IDENTIFICATION OF SPECIFIC POLLUTANTS IN YESILIRMAK RIVER BASIN BY USING COMMPS AND NORMAN PRIORITIZATION METHODS

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ABSTRACT

IDENTIFICATION OF SPECIFIC POLLUTANTS IN YESILIRMAK RIVER BASIN BY USING COMMPS AND NORMAN PRIORITIZATION METHODS

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According to the Water Framework Directive (2000/60/EC), there is a need for the identification of substances posing a relatively higher risk to the aquatic environment and human health to be included in monitoring and risk assessment studies. Thus, river basin specific pollutants must be identified and regularly monitored by the EU Member States to achieve good ecological water status. This study aims to determine specific pollutants in the Yesilirmak River Basin. The national list of 250 river basin specific pollutants for Turkey, which takes part in Surface Water Quality Regulation, was used as the list of candidate substances. Then, the COMMPS and NORMAN prioritization methods, which are commonly applied in the EU Member States, were separately applied for the identification of Yesilirmak River Basin specific pollutants. A set of 1.5-year surface water quality monitoring data collected from 42 monitoring stations in between August 2016 and January 2018 was used. The candidate 250 chemicals were scored and ranked. Since the ranking results by the COMMPS and NORMAN prioritization methods

differed, the COMMPS and NORMAN scores of each substance were combined by using a weighting factor approach in order to obtain a single ranking list and score for each substance. These integrated scores were then ranked again, and 52 dangerous substances were proposed as water phase relevant specific pollutants for the Yesilirmak River Basin. It was seen that especially metals (arsenic, chromium, zinc) and pesticides (DDT, fenarimol, permethrin) attracted the attention in the river basin.

Keywords: River basin specific pollutants, prioritization, risk assessment

ÖZ

COMMPS VE NORMAN ÖNCELİKLENDİRME YÖNTEMLERİ KULLANILARAK YEŞİLIRMAK HAVZASI BELİRLİ (SPESİFİK) KİRLETİCİLERİNİN BELİRLENMESİ

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Su Çerçeve Direktifine göre (2000/60/EC), izleme ve risk değerlendirme çalışmalarına dahil edilmek üzere, sucul ortam ve insan sağlığı açısından nispeten yüksek risk teşkil eden kimyasal maddelerin belirlenmesine ihtiyaç vardır. Bu nedenle, AB üye ülkeleri, iyi ekolojik su durumuna ulaşmayı hedefleyerek kendi havza bazlı belirli kirleticilerini tespit etmek ve düzenli olarak kontrol etmek zorundadır. Bu kapsamda, bu çalışma Yeşilırmak havzası belirli kirleticilerini tespit etmeyi amaçlamaktadır. Aday maddeler/kimyasallar olarak, Yerüstü Su Kalitesi Yönetmeliğinde yer alan Türkiye geneli için belirlenmiş ulusal 250 belirli kirleticinin kullanılmasına karar verilmiştir. Daha sonra, Yeşilırmak Havzası belirli kirleticilerini tespit etmek için AB üye ülkelerinde yaygın olarak kullanılan COMMPS ve NORMAN önceliklendirme yöntemleri ayrı ayrı uygulanmıştır. Ağustos 2016 ve Ocak 2018 tarihleri arasında 42 izleme noktasından toplanan 1,5 yıllık yüzeysel su kalitesi izleme verileri baz alınmıştır. Aday 250 kimyasal bu doğrultuda skorlanıp sıralanmıştır. COMMPS ve NORMAN önceliklendirme

yöntemleri ile elde edilen sıralama sonuçlarının farklılığından dolayı, her bir madde için tek bir sıralama skoru ve sıralama listesi oluşturmak için ağırlık faktörü yaklaşımı uygulanarak COMMPS ve NORMAN skorları kombine edilmiştir. Elde edilen bütüncül skorlara göre tekrardan sıralama yapılmış ve 52 tehlikeli madde Yeşilırmak Havzası (su fazı) belirli kirleticileri olarak önerilmiştir. Nehir havzasında özellikle metallerin (arsenik, krom, çinko) ve pestisitlerin (DDT, fenarimol, permetrin) ön plana çıktığı görülmüştür.

Anahtar Kelimeler: Nehir havzası belirli kirleticileri, önceliklendirme, risk değerlendirmesi

To my family

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ACC: American Chemistry Council

ADI: Acceptable Daily Intake

AF: Assessment Factor

AT: Animal Toxicology

ATSDR: Agency for Toxic Substances and Disease Registry

BCF: Bioconcentration Factor

BIKOP: Determination of Water Pollution Resulting from Usage of Plant Protection Products and Determination of Environmental Quality Standards on the Basis of Substance or Substance Group Project

BREF: Best Available Techniques Reference Document

C_i: Concentration of a Chemical/Substance in the Water Phase

CMR: Carcinogenic, Mutagenic and Toxic for Reproduction (or Carcinogenicity, Mutagenicity and Reproductive Toxicity)

COMMPS: Combined Monitoring-based and Modelling-based Priority Setting Scheme

CRPHR: Consumption Rate Posing Health Risk

D: Application Dose

DT_{50}: Dissipation Half-Life

DYNAMEC: Dynamic Selection and Prioritization Mechanism for Hazardous Substances

EC: European Commission

ED: Endocrine Disruption

EEP: Environmental Exposure Potential

EFS_d: Direct Aquatic Effect Score

EFS_h: Effect on Humans Score

EFS_i: Indirect Aquatic Effect Score

EOC: Emerging Organic Contaminants

EQS: Environmental Quality Standards

ERI: Environmental Risk Index

EU: European Union

EURAM: European Risk Ranking Method

f: Fugacity

GC/MS: Gas Chromatography / Mass Spectrometry

GESAMP: The Joint Group of Experts on the Scientific Aspects of Marine Environmental Protection

GHS: Globally Harmonized System of Classification and Labeling

H: Henry's Law Constant

HELCOM: Helsinki Convention on the Protection of the Marine Environment of the Baltic Sea

HNS: Hazardous and Noxious Substances

HP: Hazard Potential

HQ: Hazard Quotient

I_eff: Effect Index/Score

I_exp: Exposure Index/Score

I_prio: Priority Index/Score

IEH: Institute for Environment and Health

IRICAP: Integrated Risk Index of Chemical Aquatic Pollution

JRC: Joint Research Center

KIYITEMA: Determination of Hazardous Substances in Coastal and Transitional Waters and Ecological Coastal Dynamics Project

K_{oc}: Organic Carbon-Water Partition Coefficient

K_{ow}: Octanol-Water Partition Coefficient

L: Leaching

$L(E)C_{50}$: Lethal (Effective) Concentration

LD_{50}: Lethal Dose

LOAEL: Lowest Observed Adverse Effect Level

LOD: Limit of Detection

LOQ: Limit of Quantification

LRTP: Long-Range Transport Potential

MEC_{95}: 95^{th} Percentile of Maximum Environmental Concentrations

NOAEL: No Observed Adverse Effect Level

NOEC: No Observed Effect Concentration

NORMAN: Network of Reference Laboratories, Research Centers and Related Organizations for Monitoring of Emerging Environmental Substances

NPL: National Priorities List

OECD: Organization for Economic Co-operation and Development

OSPAR: Oslo Paris Convention for the Protection of the Marine Environment of the North-East Atlantic

PBT: Persistent, Bioaccumulative and Toxic (or Persistency, Bioaccumulation and Toxicity)

PEC: Predicted Environmental Concentration

PNEC: Predicted No Effect Concentration

POP: Persistent Organic Pollutants

QSAR: Quantitative Structure- Activity Relationship

R: The Gas Constant

REACH: Registration, Evaluation, Authorization and Restriction of Chemicals

RfD: Reference Dose

RQ: Risk Quotient

S: Water Solubility

SWQR: Surface Water Quality Regulation

T: Temperature

TES: Toxicity/Environmental Score

THVS: Total Hazard Value Score

TMMK: Control of Hazardous Substances Pollution Project

TOBB: Turkish Union of Chambers and Commodity Exchanges

TP: Toxicological Profile / Toxicity Potential

TUBITAK: Scientific and Technological Research Council of Turkey

TUBITAK MAM: TUBITAK Marmara Research Center

UF: Uncertainty Factor

US EPA: United States Environmental Protection Agency

V: Volatility

V_p: Vapor Pressure

WF: Weighting Factor

WFD: Water Framework Directive

WHP: Weighted Hazard Potential

Z: Fugacity Capacity

CHAPTER 1

INTRODUCTION

1.1. Concept of Specific Pollutants and Prioritization of Substances

Aquatic ecosystems have been exposed to a great number of pollutants formed as a result of naturally occurring events and anthropogenic activities. In order to take necessary precautions against pollution and protect the environment, environmentally responsible/relevant substances must be determined depending on the intensity of the risk they pose from the available evidence.

In the context of the EU Water Framework Directive (WFD, 2000/60/EC), there is a need for the identification of substances or group of substances posing relatively higher risk to or via the aquatic environment for monitoring and risk assessment purposes. The WFD sets the first list of "priority substances" and defines the Environmental Quality Standards (EQS) for surface waters with the EQS Directive (2013/39/EU). The WFD also requires the Member States to identify their own second lists of substances to be controlled at the river basin scale; so-called "river basin specific pollutants". Member states are to set EQS for these pollutants at a national level. The EQS are taken into account when assessing risks to the aquatic environment, classifying the status of surface waters and controlling discharges within the framework of river basin management plans.

The EU WFD aims to achieve good status for all waters. It emphasizes the necessity of management plans which are based on river basins with a requirement of an update for every six years. Good ecological status and good chemical status are the main components of good water status. Ecological status

regards the chemical characteristics (by evaluating specific pollutants levels), the hydrological characteristics and the quality of the biological community of the surface waters, whereas the chemical status considers priority substances' levels of the respective surface waters. Each member state must determine its own river basin specific pollutants for the evaluation of the ecological status. On the other hand, priority pollutants are determined by the European Commission, and they are same for all member states (European Commission, n.d.). Since priority and specific pollutants have persistence, bioaccumulation and toxicity (PBT) properties, and they are discharged to surface waters in significant quantities; hence, they must be monitored regularly and checked for compliance with EQS.

