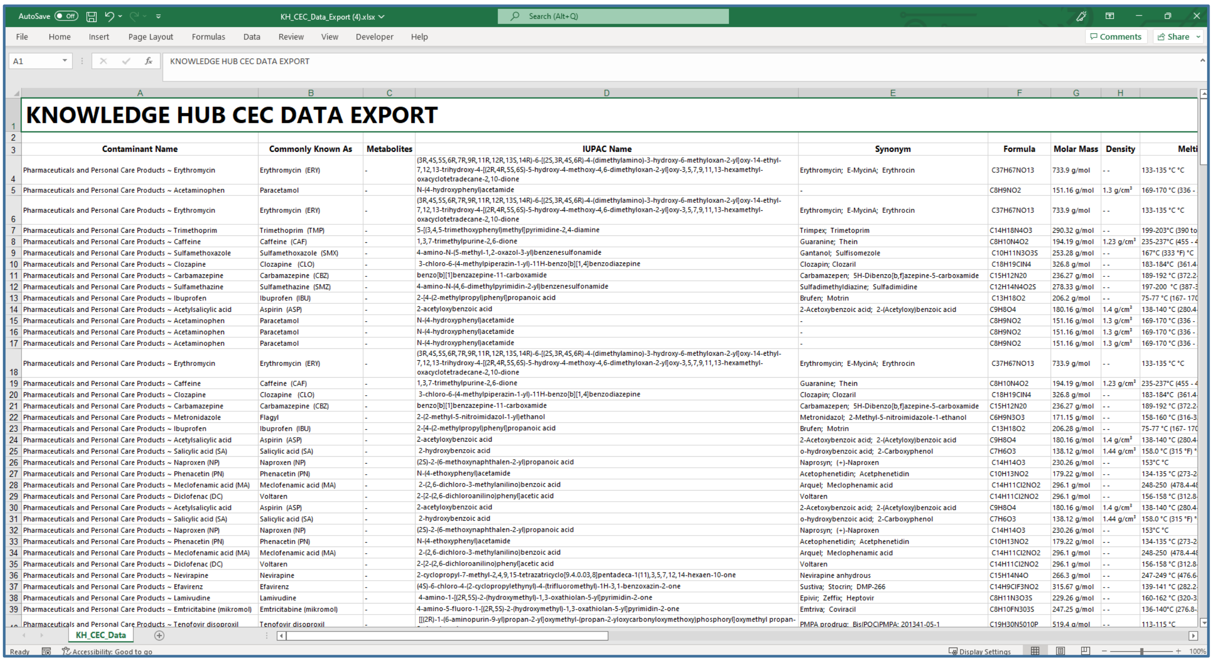


Figure 35: Export Select Contaminant

The selected contaminant type will be exported to a MS Excel file as shown in the example below:



KH_CEC_Data_Export (4).xlsx

KNOWLEDGE HUB CEC DATA EXPORT

	Contaminant Name	Commonly Known As	Metabolites	IUPAC Name	Synonym	Formula	Molar Mass	Density	Melti
4	Pharmaceuticals and Personal Care Products ~ Erythromycin	Erythromycin (ERY)	-	(3R,4S,5S,6R,7R,9R,11R,12R,13S,14R)-6-[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy-14-ethyl-7,12,13-trihydroxy-4-[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy-3,5,7,9,11,13-hexamethyl-oxacyclotetradecane-2,10-dione	Erythromycin; E-MycinA; Erythrocin	C37H67NO13	733.9 g/mol	- -	133-135 °C °C
5	Pharmaceuticals and Personal Care Products ~ Acetaminophen	Paracetamol	-	N-(4-hydroxyphenyl)acetamide	-	C8H9NO2	151.16 g/mol	1.3 g/cm³	169-170 °C (336 -
6	Pharmaceuticals and Personal Care Products ~ Erythromycin	Erythromycin (ERY)	-	(3R,4S,5S,6R,7R,9R,11R,12R,13S,14R)-6-[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy-14-ethyl-7,12,13-trihydroxy-4-[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy-3,5,7,9,11,13-hexamethyl-oxacyclotetradecane-2,10-dione	Erythromycin; E-MycinA; Erythrocin	C37H67NO13	733.9 g/mol	- -	133-135 °C °C
7	Pharmaceuticals and Personal Care Products ~ Trimethoprim	Trimethoprim (TMP)	-	5-[(3,4,5-trimethoxyphenyl)methyl]pyrimidine-2,4-diamine	Trimpex; Trimetoprim	C14H18N4O3	290.32 g/mol	- -	199-203°C (390 to
8	Pharmaceuticals and Personal Care Products ~ Caffeine	Caffeine (CAF)	-	1,3,7-trimethylpurine-2,6-dione	Guaranine; Thein	C8H10N4O2	194.19 g/mol	1.23 g/cm³	235-237°C (455 - 4
9	Pharmaceuticals and Personal Care Products ~ Sulfamethoxazole	Sulfamethoxazole (SMX)	-	4-amino-N-(5-methyl-1,2-oxazol-3-yl)benzenesulfonamide	Gantanol; Sulfisomezole	C10H11N3O3S	253.28 g/mol	- -	167°C (333 °F) °C
10	Pharmaceuticals and Personal Care Products ~ Clozapine	Clozapine (CLO)	-	3-chloro-6-(4-methylpiperazin-1-yl)-11H-benzo[b][1,4]benzodiazepine	Clozapin; Clozaril	C18H19ClN4	326.8 g/mol	- -	183-184°C (361.4
11	Pharmaceuticals and Personal Care Products ~ Carbamazepine	Carbamazepine (CBZ)	-	benzo[b][1]benzazepine-11-carboxamide	Carbamazepen; 5H-Dibenzo[b,f]azepine-5-carboxamide	C15H12N20	236.27 g/mol	- -	189-192 °C (372.2
12	Pharmaceuticals and Personal Care Products ~ Sulfamethazine	Sulfamethazine (SMZ)	-	4-amino-N-(4,6-dimethylpyrimidin-2-yl)benzenesulfonamide	Sulfadimethyldiazine; Sulfadimidine	C12H14N4O2S	278.33 g/mol	- -	197-200 °C (387-3
13	Pharmaceuticals and Personal Care Products ~ Ibuprofen	Ibuprofen (IBU)	-	2-[4-(2-methylpropyl)phenyl]propanoic acid	Brufen; Motrin	C13H18O2	206.2 g/mol	- -	75-77 °C (167- 170
14	Pharmaceuticals and Personal Care Products ~ Acetylsalicylic acid	Aspirin (ASP)	-	2-acetyloxybenzoic acid	2-Acetoxybenzoic acid; 2-(Acetyloxy)benzoic acid	C9H8O4	180.16 g/mol	1.4 g/cm³	138-140 °C (280.4
