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SELECTION AND PRIORITIZATION OF ORGANIC CONTAMINANTS FOR MONITORING IN THE DRINKING WATER VALUE CHAIN

By

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CO-PROMOTER: Prof Hein du Preez

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DECLARATION

"I declare that the thesis, "Selection and prioritization of organic contaminants for monitoring in the drinking water value chain" **Protocol no. 22/2007** that I hereby submit to the PhD in Public Health degree at the University of Pretoria, is my own work and has not previously been submitted by me for a degree at this or any other tertiary institution. All the sources used or quoted in this research study have been indicated and reflected".

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Esper Jacobeth Ncube

Student no. 99130590

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Witness's signature

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Date signed

DEDICATION

I dedicate this Thesis work to those that have worked very hard to prove the causal link between the exposure to contaminated water and human health especially through the ingestion route and still fight to ensure successful Public Health Protection for the vulnerable and defenceless masses.

New diseases, including water-related diseases, periodically "emerge" either because they are newly recognized or because their importance increases.

http://www.who.int/water_sanitation_health/emerging/en/last visited 6 Sept 2007

ABSTRACT

The occurrence of organic contaminants in the drinking water value chain (from source to tap) is a growing concern for the Drinking Water industry and its consumers given the high risk these contaminants can cause to the general public. These adverse health effects include such as endocrine disruption, toxicity teratogenicity, mutagenicity and carcinogenicity. Some of these organic contaminants are included in national and international drinking water quality guidelines or standards. However, although there are similarities in the list of organic contaminants used by each organization or country, the organic contaminants are never the same given the local conditions. There are also noticeable differences in the concentration limits set as targets or criteria for organic contaminants for public health protection via the use of drinking water. A further question requiring the response from drinking water regulators was whether the standards listed in the international literature would be applicable in other countries like South Africa. Complicating this decision is the fact that the South African National Drinking Water Standard (SANS 241) does not adequately address this component of drinking water quality management. The current standard only provides for dissolved organic carbon (DOC), total trihalomethanes (TTHMs) and phenols. However, the standard contains a statement which specifies that if there is a known organic contaminant, that may pose a health threat, it should be included in the monitoring programme and evaluated against World Health Organization (WHO) guidelines. To safeguard Drinking Water industry customers, it was deemed necessary to investigate this matter and establish a tool to assist with the identification of a list of organic contaminants to be monitored in the drinking water value chain.

To achieve this a specific procedure/protocol needed to be developed, hence the aim of this study which was to develop a generic protocol for the selection and prioritization of organic contaminants for monitoring in the drinking water value chain (from source to tap). To achieve this, a critical evaluation and synthesis of the available literature on the approaches for the selection and prioritization of organic variables of priority to the drinking water industry was undertaken as a first step. From the literature review it was evident that there are currently many selection and prioritization approaches which are characterized mainly by the purpose for which the exercise has been conducted for. Approaches that prioritize chemicals according to their importance as environmental contaminants have been developed by government agencies and private industries such as the Health Canada's Canadian Environmental Protection Agency (CEPA), the United Kingdom's Institute for Environmental Health (IEH), the European Community's Oslo and Paris (OSPAR) convention exercise for the protection of the Northeast Atlantic marine environment and the European Union (EU)'s combined monitoring based and modelling based priority setting scheme (EU-COMMPs). A few approaches such as ones published by the United States Environmental Protection Agency (USEPA), address the needs of the Drinking Water industry and there is no generic approach to the selection, prioritization and monitoring of organic contaminants in the drinking water value chain.

From the review of selection and prioritization approaches, a generic model was developed. The model consists of three main steps, the compilation of a "pool of organic contaminants, the selection of relevant parameters and criteria to screen organic contaminants and finally the application of criteria to select priority organic contaminants. It was however realized that these steps were not enough if the protocol to be develop will serve its purpose. Selection and prioritization approaches are typically intended to be fairly simple and quick methods for determining the health and environmental hazards posed by the use and release of chemical substances into different environmental systems. This was taken into account during the development of the current protocol. Understanding that a protocol is a predefined written procedural method in the design and implementation of tasks and that these protocols are

written whenever it is desirable to standardize a method or procedure to ensure successful reproducibility in a similar set up, a generic protocol was developed based on the model. The protocol developed in this study, operates as a multidisciplinary contaminants management and proactive protocol, thus exchanges toxicological, water quality, agricultural, chemical and public health information. The protocol uses previous or readily available information as a point of departure. It seeks to address the challenge facing the water industry in managing the current and emerging organic contaminants that are relevant to public health protection via the use of drinking water.