In our country, as a requirement of the Surface Water Quality Regulation (SWQR)[1], river basin specific pollutants must be determined by the Ministry of Agriculture and Forestry (The General Directorate of Water Management) and necessary actions must be taken in order to achieve good ecological water status at the appointed time (2027- EC final deadline for fulfilling objectives).

During the determination of priority and river basin specific pollutants/substances, prioritization techniques are used to choose relevant substances among great numbers of substances in terms of the risk they posed to the environment and human health. Due to financial and workforce limitations as well as deficiency of reliable data for quantitative assessment, it is not possible to evaluate all chemicals which are used/produced in different quantities and discharged to surface waters. Therefore, chemicals are subjected to screening (elimination) and prioritization processes by means of scoring, ranking and risk evaluation models regarding environmental significance or concern. A priority chemical should be dealt with greater urgency in comparison with other chemicals due to its importance (Kuzmanovic, 2014).

Basically, prioritization is carried out by regarding physicochemical and toxicological properties of chemicals and evaluating:

[1] Official Journal dated August 10, 2016, No: 29797

- ❖ Exposure data of chemicals
  - Predicted environmental concentration (by using production amount and use pattern)
  - Measured environmental concentration (concentration level in surface waters and/or sediments)
- ❖ Risk/hazard data of chemicals in terms of
  - Environmental risk (mostly aquatic ecosystem)
  - Human health risk including different toxicological endpoints related to acute, chronic, carcinogenicity, mutagenicity, reproductive toxicity (CMR) and endocrine disruption effects as well as effects on neurotoxicity and teratogenicity.

After identified criteria are combined through weighing approach for each chemical, corresponding scores are given depending on the magnitudes of the data. Then, a relative ranking procedure of chemicals is carried out (Davis et al., 1994).

Alternatively, a risk-based ranking process can be done according to risk quotient (RQ) value which indicates the ratio between measured (or predicted) environmental concentration and predicted no effect concentration value (PNEC) by considering water, sediment or biota compartments (JRC, 2015; JRC, 2016).

The present study was carried out to prioritize dangerous pollutants, which are relevant to the Yesilirmak River Basin. In the following section, an overview of the Yesilirmak River Basin is provided.

1.2. General Overview of the Yesilirmak River Basin

Yesilirmak River Basin, which is one of the twenty-five main basins in Turkey, is located in the north of Turkey as a fifth largest basin with roughly 38,000 km^2 surface area. Major provinces of the basin are Tokat, Corum, Amasya and Samsun. Certain parts of Yozgat, Giresun, Ordu, Sivas, Gumushane and Erzincan also fall within the boundaries of the river basin. Yesilirmak River is almost 519

km in length, and its tributaries are composed of Kelkit, Cekerek, Corum and Tersakan Creeks as shown in Figure 1. It discharges into the Black Sea at the end of the flow. Depending on seasonal snowmelt, rainfall and runoff as a result of semi-arid and subtropical climate, high annual streamflow occurs between March and May whereas low streamflow takes place between July and February in the Yesilirmak River Basin (Kurunc et al., 2005; Jin et al., 2013). The population of the river basin is approximately 2,8 million people (YHKB, n.d.).

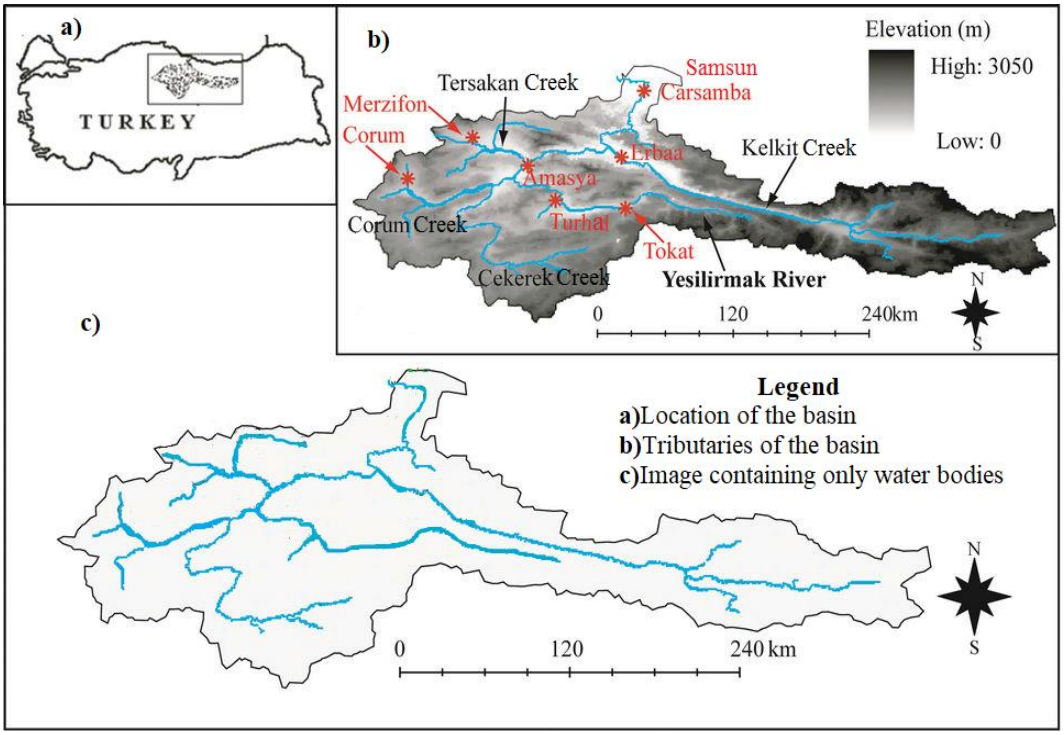

Figure 1. Map of the Yesilirmak River Basin and Its Tributaries (Jin et al, 2013)

According to a report prepared by TUBITAK MAM (2010), water in the basin serves many purposes, and it is used for

- Drinking water supply
- Agricultural irrigation water
- Industrial water supply
- Recreational activities such as fishing and swimming

In terms of pressures and effects, main polluting activities include

- Discharge of domestic and industrial wastewaters (especially food industries and industries related to soil, stone and metal) which are not treated or partially treated (insufficiently) into receiving water body
- Mining activities
- Intensive agricultural and livestock activities
- Leachate from solid waste dump sites
- Hydroelectric power plants
- Soil erosion and drought

TUBITAK 1003 Project called "Management of Point and Diffuse Pollutant Sources in the Yesilirmak River Basin" is currently being carried out. The project aims to provide technical support to Ministry of Agriculture and Forestry (The General Directorate of Water Management) about developing a strategy for the management plan of the Yesilirmak River Basin as a requirement of the WFD.

Within the scope of the project, the following actions were planned to be done:

- Determination of general pollutants by considering both point and diffuse pollutant sources in the basin and creation of pollutant inventory
- Prioritization of the pollutants and identification river basin specific pollutants
- Determination of EQS by regarding background concentrations for specific pollutants whose EQS have not been assigned by the ministry
- Determination of EQS-based discharge standards via Tiered approach described in the EU EQS Directive and related technical guidance documents by using a software such as Discharge-Test
- Evaluation and modification/improvement of the processes applied in existing wastewater treatment plants (WWTP) in order to decrease pollutant loads
- Evaluation of options for tertiary/advanced treatment processes in case of exceedance of EQS by specific and priority pollutants in the water bodies

1.3. Aim and Scope of the Thesis

The aim of the study is to identify water phase relevant specific pollutants in the Yesilirmak River Basin. It is expected that the results of this study will contribute to the development of river basin management plan, risk assessment strategies and water protection policies. Since only environmentally relevant chemicals are considered for monitoring and auditing purposes by eliminating chemicals which pose a relatively lower risk and chemicals which are not used or detected among 250 national specific pollutants via the COMMPS[2] and NORMAN[3] prioritization methods by adopting monitoring-based approach using 1.5-year surface water quality monitoring data (August 2016-January 2018); issues about budget, workforce and time will be significantly overcome.

The COMMPS and NORMAN methods enable the substances to be scored and relatively ranked by prioritizing them as a result of exposure, hazard and risk assessments. The substances are evaluated depending on the magnitudes of physicochemical and toxicological properties along with their concentration levels in the environment. In this manner, environmentally significant chemicals posing a higher risk are highlighted.

Within this scope, this thesis involves six chapters. In Chapter 1 (Introduction), description of specific pollutants, the necessity of prioritization process and general information about the Yesilirmak River Basin are given. In addition, the aim and scope of the study are stated. In Chapter 2 (Background Studies), literature review on prioritization and risk assessment approaches is given along with the status of Turkey and Europe about the determination of river basin specific pollutants. In Chapter 3 (Methodology), the COMMPS and NORMAN prioritization methods are explained along with the assumptions made for their applications. Moreover, the weighting factor approach is introduced. In Chapter 4

[2] Combined Monitoring-Based and Modeling-Based Priority Setting

[3] Network of Reference Laboratories, Research Centers and Related Organizations for Monitoring of Emerging Environmental Substances

(Results and Discussion), the ranking of candidate substances/chemicals via the COMMPS and NORMAN methods are presented. In addition, final ranking results by using the weighting factor approach are shown. In Chapter 5 (Conclusion), proposed specific pollutants for the Yesilirmak River Basin are listed. Finally, necessary steps to be taken for future studies are suggested in Chapter 6 (Recommendations for Future Studies).

CHAPTER 2

BACKGROUND STUDIES

2.1. Literature Review on Prioritization and Risk Assessment Approaches

In this part, studies related to prioritization of substances/chemicals, which were carried out between years of 2000 and 2018, are explained in detail. Since studies have different algorithms and use different techniques/procedures in order to rank/score the substances, they are evaluated separately in chronological order. In cases studies use similar approaches or apply modifications to existing methods, they are emphasized in the text by giving references.