15	Pharmaceuticals and Personal Care Products ~ Acetaminophen	Paracetamol	-	N-(4-hydroxyphenyl)acetamide	-	C8H9NO2	151.16 g/mol	1.3 g/cm³	169-170 °C (336 -
16	Pharmaceuticals and Personal Care Products ~ Acetaminophen	Paracetamol	-	N-(4-hydroxyphenyl)acetamide	-	C8H9NO2	151.16 g/mol	1.3 g/cm³	169-170 °C (336 -
17	Pharmaceuticals and Personal Care Products ~ Acetaminophen	Paracetamol	-	N-(4-hydroxyphenyl)acetamide	-	C8H9NO2	151.16 g/mol	1.3 g/cm³	169-170 °C (336 -
18	Pharmaceuticals and Personal Care Products ~ Erythromycin	Erythromycin (ERY)	-	(3R,4S,5S,6R,7R,9R,11R,12R,13S,14R)-6-[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy-14-ethyl-7,12,13-trihydroxy-4-[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyloxan-2-yl]oxy-3,5,7,9,11,13-hexamethyl-oxacyclotetradecane-2,10-dione	Erythromycin; E-MycinA; Erythrocin	C37H67NO13	733.9 g/mol	- -	133-135 °C °C
19	Pharmaceuticals and Personal Care Products ~ Caffeine	Caffeine (CAF)	-	1,3,7-trimethylpurine-2,6-dione	Guaranine; Thein	C8H10N4O2	194.19 g/mol	1.23 g/cm³	235-237°C (455 - 4
20	Pharmaceuticals and Personal Care Products ~ Clozapine	Clozapine (CLO)	-	3-chloro-6-(4-methylpiperazin-1-yl)-11H-benzo[b][1,4]benzodiazepine	Clozapin; Clozaril	C18H19ClN4	326.8 g/mol	- -	183-184°C (361.4
21	Pharmaceuticals and Personal Care Products ~ Carbamazepine	Carbamazepine (CBZ)	-	benzo[b][1]benzazepine-11-carboxamide	Carbamazepen; 5H-Dibenzo[b,f]azepine-5-carboxamide	C15H12N20	236.27 g/mol	- -	189-192 °C (372.2
22	Pharmaceuticals and Personal Care Products ~ Metronidazole	Flagyl	-	2-(2-methyl-5-nitroimidazol-1-yl)ethanol	Metronidazol; 2-Methyl-5-nitroimidazole-1-ethanol	C6H9N3O3	171.15 g/mol	- -	158-160 °C (316-3
23	Pharmaceuticals and Personal Care Products ~ Ibuprofen	Ibuprofen (IBU)	-	2-[4-(2-methylpropyl)phenyl]propanoic acid	Brufen; Motrin	C13H18O2	206.28 g/mol	- -	75-77 °C (167- 170
24	Pharmaceuticals and Personal Care Products ~ Acetylsalicylic acid	Aspirin (ASP)	-	2-acetyloxybenzoic acid	2-Acetoxybenzoic acid; 2-(Acetyloxy)benzoic acid	C9H8O4	180.16 g/mol	1.4 g/cm³	138-140 °C (280.4
25	Pharmaceuticals and Personal Care Products ~ Salicylic acid (SA)	Salicylic acid (SA)	-	2-hydroxybenzoic acid	o-hydroxybenzoic acid; 2-Carboxyphenol	C7H6O3	138.12 g/mol	1.44 g/cm³	158.0 °C (315 °F) °
26	Pharmaceuticals and Personal Care Products ~ Naproxen (NP)	Naproxen (NP)	-	(2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid	Naprosyn; (+)-Naproxen	C14H14O3	230.26 g/mol	- -	153°C °C
27	Pharmaceuticals and Personal Care Products ~ Phenacetin (PN)	Phenacetin (PN)	-	N-(4-ethoxyphenyl)acetamide	Acetophenetidin; Acetphenetidin	C10H13NO2	179.22 g/mol	- -	134-135 °C (273-2
28	Pharmaceuticals and Personal Care Products ~ Meclofenamic acid (MA)	Meclofenamic acid (MA)	-	2-(2,6-dichloro-3-methylanilino)benzoic acid	Arquel; Meclophenamic acid	C14H11Cl2NO2	296.1 g/mol	- -	248-250 (478.4-48