Once the protocol was developed, it was validated in a prototype drinking water value chain. The exercise comprised of testing each step of the protocol from the selection of the "pool of organic contaminants (Step I) to recommending the final priority list of organic contaminants (Step VII). The implementation was successfully conducted in the Rand Water drinking water value chain. Emphasis of expert judgment was made as each step was validated and the opinion of key stakeholders used to shape the process. During Step III of the protocol, an intensive literature review was conducted to determine organic contaminants that have been identified in ground and surface water systems across the world. As a result of this review, major groups of organic contaminants that have been found to occur in source water resources across the world were identified. The identified groups of organic contaminants include, pesticides, polynuclear aromatic hydrocarbons, per and polyfluoroorganic compounds, polycyclic aromatic hydrocarbons, alkanes and alkenes, C10-C13 Chloroalkanes, pharmaceuticals and personal care products [PPCPs], surfactants, benzotriazoles, cyanotoxins and Carbon-based engineered nanoparticles. The risk profile of the identified organic contaminants was established using the persistence, bio-accumulation and toxicity criteria and the development of water quality monographs as an information dissemination tool. A conceptual framework for the implementation of the protocol by water utilities and relevant institutions has been developed from the experiences learnt during the validation exercise and a priority list of organic contaminants for the monitoring in the drinking water value chain to be used by Rand Water and other water utilities was identified. Some of the organic contaminants on this are currently being analyzed for in The Rand Water's routine organic monitoring programme.

During the validation exercise, the following were noted,

- During the identification of the "pool of organic contaminants" from the consulted information sources such as the WHO guidelines for drinking water quality, Health Canada drinking water quality guidelines, the USEPA drinking water quality standards, the New Zealand drinking water quality standards, USEPA IRIS database, the PAN-UK list of registered pesticides for South Africa, the IARC list for recognized carcinogens and the Department of Agriculture pesticides manuals duplications were observed.

- The time allocated could not allow for the development of water quality monographs for all organic contaminants of concern but for a few selected contaminants whose information was inadequate to allow for decision-making.

- The determination of concentration levels of organic contaminants in fish, sediment and water samples could have been limited by the failure of current analytical instruments to go down to lower levels at which they occur in the drinking water value chain.

- Only two events could be planned, during the wet season (high flow) and dry season (low flow) based on time and budget constraints.

- Although various experts were consulted and invited to attend workshops in order to validate the process, the attendance could not be extended to all nine provinces given the time and budget constraints.

Based on the above, recommendations were made for the dissemination and use of the products emanating from this study. For example, it is recommended that the current protocol be made available to water utilities and the process of revising the current priority list be repeated every 5 years. Further research should be conducted to obtain full coverage of organic contaminants impacting on source water quality in all ground water and surface water systems used as sources for drinking water production. Another major recommendation is the investigation of potential analytical methods that current chromatographic methods with high resolution mass spectrometry to ensure that organic contaminants can be detected at the ng/l to ρg/l using a single enrichment method in order to make sure that those organic contaminants that occur at very low concentration in environmental samples can be detected. For example, the realisation that compounds such as synthetic organic polymer residues, emerging disinfectant by-products, detergent metabolites, chlorinated benzenes**,** alkyl phenol**,** polyethoxylates**,** their metabolites and cyanotoxins are continuously discharged into the environment via wastewater and industrial effluent discharges which increases their concentration in aquatic environment and concomitantly their potential to exert adverse health effects in water used as source for the production of drinking water necessitates that each of these groups be added to the current monitoring programme. The current water quality monographs can be used for the benefit of the Drinking Water industry. It is also recommended that a training manual on the production and use of water quality monographs is produced to facilitate their dissemination. CD-ROMs on the water quality monographs can be produced and distributed with the manual.