OSPAR Commission (2000) developed DYNAMEC (Dynamic Selection and Prioritization Mechanism for Hazardous Substances) approach in order to identify hazardous substances and prioritize them by taking into account their persistence, bioaccumulation, toxicity, endocrine disruption and CMR (Carcinogenic, Mutagenic and Toxic for Reproduction) properties. The COMMPS procedure was used as a base. As a result of the combination of exposure and effect score calculations, substances were ranked. Exposure score considers either predicted (via the amount of use and use pattern of substances) or measured (monitored) concentration levels of substances by using a modified version of EURAM (European Risk Ranking Method) model. On the other hand, effect score regards the direct and indirect effects of substances on aquatic life and human health. Substances which were selected via this procedure were listed for water and sediment phases both using monitoring-based and modelling-based exposure assessments.

Guiner et al. (2001) conducted a study that focuses on childhood cancer risk in order to prioritize pesticides used in California by using PUR (Pesticide Use Report) database. Toxicity (carcinogenic potential) and exposure potentials of pesticides were evaluated in their study. After pesticides had been classified according to their toxicological (as probable carcinogens, possible carcinogens, genotoxic substances and developmental/reproductive toxicants) and chemical (as carbamates, organochlorides, organophosphates and dithiocarbamates) properties, they were ranked by using criteria and scores (weights) that are shown in Table 1.

Table 1. Criteria and Corresponding Scores for the Cancer Hazard Assessment of Pesticides (Guiner et al., 2001)

Score (Weights)	**Toxicity**		**Exposure**	
	Cancer Class*	Potency of cancer (mg/kg/d)*	Volatilization Flux**	Field half-life (days)***
10	A	>1	$>10^{-1}$	-
8	B1	> 0.1-1	$>10^{-3}$ - 10^{-1}	-
7	B2	-	-	-
5	C	>0.01-0.1	$>10^{-5}$ - 10^{-3}	>100
4	-	-	-	76-100
3	Genotoxic or and developmental/ reproductive toxicants	0.001-0.01	$>10^{-7}$ - 10^{-5}	51-75
2	-	-	-	26-50
1	No data	<0.001 or no data	$<10^{-7}$ or no data	< 25 or no data

*Cancer slope factor (values in the US EPA documents)

**Flux rate = Vapor pressure / (water solubility x coefficient of soil absorption)

***Persistence data from US Department of Agriculture

For the calculation procedure (Equation (1)), corresponding scores for specified four criteria are multiplied then divided by 500 for each chemical in order to find cancer hazard factor that ranges between 0.002 and 10.

$$\textbf{Cancer Hazard Factor} = \frac{\text{Cancer class} \times \text{Cancer potency} \times \text{Flux} \times \text{Persistence}}{500} \quad (1)$$

Then, cancer hazard factor and annual average pesticide usage value are multiplied for each pesticide, and hazard-based pesticide use values are calculated (Equation (2)). The ranking is done by using these values.

$$\textbf{Hazard Based Pesticide Use} = \text{Cancer Hazard Factor} \times \text{Annual average pesticide use} \quad (2)$$

According to the study carried out by Lerche et al. (2004), chemical substances in Japanese Pollutant Release and Transfer Register (PRTR) database were ranked by using Partial Order Theory (POT) and Random Linear Extension (RLE) methodology and by the help of Hasse diagram (WHASSE computer program). This approach is based on a comparison of substances between each other, and average ranks (scores) of each substance are found by calculating ranking frequency and ranking probability for each criterion/parameter/property stated. In contrary to other types of multi-criteria analysis, POT/RLE approach does not need to associate parameters using weighting coefficients by evaluating functional relationships, and it gives more detailed information about chemicals via offering ranking probabilities for each substance. In their study, chemicals were ranked by considering the impacts of chemicals on human health and the environment. Production/usage amount of substances, emissions data (to air, water and soil), transfer data (to sewage, solid waste, landfill and recycling) and toxicity data (aquatic ecotoxicity, chronic oral toxicity, inhalation toxicity, cancer, mutagenicity, reproductivity and allergy) of substances were selected as evaluation criteria.

The UK Institute for Environment and Health (IEH, 2004) developed a method in which chemicals are scored and ranked according to their exposure and toxic effects on human health by considering fate and behavior of chemicals in the environment. This method regards environmental distribution data (into compartments/phases of water, air, suspended solids, sediments and fish), exposure data (via inhalation, water consumption, food consumption and soil) and toxicity data (acute and chronic) of chemicals. During environmental distribution calculation, after fugacity capacity and fugacity values of chemicals have been found for each compartment by using Mackay Level I model, fractions of chemicals in each phase ($fraction_{water}$, $fraction_{air}$, $fraction_{soil}$ and $fraction_{fish}$) at equilibrium are calculated. Score for each phase is normalized to be in between 0 and 10. Necessary formulas and values are shown in Table 2 and Table 3.

Table 2. Mackay Level I Model (Mackay et al., 1996; Mackay, 2001)

	Model
Fugacity Capacity (Z) ($mol/m^3 \cdot Pa$) Affinity of a chemical for each environmental compartment	$Z_{air} = 1 / RT$
	$Z_{water} = Z_{air} / K_{aw} = 1 / H = S / V_p$
	$Z_{soil} = (Z_{water} \times \rho \times f_{oc} \times K_{oc}) / 1000$
	$Z_{sediment} = (Z_{water} \times \rho \times f_{oc} \times K_{oc}) / 1000$
	$Z_{ss} = (Z_{water} \times \rho \times f_{oc} \times K_{oc}) / 1000$
	$Z_{fish} = (Z_{water} \times \rho \times L \times K_{ow}) / 1000$
Fugacity (f) (Pa) Escaping tendency of a chemical from particular compartment	$f = M / \Sigma (V_i \times Z_i)$ M: 10^8/ Molecular weight of a chemical
Concentration in each phase (C) (mol/m^3)	$C_i = f \times Z_i$

*ρ: density of phase (kg/m^3), f_{oc}: mass fraction of organic carbon in phase, H: Henry's Law constant ($Pa.m^3/mol$), L: lipid fraction (0,048), V: volume of the environmental phase (m^3), S: solubility (m^3/mol), V_p: vapor pressure (Pa), R: ideal gas constant (8.314 J/mol.K), T: temperature (K), K_{ow}: octanol-water partition coefficient , K_{oc}: organic carbon-water partition coefficient, K_{aw}: air-water partition coefficient

Table 3. Mackay Level I Environmental Compartments and Properties (Mackay et al., 1996; Mackay, 2001)

Environmental Compartments	Volume (m^3)	Depth (m)	Area (m^2)	Mass fraction of organic carbon (f_{oc})	Density (kg/m^3)
Air	10^{14}	1000	10^{11}	-	1.2
Water	2×10^{11}	20	10^{10}	-	1000
Soil	9×10^{9}	0.1	90×10^{9}	0.02	2400
Sediment	10^{8}	0.01	10^{10}	0.04	2400
Suspended solids	10^{6}	-	-	0.2	1500
Fish (Biota)	2×10^{5}	-	-	-	1000

Exposure via inhalation score ($E_{inhalation}$) is obtained for each chemical by evaluating volatilization potential (Henry's Law constant- H_c', unitless), air persistence (half-life) and air fraction values of chemicals (Equation (3)). Criteria and corresponding values are shown in Table 4 and Table 5.

$$\mathbf{E_{inhalation}} = \text{Volatilization potential score} \times \text{Persistence (in air) score} \times \text{fraction}_{air}\text{ score} \quad \text{(Maximum score 150)} \tag{3}$$

Table 4. Volatilization Potential (IEH, 2004)

Criteria	**Ranking**	**Score**
$H_c' > 1x10^{-4}$	High	3
$H_c' = 1x10^{-4}$	Medium	2
$H_c' < 1x10^{-4}$	Low	1

Table 5. Persistence in Water and Air (IEH, 2004)

Half-life (median)	Ranking	Score
>40 days	Extremely persistent	5
4-40 days	Moderately persistent	4
0.42-4 days	Moderately short lived	3
0.042-0.42 days	Short lived	2
< 0.042 days (1 hour)	Very short lived	1

Exposure via water consumption score (E_{water}) is obtained for each chemical by evaluating partition behaviors related to air and organic phases (H_c' and K_{ow}), water persistence (half-life) and water fraction values of a chemical (Equation (4)). Criteria and corresponding values are shown in Table 5 and Table 6.

$$\mathbf{E_{water}} = \text{Tendency (to remain in water) score} \times \text{Persistence (in water) score} \times \text{fraction}_{water}\text{ score} \quad \text{(Maximum score 150)} \tag{4}$$

Table 6. Tendency to Remain in Water (IEH, 2004)

Criteria	Ranking	Score
$H_c' < 1x10^{-4}$ or $K_{ow} < 2,5$	High	3
$H_c' \geq 1x10^{-4}$ and $2,5 < K_{ow} < 4$	Medium	2
$H_c' > 1x10^{-4}$ and $K_{ow} > 4$	Low	1

Exposure via soil score (E_{soil}) is obtained for each chemical by evaluating soil adsorption potential (K_{ow}), soil persistence (half-life) and soil fraction values of chemicals (Equation (5)). Criteria and corresponding values are shown in Table 7 and Table 8.

$$\mathbf{E_{soil}} = \text{Soil adsorption potential score} \times \text{Persistence (in soil) score} \times \text{fraction}_{soil}\ \text{score} \quad \text{(Maximum score 150)} \tag{5}$$

Table 7. Soil Adsorption Potential (IEH, 2004)

Criteria	Ranking	Score
Log K_{ow}> 4	High	3
2.5 <Log K_{ow}< 4	Medium	2
Log K_{ow}< 2.5	Low	1

Table 8. Persistence in Soil (IEH, 2004)

Half-life (median)	Ranking	Score
>100 days	Extremely persistent	5
30-100 days	Moderately persistent	4
15-30 days	Moderately short lived	3
5-15 days	Short lived	2
< 5 days	Very short lived	1

Exposure via food consumption score (E_{food}) is obtained for each chemical by evaluating bioaccumulation potential (BCF and K_{ow}) and biota (fish) fraction values of chemicals. (Equation (6)). Criteria and corresponding values are shown in Table 9 and Table 10. The average score from BCF and K_{ow} assessments is used.

$$\mathbf{E_{food}} = 3 \times \text{Bioaccumulation potential score (average)} \times \text{fraction}_{fish}\ \text{score} \quad \text{(Maximum score 150)} \tag{6}$$