29	Pharmaceuticals and Personal Care Products ~ Diclofenac (DC)	Voltaren	-	2-[2-(2,6-dichloroanilino)phenyl]acetic acid	Voltaren	C14H11Cl2NO2	296.1 g/mol	- -	156-158 °C (312.8
30	Pharmaceuticals and Personal Care Products ~ Acetylsalicylic acid	Aspirin (ASP)	-	2-acetyloxybenzoic acid	2-Acetoxybenzoic acid; 2-(Acetyloxy)benzoic acid	C9H8O4	180.16 g/mol	1.4 g/cm³	138-140 °C (280.4
31	Pharmaceuticals and Personal Care Products ~ Salicylic acid (SA)	Salicylic acid (SA)	-	2-hydroxybenzoic acid	o-hydroxybenzoic acid; 2-Carboxyphenol	C7H6O3	138.12 g/mol	1.44 g/cm³	158.0 °C (315 °F) °
32	Pharmaceuticals and Personal Care Products ~ Naproxen (NP)	Naproxen (NP)	-	(2S)-2-(6-methoxynaphthalen-2-yl)propanoic acid	Naprosyn; (+)-Naproxen	C14H14O3	230.26 g/mol	- -	153°C °C
33	Pharmaceuticals and Personal Care Products ~ Phenacetin (PN)	Phenacetin (PN)	-	N-(4-ethoxyphenyl)acetamide	Acetophenetidin; Acetphenetidin	C10H13NO2	179.22 g/mol	- -	134-135 °C (273-2
34	Pharmaceuticals and Personal Care Products ~ Meclofenamic acid (MA)	Meclofenamic acid (MA)	-	2-(2,6-dichloro-3-methylanilino)benzoic acid	Arquel; Meclophenamic acid	C14H11Cl2NO2	296.1 g/mol	- -	248-250 (478.4-48
35	Pharmaceuticals and Personal Care Products ~ Diclofenac (DC)	Voltaren	-	2-[2-(2,6-dichloroanilino)phenyl]acetic acid	Voltaren	C14H11Cl2NO2	296.1 g/mol	- -	156-158 °C (312.8
36	Pharmaceuticals and Personal Care Products ~ Nevirapine	Nevirapine	-	2-cyclopropyl-7-methyl-2,4,9,15-tetrazatricyclo[9.4.0.03,8]pentadeca-1(11),3,5,7,12,14-hexaen-10-one	Nevirapine anhydrous	C15H14N4O	266.3 g/mol	- -	247-249 °C (476.6
37	Pharmaceuticals and Personal Care Products ~ Efavirenz	Efavirenz	-	(4S)-6-chloro-4-(2-cyclopropylethynyl)-4-(trifluoromethyl)-1H-3,1-benzoxazin-2-one	Sustiva; Stocrin; DMP-266	C14H9ClF3NO2	315.67 g/mol	- -	139-141 °C (282.2
38	Pharmaceuticals and Personal Care Products ~ Lamivudine	Lamivudine	-	4-amino-1-[(2R,5S)-2-(hydroxymethyl)-1,3-oxathiolan-5-yl]pyrimidin-2-one	Epivir; Zeffix; Heptovir	C8H11N3O3S	229.26 g/mol	- -	160-162 °C (320-3
39	Pharmaceuticals and Personal Care Products ~ Emtricitabine (mikromol)	Emtricitabine (mikromol)	-	4-amino-5-fluoro-1-[(2R,5S)-2-(hydroxymethyl)-1,3-oxathiolan-5-yl]pyrimidin-2-one	Emtriva; Coviracil	C8H10FN3O3S	247.25 g/mol	- -	136-140°C (276.8
40	Pharmaceuticals and Personal Care Products ~ Tenofovir disoproxil	Tenofovir disoproxil	-	[[(2R)-1-(6-aminopurin-9-yl)propan-2-yl]oxymethyl-(propan-2-yloxycarbonyloxymethoxy)phosphoryl]oxymethyl propan-	PMPA prodrug; Bis(POC)PMPA; 201341-05-1	C19H30N5O10P	519.4 g/mol	- -	113-115 °C

KH_CEC_Data

Figure 36: Exported Data as MS Excel Format

APPENDIX B: CONTAMINANT OF EMERGING CONCER KNOWLEDGE HUB CODE

****************************coding files cannot be read in word****************************