Key words
Organic contaminants, selection and prioritization, drinking water value chain, adverse human health effects, pool of contaminants, screening, protocol

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CONCEPTUAL DEFINITIONS

Water quality: the physical, chemical, biological and organoleptic properties of water that makes it fit for its intended use. Organoleptic properties are understood as those properties, which involve the use of senses, such as taste, smell, feel, sight in order to describe them. These are collectively, taste, odour, colour and turbidity.

The toxicity of a compound is its intrinsic capacity to cause injury, including the potential to induce carcinogenic, mutagenic and teratogenic effects.

The hazard presented by a compound is the capacity of that compound to cause injury under the circumstances of exposure. A toxic compound found in water does not necessarily present a hazard. It will present a risk only if exposure to the target organ(s) of an organism occurs.

Risk: The probability that in a certain time frame, an adverse outcome will occur in a person; group of people, plants, animals and/or the ecology of a specified area that is exposed to a particular dose or concentration of a hazardous agent, that is, it depends on both the level of toxicity of the agent and the level of exposure.

Validation: is an element of system assessment. It is undertaken to assess the feasibility of the protocol. It is also done to assess if the information supporting the protocol is correct and is mainly concerned with the assessment of the scientific and technical inputs into the protocol.

Prioritization: A prioritization exercise's function is to identify a short list of chemicals that rank highest when scored against a number of different screening criteria.[98] It gives an idea of magnitude of the problem associated with a potential contaminant and allows energy and resources to be directed to better understanding, regulating or engineering control measures for the most serious threats.[98] To produce an overall ranking of chemicals, scores resulting from application of individual screening criteria are weighted and the chemicals are ranked in order of increasing total score.

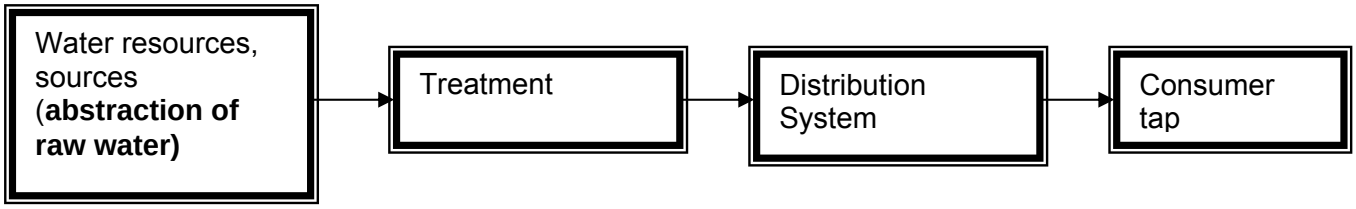
Critical control point: an activity, procedure at which control can be applied and which is essential to prevent a hazard or reduce it to an acceptable level. In the drinking water value chain, this will be the point at which the quality of water is expected to change. Hence, control at this point is crucial in terms of all system parameters.

Expert opinion

Expert opinion usually refers to the views of professionals who have expertise in a particular form of practice or field of inquiry, such as clinical practice or research methodology. Expert opinion may refer to one person's views or to the consensus view of a group of experts. When the concept of evidence based practice was first introduced, expert opinion was identified as the least reliable form of evidence on the effectiveness of interventions, and positioned at the lowest level in "levels of evidence" hierarchies. Other developments have determined that ranking expert opinion with levels of evidence is not useful or appropriate because expert opinion is qualitatively different to the forms of evidence that are derived from research.

Drinking water value chain (from source to tap)

This is traditionally known as the drinking water supply chain. The word "value" is added to emphasize the value add from one step to another from a process and water quality point of view. As the water progresses from the source, the water quality improves until it reaches the consumer at a quality that is acceptable and complies with the drinking water quality guidelines or standards. The figure below illustrates the chain.