Table 9. Bioaccumulation Potential (BCF) (IEH, 2004)

BCF_{fish}	**Bioaccumulation Possibility**	**Score**
>10000	High	5
1000-10000	Moderately high	4
100-1000	Moderately low	3
10-100	Low	2
<10	Unlikely	1

Table 10. Bioaccumulation Potential (K_{ow}) (IEH, 2004)

Log K_{ow}	**Bioaccumulation Possibility**	**Score**
>5	High	5
4-5	Moderately high	4
3-4	Moderately low	3
2-3	Low	2
< 2	Unlikely	1

For evaluation of human health's effects, total toxicity score (TTS) is calculated by regarding risk phrases of each chemical (Equation (7)). The highest score that corresponds to the chemical's effects is taken into consideration. Table 11 shows/summarizes toxicity criteria for human health and corresponding risk phrases and scores.

$$\mathbf{TTS} = 15 \times \text{Effect score in Table 11} \quad (7)$$

(Maximum score 150)

Table 11. Toxicity Criteria, Risk Phrases and Scores (IEH, 2004)

Evidence for Toxicology	**Risk phrases**	**Score**
Significant evidence in animals related to genetic damage/carcinogenicity/effects on reproduction or evidence for human	R45, R46, R49, R60 or R61	10

Table 11. Toxicity Criteria, Risk Phrases and Scores (IEH, 2004) (cont'd)

Evidence for Toxicology	Risk phrases	Score
Evidence for animals about carcinogenicity/mutagenicity (in vivo)/ reproductive effects or evidence for human about the genetic damage of somatic cell	R40, R62, R63 or R64	9
Positive results in mutagenicity test (in vitro) or screening test for reproduction (in vivo) or OECD screening test for reproduction		8
90-day oral toxicity study is ≤ 5 mg/kg bw/d or respiratory sensitization evidence	R42 or 48	7
90-day oral toxicity study is ≤ 50 mg/kg bw/d or skin sensitization evidence	R43 or R48	6
Evidence for cumulative effects or no data about mutagenicity/reproductive effects	R33	5
No data for eyes, skin and respiratory system irritations		5
A negative result in one mutagenicity test (in vivo) but also positive in at least one in vitro test or negative result for the reproductive screening test (in vivo) or no data about repeat dose toxicity		4
Oral LD_{50} ≤ 25 mg/kg for rat or negative for only teratogenicity	R28	3
Oral LD_{50} ≤ 200 mg/kg for rat or cause skin corrosion/eye irritation or negative for only gene mutation/for only chromosomal aberrations (in vitro)/for only fertility	R25, R34, R35 or R41	2
Detrimental by skin contact, inhalation or oral ingestion LD_{50} ≤ 2000 mg/kg for rat	R20, R21, R22	1

*Adapted from Hansen et al. (1999) and Wearne et al. (1996)

Finally, the total score for prioritization process is calculated for each chemical by giving equal weight to chemicals' exposure and toxicity criteria and summing them as follows (Equation (8)):

$$\textbf{Total score} = \frac{E_{inhalation} + E_{water} + E_{soil} + E_{food}}{4} + TTS \quad (8)$$

(Maximum score 300)

Alister and Kogan (2006) conducted a study that ranks agrochemicals according to environmental risk index (ERI) value, which reflects the main superiorities/weaknesses/limitations of agrochemicals in comparison with others. During ERI assessment, soil persistence (P), volatility (V), leaching (L), application dose/rate (D) and toxicity profile (TP) (including octanol-water partition coefficient- K_{ow}, reference dose- Rfd and lethal dose- LD_{50} for human as dermal lethal dose and for animals such as fish, mallard duck and honey bee) criteria were taken into consideration for each agrochemical in their study. Following Equation (9) is used for ERI calculation by using corresponding scores according to the range of the magnitude for each criterion. Criteria and corresponding score/assigned values are shown in Table 12 and Table 13.

$$\textbf{ERI} = (P + L + V + TP) \times D \quad (9)$$

Where

$L = LIX\ index = \exp^{(-k \times Koc)}$

$V = 2.9 \times 10^{-3} \times P \times M^{0.5}$

$TP = K_{ow} + Rfd + LD_{50} + AT$

$Rfd = {}^{NOEL}/_{(UF \times MF)}$

(P: vapor pressure, M: molecular weight of related agrochemical, k: rate of degradation ($k = 0.693/DT_{50}$), K_{oc}: organic carbon adsorption coefficient, NOEL: no observed effect level, UF: uncertainty factor (extrapolation of findings in animals to humans, 10), MF: modifying factor (expert assessment about study uncertainties, $0 \leq 10$ and default value 1))

Table 12. Criteria and Scores for ERI (Alister & Kogan, 2006)

	Ranking intervals				
Scores/ assigned values	Persistence (P) DT_{50}, day	Application dose/rate (D) kg ai ha^{-1}	Leaching (L) LIX index	Volatility (V) mm Hg	Toxicological Profile (TP)
4	≥ 90	≥ 3	≥ 0.5	≥ 10^{-4}	≥ 20
3	60< 90	2<3	0.25 < 0.5	10^{-5} <10^{-4}	14<20
2	30≤ 60	1≤ 2	0.09 ≤ 0.25	10^{-6} ≤ 10^{-5}	8≤14
1	≤ 30	≤ 1	≤ 0.09	≤ 10^{-6}	≤ 8

Table 13. Criteria and Scores for TP (Alister & Kogan, 2006)

	Ranking intervals					
Scores/ assigned values	Log K_{ow}	Rfd (mg/kg/ d)	LD_{50} (mg/kg) (human acute dermal dose)	AT (Animal Toxicology)		
				LD_{50} (mg/kg) (Mallard duck)	LC_{50} (mg/L) (Rainbow trout)	LD_{50} (mg/kg) (Honey bee)
4	≥ 3	≤ 0.001	≤ 40	≤ 50	≤ 10	≤ 25
3	2<3	0.01> 0.001	400>40	500>50	50>10	50>25
2	1≤2	0.1≥ 0.01	4000≥400	5000≥500	100≥50	100≥50
1	≤1	≥ 0.1	≥ 4000	≥ 5000	≥100	≥100

In addition, a good correlation was observed between ERI (excluding TP criteria) values and detection percentages in surface waters and groundwater for several agrochemicals.

Juraske et al. (2007) developed a method called PestScreen, which is based on scoring and ranking of pesticides, by reviewing and incorporating current approaches. They used criteria related to fate (overall persistence and long-range transport potential-LRTP), exposure (human intake fraction) and toxicity (LC_{50} for fish, LD_{50} for rat and honey bee and acceptable daily intake-ADI for human) of pesticides along with application dose (as an indicator of chemical loading). While SimpleBox 3.0 multimedia fate model was used for the calculation of overall persistence and LRTP, human intake fractions were calculated employing USES-LCA 2.0 multimedia fate/exposure/effect model. Criteria, ranking intervals and scores are shown in Table 14 and Table 15.

Table 14. PestScreen Criteria for Fate and Exposure (Juraske et al., 2007)

Subscores	**Ranking Intervals**		
	Overall Persistence (day) (F_1)	LRTP (-) (F_2)	Human intake fraction ($kg.d^{-1}/kg.d^{-1}$) (E)
4	≥ 106	$\geq 6x10^{-3}$	$\geq 10^{-5}$
3	$61 < 106$	$10^{-3} \leq 6x10^{-3}$	$4x10^{-6} < 10^{-5}$
2	$44 \leq 61$	$10^{-4} \leq 10^{-3}$	$2x10^{-6} \leq 4x10^{-6}$
1	≤ 44	$\leq 10^{-4}$	$\leq 2\ x10^{-6}$

Table 15. PestScreen Criteria for Toxicity (Juraske et al., 2007)

Subscores	**Ranking Intervals**			
	LC_{50} (mg/L, fish) (T_1)	ADI (mg/kg body weight/day) (T_2)	LD_{50} (mg/kg body weight, rat) (T_3)	LD_{50} (μg/bee) (T_4)
4	≤ 0.2	≤ 0.005	≤ 250	≤ 1.5
3	$2.5 > 0.2$	$0.01 > 0.005$	$1800 > 250$	$20 \geq 1.5$
2	$25 \geq 2.5$	$0.05 \geq 0.01$	$5000 \geq 1800$	$100 \geq 20$
1	≥ 25	≥ 0.05	≥ 5000	≥ 100

Total score for each pesticide was found by using corresponding subscores for each indicator as follows (Equation (10)):

$$\textbf{PestScore} = D \times \left(\frac{F_1 + F_2}{2} + E + \frac{T_1 + T_2 + T_3 + T_4}{4} \right) \quad (10)$$

Where D: application dose/rate (kg active ingredient / ha)

Finally, pesticides were classified according to the level of concern depending on PestScores as shown in Table 16.

Table 16. PestScores and Corresponding Degrees of Importance (Juraske et al., 2007)

Degree of importance	**Category**	**PestScore**
Very high	IV	≥ 12
High	III	$5.9 \leq 12$
Medium	II	$2.5 \leq 5.9$
Low	I	≤ 2.5

Environment Agency (2007) carried out a prioritization study for 300 organic chemicals compiled from different legislations, regulations, directives and databases within the scope of Water Framework Directive Annex VIII. Exposure (monitoring and/or usage data) and hazard score were determined for each chemical and final score was obtained by combining them. For exposure assessment, monitored environmental concentrations and data for usage amount/use pattern of chemicals were examined, and the highest score was taken into account. For hazard assessment, PBT properties of chemicals were analyzed by considering effects on the aquatic environment (dominantly) and human health. Moreover, fugacity model was used in order to observe the distribution of chemicals into environmental compartments (Fugacity-Based Environmental Equilibrium Partitioning Model Version 3, Level 1 simulation- Trent University

(Canada)). In case data from different sources were different or during evaluation of indicators/parameters, the worst-case scenario was regarded. Criteria and scores for prioritization process are shown in following Table 17, Table 18 and Table 19.

Table 17. Exposure Assessment (Environment Agency, 2007)

Usage data-based exposure*		**Monitoring data-based exposure**	
Criteria	**Score**	**Criteria**	**Score**
0-1	0	Not detected	0
1-10	1	Detected (0.1 µg/L for surface water and any concentration for groundwater)	1 (2 for biota)
10-100	2	Detected nationally (at least 2 region)	2
100-1000	3	>ES or PNEC	3
>1000	4	>ES or PNEC (nationally)	4

*Corresponding scores which are obtained by multiplying usage amount of chemicals by coefficients related to usage pattern are used. Coefficients are 0.1 for a controlled system, 0.2 for non-dispersive (industrial) use, 0.5 for wide dispersive use (mostly diffuse sources) and 1 for usage in the environment.

Table 18. Hazard Assessment (Environment Agency, 2007)

Criteria	**Score**
Not classified	0
T	1
PT or BT or (HT)	2
PBT or P(HT) or B(HT) or v(HT)	3
P(HB)(HT) or vPvB	4

*H: highly, v: very

Table 19. Categorization of PBT Criteria (Environment Agency, 2007)

Persistence (P)		**Bioaccumulation (B)**		**Toxicity (T)**	
Criteria	**Class**	**Criteria**	**Class**	**Criteria (mg/L)**	**Class**
- >20 days (for fresh or marine water) - >60 days (for fresh or marine water sediment)	P	BCF> 500 or log K_{ow} > 4	B	- < 1 (acute $L(E)C_{50}$ test) - < 0.1 (chronic NOEC test)	T
- >40 days (for fresh water) or >60 days (for marine water) - >120 days (for freshwater sediment) or >180 days (for marine water sediment)	HP	BCF>2000 or log K_{ow} >4.5	HB	- < 0.1 (acute $L(E)C_{50}$ test) - < 0.01 (chronic NOEC test) - Known or suspected endocrine disruptors (ED)	HT
- >60 days (for fresh or marine water) - >180 days (for fresh or marine water sediments) - Limitation/ absence of ready biodegradability	vP	BCF>5000 or log K_{ow} >5	vB	- < 0.01 (acute $L(E)C_{50}$ test) - < 0.001 (chronic NOEC test)	vHT

Finally, the final risk score was determined by combining exposure and hazard scores as shown in Table 20 where 1 indicates the highest priority whereas 5 represents the lowest priority. Chemicals with 1 and 2 ranking scores were chosen to derive EQS.

Table 20. Final Risk Ranking Scores (Environment Agency, 2007)

	Exposure Score					
Hazard Score		**4**	**3**	**2**	**1**	**0**
	4	***1***	***1***	***2***	3	5
	3	***1***	***2***	***2***	3	5
	2	***2***	***2***	3	4	5
	1	3	3	4	4	5
	0	5	5	5	5	5

Arnot and Mackay (2008) prioritized 200 chemicals (that are included the list of Canadian Domestic Substances (DSL)) and 12 persistent organic pollutants (identified by United Nations Stockholm Convention) by using holistic mass balance model. Exposure assessment factors (EAF), hazard assessment factors (HAF) and risk assessment factors (RAF) were calculated for each chemical considering most vulnerable species through RAIDAR (Risk Assessment, Identification and Ranking- level II and III) model. In addition, they compared this holistic approach with current methods. Formulas and criteria used in the model are summarized as noted below (Equations (11), (12) and (13)):

$$\textbf{EAF} = {}^{C_U}/_{E_U} = \text{f (persistence and bioaccumulation)} \quad (11)$$

$$\textbf{HAF} = {}^{C_U}/_{C_T} = \text{f (persistence, bioaccumulation and toxicity)} \quad (12)$$

$$\textbf{RAF} = ({}^{C_U}/_{C_T}) \times ({}^{E_A}/_{E_U}) = \text{f (persistence, bioaccumulation, toxicity and quantity)} \quad (13)$$

Where

C_U: computed unit concentration in the representative species (mol/m^3) (via food web bioaccumulation model), E_U: arbitrary unit rate of emission (1 mol/h), C_T: threshold toxic effect concentration of a chemical (acute or chronic) (mol/m^3), E_A: actual emission rate (mol/h)

According to the prioritization exercise conducted by INERIS/IOW consortium (James et al., 2009), risk ratios (PEC/PNEC) were calculated for each substance (determined metals and organics) for water, sediment and biota compartments. During the determination of PEC, two cases were considered by using monitoring data. In the first case, only measurements having concentrations above detection limits were used, arithmetic means of all measurements were calculated for each monitoring site, and then 90^{th} percentile approach was applied. In the second case, the same procedure was applied but non-quantified concentrations were also taken into consideration by taking their values as detection limit/2. PNEC values were calculated for each phase following the EU Technical Guidance Document on risk assessment. Depending on the magnitude of risk ratio for each case and each compartment, substances were grouped as very high (with risk ratios >100), high (with risk ratios >10), medium (with risk ratios >1) and low priority.

Götz et al. (2010) prioritized aquatic microcontaminants that exist in Swiss surface waters based on exposure assessment. After candidate substances had been determined by considering the EU WFD, results of monitoring studies and relevant substances used in that country; substances were categorized depending on their physicochemical properties (environmental distribution from Mackay model and degradation behaviors from BIOWIN model in EPI Suite) and input dynamics (point and diffuse source analysis as continuous or complex input). Then, water phase relevant chemicals in Swiss waters were identified as a result of analysis of exposure category of each substance.

Murray et al. (2010) prioritized trace pollutants and emerging contaminants (including pesticides, industrials, personal care products and pharmaceuticals) that exist in the freshwater environment by evaluating the relative risk of chemicals to human health. Frequency of detection, average or maximum concentration values and risk on human health criteria were used for prioritization process. For each chemical, they calculated the consumption rate posing health risk (CRPHR) value (Equations (14) and (15)). Chemicals with CRPHR of less than 2 L/d were

identified as a very high priority, whereas those with CRPHR of less than 20 L/d and 200 L/d were determined as high and intermediate priority pollutants, respectively.

$$\mathbf{CRPHR} = \frac{\mathrm{ADI} \times 70\ \mathrm{kg}}{\mathrm{C} \times 0.001} \tag{14}$$

$$\mathbf{ADI} = \frac{\mathrm{LOAEL}}{\mathrm{UF}} \tag{15}$$

Where

ADI: acceptable daily intake (mg/kg/day), C: concentration of pollutant in freshwater (μg/L) (either average or maximum observed value), 70: average human weight (kg), 0.001: unit conversion for mass, LOAEL: lowest observed adverse effect level (oral exposure to fauna), UF: uncertainty factor (100) (to compensate difference in effect between animal and human)

Kumar and Xagoraraki (2010) developed a comprehensive ranking method (EOCRank system) with multiple criteria for prioritization of emerging organic contaminants (EOC) including endocrine disrupting chemicals, personal care products and pharmaceuticals in surface water (stream/source water) and finished drinking water for treatment and monitoring purposes. Four criteria, which are occurrence, treatment (removal) in treatment plants for drinking water, ecological and health effects, were used for the evaluation of EOCs. Occurrence criterion consists of prevalence and magnitude properties. Ecological effect criterion includes bioaccumulation and ecotoxicity properties whereas health effect criterion considers effect and pregnancy category properties. Moreover, the property of effect category contains seven subproperties which are developmental impacts, immunotoxicity, endocrine disrupting impacts, effects on central nervous system, carcinogenicity, mutagenicity and fertility impairment.

During calculation of the total score for each EOC (step by step), firstly property-based score is calculated by multiplying related utility functions by importance weights for each subproperty and summing them. Secondly, the criterion-based

score is found by multiplying related property based score by importance weights for each property and summing them. Finally, the total rank score is calculated by multiplying related criterion based score by importance weights for each criterion and summing them. Utility functions, criteria, properties and importance weights are shown in Table 21. Treatment criterion is neglected during calculation of ranking score for source/stream water, whereas ecological effects criterion is excluded during calculation of ranking score for finished drinking water.

Table 21. Criteria, Data and Values in EOCRank System
(Kumar & Xagoraraki, 2010)

Criteria, properties and subproperties*	**Importance weights**	**Utility Functions****
1) Occurrence	1/3	
a) Prevalence	1/2	$U(O_1) = (fod/100)$ fod: frequency of detection of a chemical in water
b) Magnitude	1/2	$U(O_2) = (C-C_{min}) / (C_{max}- C_{min})$ C: Concentration value of a chemical in water C_{min} and C_{max}: Minimum and maximum concentration values in the entire list
2) Treatment	-Not applicable for source/stream water -1/3 (for finished drinking water)	$U(T) = 1- (T/100)$ T: removal efficiency of a chemical in specific treatment plant for drinking water
3)Ecological Effects	- Not applicable for finished drinking water -1/3(for source/stream water)	

Table 21. Criteria, Data and Values in EOCRank System (cont'd)

(Kumar & Xagoraraki, 2010)

Criteria, properties and subproperties*	**Importance weights**	**Utility Functions****	
a) Bioaccumulation	1/2	If Log K_{ow}> 3, $U(E_1)$=1 If Log K_{ow}< 3, $U(E_1)$=0	
b) Ecotoxicity (only acute effects were considered)	1/2	$U(E_2) = 1/3 \times (E_{fish}+E_{daphnia}+E_{algae})$ E (for each one) = 1- ((LC_{50}- $LC_{50\text{-}min}$) / ($LC_{50\text{-}max}$- $LC_{50\text{-}min}$)) LC_{50}= Lethal concentration value for 50 % kill $LC_{50\text{-}min}$ and $LC_{50\text{-}max}$: Minimum and maximum LC_{50} value in the entire list (for that species)	
4)Health Effects	1/3		
a) Pregnancy Category	1/2	Low possibility of fetal harm	$U(H_1)$=0.2
		No risk for animals or risk for animals but no risk for humans	$U(H_1)$=0.4
		Risk for animals but insufficient human studies or lack of sufficient studies	$U(H_1)$=0.6
		Risk indication for humans	$U(H_1)$=0.8
		Fetal harm risk for animal or humans	$U(H_1)$=1
b) Effect Category	1/2		
- Developmental effects	1/7		
- Immunotoxicity	1/7		

Table 21. Criteria, Data and Values in EOCRank System (cont'd)

(Kumar & Xagoraraki, 2010)

Criteria, properties and subproperties*	**Importance weights**	**Utility Functions****
- Endocrine effects	1/7	$U(H_2)$= If effect exist, 1 If no effect, 0 (for each one)
- Effect on central nervous system	1/7	
- Carcinogenicity	1/7	
- Mutagenicity	1/7	
- Fertility impairment	1/7	

*In case there is no data, 0.5 default value was used in the calculations.