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SYMBOLS AND ABBREVIATIONS

ADI	Acceptable daily intake
AhR	Aryl hydrogen receptor
AI	Adaptive implementation
$Al_2 (SO_4)_3$	Aluminium sulphate
$Al_2 (SO_4)_3.18H_2O$	Hydrated Aluminium sulphate
ANN	Artificial Neural Network
AOP	Advanced oxidation process
AOS	Alpha-olefin sulfonates
APs	Alkylphenols
APCI	Atmospheric chemical ionization
APE	Alkyl phenol ethoxylate
APPEOs	Alkyl phenol polyethoxylates
ARC	Agriculture Research Council
Arg	Arginine
As	Arsenic
AS	Alkyl sulfonates
ATSDR	Agency for Toxic Substances and Disease Registry
BBP	Butylbenzylpthalate
BPA	Bisphenol A
BTEX	Benzene, toluene, ethylbenzene and xylenes
BA	Bioassay
BaP	Benz[a]pyrene
BCF	Bioconcentration factor
BCF_{fish}	Bioconcentration factor in fish
BDEs	Brominated diphenyl ethers
BHC	Benzene hexachloride
BOC (M)	Biodegradable organic carbon (matter)
BP	Butyl phenol
BT	Benzotriazole
CAFOs	Confined animal feeding operations
CART	Classification and regression tree
CASRN	Chemical abstracts services registration number

CCL	Contaminants candidate list
CDBPs	Chlorinated disinfectant by-products
CEC	Commission for Environmental Cooperation
CEPA	Canadian Environmental Protection Agency
CH_3Sn^{3+}	Monomethyl tin
$(CH_3)_2Sn^{3+}$	Dimethyltin
ChV	Chronic values
Cl_2	Chlorine
ClO_2	Chlorine dioxide
COMMPS	Combined monitoring and modelling based priority setting
CPAM	Cationic polyacrylamide
CSIR	Council for Science and Industrial Research
CTP	Cyanotoxin poisoning
CYN	Cylindrospermopsin
C10-C13-	Ten carbon atoms to thirteen carbon atoms chained hydrocarbons
C_{60}	Fullerene
DADKM	Deaminodiketometribuzin
DADMAC	Diallyldimethylammonium chloride
DAM	Deamino metribuzin
DBCP	Dibromochloropropane
DBP	Di-n-Butylphthalate
DBPs	Disinfection by-products
DBP-CAN	Disinfection by-products with carcinogenicity estimates
DBT	Dibutyltin
DDA	Didealkyl atrazine
DDD	(1,1-dichloro-2,2-bis(p-chlorophenol) ethane
DDE	(1,1-dichloro-2,2-bis(p-chlorophenyl) ethylene
DDHA	Didealkylhydroatrazine
DDT	Dichlorodiphenyltrichloroethane
DEA	Deethylatrazine
DEHA	Di-(2-ethylhexyl)adipate
DEHP	Di-(2-ethylhexyl) phthalate
DEP	Diethylphthalate
DES	Diethylstilbestrol
DIA	Deisopropylatrazine
DIHA	Deisopropylhydroatrazine

DKM	Diketo metribuzin
DMP	Dimethylphthalate
DMT	Dimethyltin
DNA	Deoxyribonucleic acid
DOC	Dissolved organic carbon
DOH	Department of Health (RSA)
DOP	Di-n-octylphthalate
DWAF	Department of Water Affairs and Forestry
DWI	Drinking Water Inspectorate (UK)
DES	Diethylstilberol
DOC	Dissolved Organic Carbon
DOM	Dissolved Organic Matter
DsPH	Directors of Public Health
DSL	Domestic substances list
DYNAMEC	Dynamic Mechanism
E_1	Estrone
E_2	17-ß-Estradiol
EAWAG	Swiss Federal Institute for Environmental Science and Technology
EC	Effect concentration
ECB	European chemicals bureau
EDB	Ethyl dibromide
EDC	Endocrine disrupting compounds
EDCs	Endocrine disrupting chemicals
EDTA	Ethylene dinitrotetraacetic acid
EE_2	17α-ethynylestradiol
EEC	European Economic Community
EFS_d	Direct effect scores
EFS_i	Indirect effect scores
EFS_h	Effects on human
EHOs	Environmental health officers
EPA	Environmental Protection Agency
ESI	Electron spray ionization
EU	European Union
EURAM	European Academy of Management
FA	Fulvic acid
FAO	Food and Agriculture Organization