**$0 \leq U \leq 1$

Neuparth et al. (2011) applied a weight of evidence approach to prioritize hazardous and noxious substances (HNS) taking part in marine transportation in terms of risk caused by spillage into the marine environment. For prioritization process, quantity of chemicals transported along with the frequency of transportation (to detect the probability of occurrence of accidents), reported incidents in European waters, physicochemical and toxicological properties (for marine organisms) were taken into consideration as four main criteria. Quantity information about HNS was used during the determination of chemical list as a starting point. Chemical list of 100 HNS was ranked/graded, according to the GESAMP (The Joint Group of Experts on the Scientific Aspects of Marine Environmental Protection) risk evaluation procedure that are shown in Table 22 and Table 23.

Table 22. Criteria Related to Fate and Rank Information in GESAMP Guidelines (Neuparth et al., 2011)

Rank/ Grade	Bioaccumulation			Biodegradability
	Info	Log K_{ow}	BCF	
0	No potential	≤ 1 or >ca.7	-	R: Readily biodegradable, NR: Not readily biodegradable, Inor: Inorganic
1	Very low	≥1 <2	≥1 <10	
2	Low	≥2 <3	≥10 <100	
3	Moderate	≥3 <4	≥100 <500	
4	High	≥4 <5	≥500 <4000	
5	Very high	≥5 <ca.7	≥4000	

*Adapted from GESAMP (2002)

Table 23. Criteria Related to Toxicity and Rank Information in GESAMP Guidelines (Neuparth et al., 2011)

Rank/ Grade	Aquatic Toxicity				Carcinogenicity
	Acute Toxicity		Chronic Toxicity		
	L(E)C_{50} (mg/L)	Info	NOEC (mg/L)	Info	
0	>1000	Not toxic	>1	Minor	C: Carcinogen, NC: not carcinogenic or no data
1	100-1000	Almost not toxic	>0.1 ≤1	Low	
2	10-100	Low	>0.01 ≤0.1	Moderate	
3	1-10	Moderate	>0.001 ≤0.01	High	
4	0.01-1	High	≤0.001	Very high	
5	<0.01	Extreme			

*Adapted from GESAMP (2002)

After chosen/stated criteria had been evaluated for each HNS, chemicals falling into any of the following groups were identified as priority:

(Group 1)

- Rank of bioaccumulation at least 2 (low tendency)
- Not readily biodegradable
- Rank of acute toxicity at least 3 (moderate toxicity) and/or chronic toxicity at least 2 (moderate toxicity)

(Group 2)

- Rank of bioaccumulation at least 3 (moderate tendency)
- Readily biodegradable
- Rank of acute toxicity at least 4 (high toxicity) and/or chronic toxicity at least 2 (moderate toxicity)

(Group 3)

- Rank of bioaccumulation at least 2 (low tendency)
- Readily biodegradable
- Rank of acute toxicity at least 3 (moderate toxicity) and/or chronic toxicity at least 2 (moderate toxicity)
- Appeared in past incidents

Furthermore, chemicals that show long-term carcinogenic effects on mammals were regarded for inclusion into HNS priority list.

According to the study carried out by Von der Ohe et al. (2011) within the scope of EU Water Framework Directive, organic microcontaminants were ranked and prioritized depending on their maximum environmental concentration (MEC_{95}) and the lowest PNEC values (considering both acute and chronic data for fish, daphnia and algae) after they had been classified into six action categories considering available information about exposure and risk assessment data. 95^{th} percentile of MEC values for each monitoring site (MEC_{site}) gives MEC_{95} value

for a chemical. Division of L(E)C_{50} or NOEC values by assessment factors (1000 for acute data, 100 for chronic data) gives PNEC value for each chemical. In their study, they converted total water concentration of chemicals into dissolved water concentrations by using following Equation (16) in order to obtain more realistic results by considering bioavailability factor.

$$\mathbf{C_d} = \frac{C_t}{(f_{oc} \text{ x } K_{oc}) + 1} \tag{16}$$

Where

C_t: total measured concentration of a chemical

C_d: dissolved concentration in water phase

f_{oc}: organic carbon fraction in water sample

K_{oc}: organic carbon partition coefficient

Data obtained from exposure (MEC) and hazard (PNEC) assessments were used for score determinations of exceedance frequency and exceedance extent of the lowest PNEC value for each chemical. Exceedance frequency indicates spatial distribution of contaminants whereas exceedance extent gives an idea about the severity of impacts. Following Equations (17) and (18) and Table 24 are used for the determination of scores for two indicators:

$$\textbf{Exceedance frequency score} = {}^{n}/_{N} \tag{17}$$

(0-1)

Where

n: number of monitoring points with MEC_{site} / lowest PNEC >1,

N: total number of monitoring points with analytical measurements

$$\textbf{Exceedance extent} = {}^{MEC_{95}}/_{\text{lowest PNEC}} \tag{18}$$

Table 24. Scores for Exceedance Extent (Von der Ohe et al., 2011)

Exceedance extent	**Score**
<1	0
10 > >1	0.1
100 > > 10	0.2
1000 > > 100	0.5
>1000	1

Each organic pollutant was ranked and prioritized according to the total score obtained by summing exceedance frequency and exceedance extent scores (in the range of 0 and 2).

According to the modelling-based prioritization approach (compatible with Water Framework Directive) recommended by Daginnus et al. (2011), the total score is calculated by combining hazard and exposure assessments for each substance. Hazard score equals to the summation of persistence, bioaccumulation, toxicity and endocrine disruption scores as indicated in Equation (19). Criteria for substances are shown in Table 25 for hazard evaluation. If limit values are exceeded, the score is taken as 1 for the related criterion. In other cases, the score equals to 0. The range of the hazard score is between 0 and 5. If all screening criteria are fulfilled or a substance is classified as very P and very B (vPvB), extra +1 is added to the total score.

$$\textbf{Hazard score (0-5)} = \text{Persistence (P)} + \text{Bioaccumulation (B)} + \text{Toxicity (T)} + \text{Endocrine Disruption (ED)} \quad (19)$$

Table 25. Criteria of Hazard Evaluation (Daginnus et al., 2011)

Limit values of hazard criteria			
Persistence* (P)	**Bioaccumulation (B)**	**Toxicity (T)**	**Endocrine Disruption (ED)**
Half-life of fresh (estuarine) water > 40 d or marine water > 60 d or Half-life of fresh (estuarine) sediment > 120 d or marine sediment > 180 d **-vP** if Pov (overall persistence) > 195 d and CTD (Characteristic Travel Distance) > 5097 km or TE (Transport Efficiency) > 2.25%	BCF (L/kg) > 2000 **-vB** if BCF > 5000	NOEC < 0.01 mg/L (freshwater or marine organisms) - Carcinogenicity (category 1 or 2), mutagenicity (category 1 or 2) or toxicity for reproduction (category 1, 2 or 3) - Other evidence for chronic toxicity such as R48 or Xn - Acute EC_{50} or EL_{50} standard toxicity tests < 0.1 mg/L (potentially toxic)	Yes/No

*via EPI Suite, OECD and LRTP Screening tools

*Adapted from REACH regulation and ECHA guidance documents

Exposure score is calculated by considering total production/usage and use pattern of substances. Following Equation (20), Table 26 and Table 27 are used to calculate exposure score.

$$\textbf{Annual usage (tons)} = \text{Total production} \times \text{Use index} \quad (20)$$

Table 26. Use Index for Substances (Daginnus et al., 2011)

Use Pattern	Controlled system (intermediate isolated)	Non dispersive (industrial) usage or usage ending up with matrix inclusion	Dispersive usage (mostly diffusive sources)	Environmental usage
Use index	0.1	0.2	0.5	1.0

Table 27. Exposure Score (Daginnus et al., 2011)

Annual Usage (tons)	0-1	1-10	10-100	100-1000	> 1000
Exposure Score	0	1	2	3	4

The final risk score is determined for each substance by using the matrix which combines hazard and exposure evaluation results as shown in Table 28. A score of 1 represents the highest risk condition whereas a score of 5 indicates the lowest risk condition.

Table 28. Final Risk Score (Daginnus et al., 2011)

	Exposure Score					
Hazard Score		**4**	**3**	**2**	**1**	**0**
	4-5	1	1	2	3	5
	3	1	2	2	3	5
	2	2	2	3	4	5
	1	3	3	4	4	5
	0	5	5	5	5	5

Then, substances with the final risk score 1 are ranked by using PEC (Predicted Environmental Concentration) / PNEC (Predicted No Effect Concentration) ratio.

PEC value is calculated by employing the ECETOC TRA tool and/or OECD LRTP multimedia tool whereas PNEC value is taken from experimental studies or predicted by using QSAR algorithms.

American Chemistry Council (ACC, 2011) developed a two-step risk-based prioritization method. In the first step, hazard and exposure scores are calculated. For hazard assessment, effects of chemicals on the environment and human health are considered. Environmental ranking and human health ranking scores are calculated (as shown in Table 29 and Table 30) based on The U.N. Globally Harmonized System of Classification and Labeling (GHS) procedure which is summarized in Table 31.