$FeCl_3$	Ferric chloride
GAC	Granular Activated Carbon
GC	Gas Chromatography
GC-MS	Gas Chromatography with Mass Spectrometric detection
GDWQ	Guidelines for Drinking Water Quality
GLI	Global leachability index
GUS	Groundwater ubiquity score
HA	Humic acid
HAA	Haloacetic acid
HAA5	The five regulated haloacetic acids
HABs	Harmful algal blooms
HANs	Haloacetonitrile
HCB	Hexachlorobenzene
HCH	Hexachlorocyclohexane
HDPE	High density polyethylene pipes
Hg	Mercury
Hg^{2+}	Mercury ion
HKs	Haloketones
HMW	High molecular weight
H_2O	Water molecule –Chemical formula
HRA	Health Risk Assessment
Hu	Humin
HS^-	Hydrogen sulphide ion
Hy	Hydrophilic factor
IARC	International Agency for Research on Cancer
2-IBMP	2-Isobutylmethoxy-pyrazine
IEH	Institute of Environmental Health
IMAC	Interim maximum allowable concentration (Canada)
IPCS	International Programme on Chemical Safety
2-IPMP	2-Isopropymethoxy-pyrazine
IRIS	Integrated Risk Information System (USEPA)
IS	Internal standard
ISCW	Institute for Soil, Crops and Water
IUCLID	International Uniform Chemical Information Database
IUPAC	International Union of Pure and Applied Chemistry
JMPR	The Joint FAO/WHO meetings on Pesticide Residues
KCl	Potassium chloride

LASs	Liner alkyl sulfonates
LC	Liquid chromatography
L_c	Lethal concentration
LC-MS	Liquid chromatography, Mass spectrometry
LD_{50}	Lethal dose (death of 50% of a group of test animals)
LD_{Lo}	Lowest dose of a toxic material at which the death of the exposed test animal occurs
LIN	Leaching indices
LOEL	Low observed effect level
LOAEL	Low observed adverse effect level
LSE	Liquid solid extraction
MAC	Maximum Allowable Concentration (Canada)
MAV	Maximum Acceptable Value (New Zealand)
MBT	Methylbutyltin
MCL	Maximum Contaminant Limit (USEPA)
MCLG	Maximum Contaminant Limit goal (USEPA)
MC-LR	Microcystin-LR (L-Leucine, R-Arginine)
MCF-7 cells	A breast cancer cell line
MCPA	Monochlorophenoxy acetic acid
MCYST	Microcystins
MDL	Method detection limit
MDS	Multi-dimensional scaling
MDPE	Medium density polyethylene
MeHg	Methylmercury
2-MIB	2-Methylisoborneol
MRL	Minimum Reporting Limit
MTBE	Methyl tertbutyl ether
MX	Mutagen X
NDMA	Nitrosodimethylamine
NGOs	Non-governmental organizations
NHMRC	National Health Medical Research Council (Australia)
NOAEL	No observed adverse effect level
NOC	Natural Organic Carbon
NOEC	No-observed-effect concentration
NOM	Natural organic matter
NP	Nonylphenol
NPEOs	Nonylphenol ethoxylates

NSC	North Sea conference
NTA	Nitrilo acetic acid
NTP	National Toxicity Programme
O_2	Oxygen molecule, Chemical formula
O_3	Ozone molecule, Chemical formula
OC	Organic carbon
OECD	Organization for Economic Cooperation and Development
OECD-SIDs	Organization for Economic Cooperation and Development Screening Information Databases
OP	Octylphenol
OH	Hydroxyl group
OM	Organic matter
OPEOs	Octylphenol ethoxylates
OSPAR	OSLO PARIS
PAC	Powder activated carbon
PAHs	Polynuclear aromatic hydrocarbons
p-$AlCl_3$	Polyaluminium chloride
p-AlSiS	Polyaluminium silicate sulphate
PAM	Polyacrylamide
PBB	Polybrominated biphenyl
PBDEs	Polybrominated diphenylethers
PBT	Persistence, Bioaccumulation and Toxicity
PCB	Polychorinated biphenyl
PCBs	Polychlorinated biphenyls
PCBEs	Polychlorinated biphenyl ethers
PCCL	Preliminary Candidate Contaminant List
PCDDs	Polychlorinated dibenzo-p-dioxins
PCDFs	Polychlorinated dibenzo-p-furans
PCE	Perchloroethylene
PCP	Pentachlorophenol
PDADMAC	Polydiallyldimethylammonium chloride
PEX	Cross-linked (X) Polyethylene pipe
PFAs	Polyfluorinated alkyl substances
PFACs	Perfluoroalkyl carboxylates
PFASs	Polyfluoroalkyl sulfonates
PFBES	Polyfluoro biphenyl ethers
PFOA	Perfluorooctanoic acid