Table 29. Environmental Ranking Scores (ACC, 2011)

Environmental effect score	**Ranking**	**GHS Categories**
4	High	Acute I or Chronic I or inadequate data for classification
3	Medium-High	Acute II or Chronic II
2	Medium	Acute III or Chronic III- IV or none
1	Low	Not categorized

Table 30. Human Health Ranking Scores (ACC, 2011)

Human health score	**Ranking**	**GHS Categories**
4	High	GHS CMR Category 1a, 1b; or Repeat Dose $\leq$ 10 mg/kg/d (oral); $\leq$ 20 mg/kg/d (dermal); $\leq$ 50 ppm/6 h/d (gas respiration); $\leq$ 0.2 mg/L/6 h/d (vapor respiration); $\leq$ 0.02 mg/L/6h/d (dust/mist/fume inhalation) or inadequate data for classification

Table 30. Human Health Ranking Scores (ACC, 2011) (cont'd)

Human health score	**Ranking**	**GHS Categories**
3	Medium High	GHS CMR Category 2; or Repeat Dose 10-100 mg/kg/d (oral); 20-200 mg/kg/d (dermal); 50-250 ppm/6 h/d (gas respiration); 0.2-1 mg/L/6 h/d (vapor respiration); 0.02-0.2 mg/L/6h/d (dust/mist/fume inhalation)
2	Medium	Does not show CMR properties; or Repeat Dose 100-1000 mg/kg/d (oral); 200-2000 mg/kg/d (dermal); 250-1000 ppm/6 h/d (gas respiration); 1 -5 mg/L/6 h/d (vapor respiration); 0,2-1 mg/L/6h/d (dust/mist/fume inhalation)
1	Low	Does not show CMR properties; or Repeat Dose >1000 mg/kg/d (oral); >2000 mg/kg/d (dermal); >1000 ppm/6 h/d (gas respiration); >5 mg/L/6 h/d (vapor respiration); >1 mg/L/6h/d (dust/mist/fume inhalation)

Table 31. Criteria for GHS Category (United Nations, 2011)

GHS categories (for 3 trophic level)			
Acute effect	**Long-term effect**		
(for fish, crustacea, algae or other aquatic plants, mg/L)	If sufficient chronic toxicity data exist		If sufficient chronic toxicity data does not exist (for fish, crustacea, algae or other aquatic plants, mg/L)
	Substances being degraded slowly (for fish or crustacea, mg/L)	Substances being degraded rapidly (for fish or crustacea, mg/L)	

Table 31. Criteria for GHS Category (United Nations, 2011) (cont'd)

GHS categories (for 3 trophic level)			
Acute effect	**Long-term effect**		
Category: Acute I $L(E)C_{50} \leq 1$	Category: Chronic I NOEC or equivalent $EC_x \leq 0.1$	Category: Chronic I NOEC or equivalent $EC_x \leq 0.01$	Category: Chronic I $L(E)C_{50} \leq 1$ and without fast degradability and/or BCF≥ 500 (or log $K_{ow} \geq 4$)
Category: Acute II $1 < L(E)C_{50} \leq 10$	Category: Chronic II $0.1 \leq$ NOEC or $EC_x \leq 1$	Category: Chronic II $0.01 \leq$ NOEC or $EC_x \leq 0.1$	Category: Chronic II $1 \leq L(E)C_{50} \leq 10$ and without fast degradability and/or BCF≥ 500 (or log $K_{ow} \geq 4$)
Category: Acute III $10 < L(E)C_{50} \leq 100$		Category: Chronic III $0.1 \leq$ NOEC or $EC_x \leq 1$	Category: Chronic III $10 \leq L(E)C_{50} \leq$ and without fast degradability and/or BCF≥ 500 (or log $K_{ow} \geq 4$)
	Category: Chronic IV (unless NOECs > 1 mg/L) (no rapid degradability and no acute toxicity and BCF≥ 500 (or log $K_{ow} \geq 4$))		

The highest score from environmental and human health evaluations is taken as hazard score for each chemical.

Exposure score is calculated for each chemical by considering use pattern, production amount and persistent-bioaccumulative characteristics of chemicals. Criteria for the scoring process are indicated in Table 32, Table 33 and Table 34.

Table 32. Score for Use Pattern (ACC, 2011)

Score for use pattern	Ranking	Use pattern
4	High	Consumer usage
3	Medium High	Commercial usage
2	Medium	Industrial usage
1	Low	Intermediates formed during manufacturing

Table 33. Score for Production Amount (ACC, 2011)

Score for production amount	Ranking	National total production amount
4	High	≥ 100,000,000 lbs
3	Medium High	1,000,000 lbs – 100,000,000 lbs
2	Medium	≥ 25,000 lbs and <1,000,000 lbs
1	Low	< 25,000 lbs

Table 34. Score for Persistence and Bioaccumulation (ACC, 2011)

Score for persistence and bioaccumulation	Ranking	Persistent (P) - Bioaccumulative (B)
5	High	P and B
3	Medium	P or B
1	Low	Not P and not B

In order to determine persistence property, the following procedure is followed/applied:

- For volatile substances (V_P > 1000 Pa), if air half-life < 2 days, non-persistent
- For nonvolatile substances (V_P > 1000 Pa), non-persistent if:
    - Readily biodegradable (OECD 301)

- Inherently biodegradable (OECD 301, 302, 306)
- In the light of measured data related to a substance
- Equivalent degree of abiotic degradation (> 20 % degradation in 28 days) such as hydrolysis (OECD 111) and photolysis (OECD 316)
- Consideration of simulation data regarding transformation in surface water/sediment, marine/brackish water/sediment, soil, oceanic water (OECD 308/309) , half-lives < 180 days
- The result of BIOWIN model (EPIWEB 4) evaluation

On the other hand, in order to determine bioaccumulation property, the following procedure is followed/applied:

A related substance is not bioaccumulative if:

- Trophic magnification factor (TMF) < 1 (field research)
- Biomagnification factor (BMF) for fish < 1 (lab study)
- Bioconcentration factor (BCF) for fish < 5000 (lab study)
- Predicted BCF < 5000 via EPIWIN 4 BCFBAF model

After scores for use pattern, production amount and persistence-bioaccumulation of chemicals are determined; exposure score is calculated for each chemical by combining (summing) scores of these three criteria as shown in Table 35.

Table 35. Combined Exposure Score (ACC, 2011)

Combination score of 3 criteria	**Ranking**	**Exposure score**
11-13	High	5
9-10	Medium High	4
7-8	Medium	3
5-6	Medium Low	2
3-4	Low	1

Finally, the general prioritization score for each chemical equals to the summation of hazard and exposure scores, and it is indicated in Table 36.

Table 36. General Prioritization Score (ACC, 2011)

Prioritization Score (Hazard score + Exposure score)	**Exposure score**	1 Low	2 Medium low	3 Medium	4 Medium high	5 High
Hazard score						
1(Low)		2	3	4	5	6
2(Medium)		3	4	5	6	7
3(Medium high)		4	5	6	7	8
4(High)		5	6	7	8	9

In the second step, chemicals that belong to same prioritization groups are ranked again within themselves by considering environmental monitoring/biomonitoring, emission data of chemicals to the environment, international risk management plans and usage of chemicals in products of children.

Slobodnik et al. (2012) benefited from the frequency of exceedance and extent of exceedance of the lowest PNEC approach developed by Von der Ohe (2011) during identification of river basin specific pollutants and derivation of EQS in the Slovak Republic. They applied complementary (integrated) approach for prioritization process by considering production/usage data of chemicals, monitoring/emission data of chemicals and results of non-target GC/MS (Gas chromatography/Mass spectrometry) screening studies and results of risk assessments.

According to the study conducted by Fàbrega et al. (2013), 205 organic compounds used in four Spanish River Basins were prioritized/ranked in

accordance with their PBT properties by means of Self-organizing maps (SOM) in MATLAB, which enable to visualize huge amount of information by grouping data with similar characteristics, and it is used in data analysis and environmental modelling. In their study, firstly SOM based Hazard index (HI) was estimated for each compound via the SOM toolbox for MATLAB by the help of EPI Suite program where physicochemical and toxicological properties of chemicals were obtained. Secondly, integrated risk index of chemical aquatic pollution (IRICAP) was calculated for each monitoring site and each river basin. Then, compounds with significant contribution were identified by using the Hirsch index (h index) and Zipf's law. Depending on hazard index and contribution values, chemicals of concern were suggested to be included in routine monitoring programs in the Mediterranean rivers. IRICAP was calculated after the hazard index and concentration had been rescaled to 0-10 by using following Equation (21):

$$\mathbf{IRICAP} = \sum\left(\frac{\text{Hazard index} \times \text{Normalized chemical concentration}}{\text{Number of chemicals}}\right) \qquad (21)$$

Where normalized chemical concentration= $(C_i - C_{min}) / (C_{max} - C_{min})$

Sugeng et al. (2013) modified and advanced pesticide prioritization study conducted by Guiner et al. (2001) and customized for Yuma County in Arizona. In addition to the hazard factor for cancer, they calculated hazard factors for other chronic effects such as endocrine disruption and toxicity for reproduction/ development. For cancer and endocrine disruption, hazard factor was calculated by multiplying scores for potency, persistence, volatilization flux and class evaluation and dividing by 1000 whereas hazard factor for reproductive/ developmental toxicity is calculated by multiplying scores for potency (reference dose-RfD value or cancer slope factor), persistence, volatilization flux and dividing by 100 in order to normalize score between 0 and 10. Table 37 shows the criteria for scoring/weighting process in pesticide hazard evaluation. Then, hazard-based pesticide usage value was found for each chronic effect separately by multiplying related hazard factor by pesticide use (total weight applied).

Moreover, the top 10 hazard ranked pesticides for each chronic health impact were subjected to overall chronic health effect ranking by dividing the number of related health effects caused (cancer and/or endocrine disruption and/or reproductive/developmental toxicity) by average position of hazard ranking.