PFOC	Polyfluorinated organic compounds
PFOS	Perfluoroorganic sulfonates
PFOSA	Perfluorooactane sulfoamide
PFUnDA	Perfluoroundecanoic acid
PFDoDA	Perfluorododecanoic acid
PNECs	Predicted no effect concentrations
POC	Particulate Organic Carbon
POPs	Persistent organic pollutants
PPCPs	Pharmaceuticals and personal care products
PPOPs	Priority persistent organic pollutants
PPU	Plant Protection Unit
PSL	Priority Substances List
PSPs	Paralytic shellfish poisons
PTB	Persistence, Toxic and Bioaccumulation
PVC	Polyvinyl chloride
PWSs	Public Water Systems
QSARs	Quantitative Structure Activity Relationships
QUEST	Quick, Unbiased and Efficient Statistical Tree
R_fD	Reference Dose
RDA	Regularized discriminant analysis
RQ	Risk quotients
RSA	Republic of South Africa
RW	Rand Water
SABS	South African Bureau of Standards
SANS	South African National Standard
SAR	Structure Activity Relationship
SCs	Sulfophenyl carboxylates
SCCPs	Short chain chlorinated paraffins
SDWA	Safe Drinking Water Act
Se	Selenium
Sn	Tin
sp	Species
SPE-GC-MS	Solid phase extraction Gas chromatography Mass spectrometry
SPM	Suspended particulate matter
STP	Sewage Treatment Plant
SWT	Sewage Water treatment

2,4,5-TP	2,4,5-Trichlorophenoxyacetic acid
TBA	Terbutylazine
TBP	Tri-n-butylphosphate
TBT	Tributyltin
TBTO	Tributyloxide
TCA	Trichloroacetic acid (1,1,1-Tricloroethane)
TCDD	Tetrachlorodibenzo-p-dioxin
TCE	Trichloroethylene
TD	Tumorigenicity dose
TDS	Total dissolved solids
TEFs	Toxic equivalent factors
THMs	Trihalomethanes
TOC	Total organic carbon
TOX	Total organic halide
TPP	Triphenyl phosphate
TT	Tolyltriazole
TTS	Total toxicity score
TTHMs	Total trihalomethanes
Ui	Unsaturation index
UK	United Kingdom
UN	United Nations
UNEP	United Nations Environment Programme
USEPA	United States Environment Protection Agency
VIN	Volatile indices
VMS	Volatile methylated siloxanes
VOCs	Volatile organic compounds
WHIM	Weighted holistic invariant molecular descriptors
WHO	World Health Organisation
WRC	Water Research Commission
WW	Water Works
WWTP	Waste Water Treatment Plant
XOCs	Xenobiotic organic compounds
=	Equal sign
≈	approximately
Atm.m^3/mol	Atmospheres. Cubic metres per mol
β	Beta
<	Less than

≤	Less or equal to
>	Greater than
%	Percentage
˚C	Degrees Celsius
g/mol	Gram per mole
H_c or K_h	Henry's law constant
K_d	Distribution coefficient
K_{oc}	Organic carbon-water partition coefficient
K_{ow}	Octanol/water partition coefficient
g/cm^3	Grams per cubic centimeter
lbs.yr	pounds/year
m	meter
mg/kg	Milligrams per kilogram
mg/kg/day	Milligrams per kilogram per day
mg/kg/day bw	Milligrams per kilogram per day body weight
mg/l	Milligrams per litre
MW	Molecular weight
ng/l	Nanograms per litre
ng/g	Nanograms per gram
Nm	Nanometre
ρ	Relative density
S_w	Water solubility
$T_{1/2}$	Half life
mg/l	Micrograms per litre
µg/kg	Micrograms per kilogram
µg/mol	Micrograms/mol
µm	Micrometer
V_p	Vapour pressure