Table 37. Hazard Factor Criteria for Evaluation of Pesticides (Sugeng et al., 2013)

Weight/ Score	**Potency**		**Exposure**	
			Flux	**Persistence**
	RfD value* (mg/kg-d)	**Cancer Slope Factor (mg/kg-d)**	**Volatilization Flux****	**Half-life for soil (days)**
1	>1	<0.001 or NA	$<10^{-7}$	<25 or NA
3	>0.1-1	0.001-0.01	$10^{-7} – 10^{-5}$	25-50
5	>0.01-0.1	>0.01-0.1	$>10^{-5} – 10^{-3}$	51-75
8	0.001-0.01	>0.1-1	$>10^{-3} – 10^{-1}$	76-100
10	<0.001 or NA	>1	$>10^{-1}$	>100

*For endocrine disruption and reproductive/ developmental toxicity

**Flux rate = Vapor pressure / (water solubility x coefficient of soil absorption)

(Weights/scores for cancer and endocrine disruption class is available in Supplementary Material section of the article)

Dabrowski et al. (2014) conducted a prioritization study by modifying approach applied by Valcke et al. (2005). Pesticides (with > 1000 kg/year) used in South Africa were ranked in terms of potential risk to human health by using four indices. These are quantity index (usage amount, kg), toxicity potential index (by considering five health effects: carcinogenicity, mutagenicity, teratogenicity, neurotoxicity and endocrine disruption), hazard potential (HP) index and weighted hazard potential (WHP). Top 25 pesticides occurring in each index were chosen as priority pesticides. Toxicity potential (TP) index is found by summing related scores shown in Table 38 for five different effects on human health.

Table 38. Toxicity Potential (TP) Index (Dabrowski et al., 2014)

Classification And Scores/Values	**ED**	**C**	**M**	**T**	**N**
Yes (Definitive Evidence)	8	8	6	4	4
Possible	6	6	4	2	2
No data	3	3	2	1	1
No	0	0	0	0	0

*ED: Endocrine Disruption, C: Carcinogenicity, M: Mutagenicity, T: Teratogenicity, N: Neurotoxicity

Hazard potential (HP) index is calculated as indicated in Equation (22) by multiplication of toxicity potential (TP) score and environmental exposure potential (EEP) score (GUS index- Groundwater Ubiquity Score) which shown in Table 39.

$$\mathbf{HP} = \text{TP score} \times \text{EEP score} \quad (22)$$

Table 39. Environmental Exposure Potential (EEP) Score (Dabrowski et al., 2014)

EEP	**GUS Index***	**Score/Value**
High	>2.8	4
Medium	2.8> > 1.8	2
Low	<1.8	1
No data	No K_{oc} or DT_{50} value	1.5

* GUS Index= $\log_{10}$ (half-life) x [4 - $\log_{10}$ (K_{oc})] (Gustafson, 1989)

Weighted hazard potential (WHP) is calculated for each pesticide by using Equation (23).

$$\mathbf{WHP} = \text{HP} \times \left({}^{QI}/_{Q_{total}}\right) \quad (23)$$

Where

QI: total amount of the specific pesticide usage nationally (kg), Q_{total}: total amount of all pesticides taking part in prioritization study (kg)

Moreover, site-specific risk evaluation regarding crops was done by summing related WHP values originated from specific pesticide application for the specific crop and dividing it by pesticide application area (ha).

Narita et al. (2014) ranked and selected pesticides to be included in drinking water quality regulations in Japan by taking into consideration quantity of sales information, guideline value based on acceptable daily intake (ADI), physicochemical properties of pesticides and regional precipitation characteristics. As a result of the evaluation of selected indicators based on detection rate (contains monitoring data and guideline value for pesticides), the following two indicators which showed the best correlations were determined:

- $\mathrm{Max}\left(\left(\text{Quantity of sales for upland fields} / GV_i\right)/_{\text{r.p.}}\right)_i$
- $\mathrm{Max}\left(\left(\text{Quantity of sales for rice farming} \times 10^{(Y+Z-6)} / GV_i\right)/_{\text{r.p.}}\right)_i$

  (ton/year) $(\mu g/L)^{-1}$ $(km^3/year)^{-1}$

Where

Max: maximum value obtained from 10 geographical regions in Japan, GV_i: guideline value for each pesticide (μg/L) ((ADI x body weight (kg) x 0.1) / daily water consumption (2 L/d)), r.p.: regional precipitation, Y: score for soil adsorption and degradation of pesticides (between 0-3) (values taken from Tani et al. (2012)), Z: score for degradation of pesticides in water (between 0-3) (values taken from Tani et al. (2012))

According to the risk assessments and prioritization study conducted by Kuzmanovic et al. (2014), possible pollutants in Mediterranean (Iberian) waters were ranked with regard to their calculated hazard quotients (HQ) to detect most relevant pollutants for each trophic level (fish, *Daphnia sp.*, algae). For

calculation of HQ for each pollutant, measured environmental concentration (MEC) values (either mean or maximum values) obtained from the literature are divided by PNEC value obtained from NOEC or L(E)C_{50} data for each trophic level. As a result of this study, priority pollutants which were specific to the Mediterranean aquatic system were identified and compared to those found in northern Europe and USA rivers in terms of HQ values.

Caldwell et al. (2014) proposed an approach for prioritization of pharmaceuticals. Due to the limitation of analytical techniques, lack of data about potential hazards and some uncertainties for pharmaceuticals, adverse outcome pathways (AOP) approach via fish plasma model was offered to be used by incorporating mammalian pharmacology data and modelled exposure data (based on usage data on pharmaceuticals) for risk assessment purposes. AOP is a conceptual framework that describes sequential chains of linked responses at different levels of biological organization between molecular initiating events and adverse outcome due to environmental exposure (European Commission, n.d.). Fish plasma model helps to determine whether a pharmaceutical existing in water comes up to fish internal plasma concentration which is equivalent to the remedial concentration of human and can be used as an indicator for investigation of potential risk in the field (Brooks et al., 2012; Du et al., 2014).

Donnachie et al. (2014) carried out a study in which metals observed in the United Kingdom were ranked based on risk assessments. For risk analysis calculations, the median value of measured river concentrations (μg/L) in the UK obtained from literature publications and several databases were divided by the median value of ecotoxicological thresholds (μg/L) including both acute and chronic effects for all species and all endpoints. As a precautionary approach, metals were also ranked according to risk ratio considering median river water concentrations, and 5^{th} percentile of compiled effect concentrations. Lastly, bioconcentration factor (BCF) values for each metal were used for ranking.

According to the risk-based prioritization study conducted by Kuzmanovic et al. (2015), 200 organic micropollutants in four Iberian rivers (Llobregat, Ebro, Jucar and Gualdalquivir) were prioritized by regarding their measured concentration levels and ecotoxicological risk potential. Ranking index (RI) approach was used by modifying prioritization approach developed by Von der Ohe et al. (2011). According to the RI approach, toxic unit value (TU for algae, *Daphnia sp* and fish) and ranking frequency (f_x) value are taken into account for each pollutant. Following Equations (24), (25) and (26) are used to calculate ranking index (0-100) for each species, each river and each year. Pollutants were identified as the most important compounds in case their RI were greater than 20 %.

$$\mathbf{TU} = {}^{Ci}/_{Ci(ref)} \tag{24}$$

Where

C_i: measured water phase concentration for a compound (µg/L), $C_{i(ref)}$: ecotoxicity (acute) reference concentration for same compound (µg/L, LC_{50} for fish, EC_{50} for algae and *Daphnia sp*)

According to the TU values obtained, pollutants are classified into six groups as shown in Table 40.

Table 40. Classification and Weighting Factors (Kuzmanovic et al., 2015)

Rank class (x)	**Range (log TU)**	**Weights (w_x)**
1	>0	1
2	<0, -1>	0.5
3	<-1, -2>	0.25
4	<-2, -3>	0.125
5	<-3, -4>	0.0625
6	<-4	0

$$\mathbf{f_x}\ (\%) = {}^{n_x}/_{N_{total}} \tag{25}$$

Where

n_x: number of monitoring sites belonging to rank class (x) from Table 40, N_{total}: total number of monitoring sites for each river

$$\textbf{Ranking Index (RI)} = \sum_{x=1}^{6} (f_x \times w_x) = (f_1 \times 1) + (f_2 \times 0.5) + (f_3 \times 0.25) + (f_4 \times 0.125) + (f_5 \times 0.0625) + (f_6 \times 0) \quad (26)$$

Teklu et al. (2015) conducted a risk assessment study of pesticides in surface water of Ethiopia referred as water tower of Africa due to the relative abundance of water resources. For pesticide registration procedure, pesticides were evaluated according to their predicted environmental concentrations and acute toxicity to aquatic organisms and human as a result of surface water consumption. Using modelling software (Pesticide Root Zone Model (PRZM) and Toxic Substances in Surface Waters Model (TOXSWA)), exposure concentrations were calculated by introducing inputs of physicochemical properties, irrigation-application pattern data, meteorological information, crop calendars. For environmental and human risk assessment calculations, following Equations (27) and (28) are used, respectively:

$$\textbf{ETR}_{\textbf{w-org}} = PEC_{90th} / NEC_{w\text{-}org} \quad (27)$$

Where

$ETR_{w\text{-}org}$: exposure toxicity ratio for fish, algae or Daphnia, PEC_{90th}: 90^{th} percentile of predicted environmental concentrations in the chosen surface water (µg/L), $NEC_{w\text{-}org}$: no effect toxicity concentration for fish, algae or Daphnia ($NEC_{Daphnia}$= 0.01x EC_{50}, NEC_{fish}= 0.01x LC_{50}, NEC_{algae}= 0.1x EC_{50}) (µg/L)

$$\textbf{ESTI} = \frac{PEC_{99th} \text{ x } LP_{dw}}{ARfD \text{ x } BW} \times 100 \quad (28)$$

Where

ESTI: estimated short-term intake (as percentage), PEC_{99th}: 99^{th} percentile of predicted environmental concentrations in the chosen surface water (μg/L), LP_{dw}: large portion of intake of drinking water (6 L/d), ARfD: acute reference dose (μg/kg BW/d), BW: body weight (60 kg)

Then, risk categorization was done depending on the severity of values.

Papadakis et al. (2015) carried out ecotoxicological and human risk assessment study of pesticides used in northern Greece based on monitoring data. During ecotoxicological risk assessment, risk quotient (RQ) value of each pesticide was calculated by using Equation (29), and pesticides with RQ> 1 were identified.

$$\mathbf{RQ} = {}^{MEC}/_{PNEC} \tag{29}$$

Where

MEC: measured environmental concentration (median and maximum detected concentration), PNEC: predicted no effect concentration (dividing NOEC or $L(E)C_{50}$ by related assessment factors)

For human health risk assessment, hazard quotient (HQ) value was calculated as indicated in Equation (30) for each pesticide by considering carcinogenic and non-carcinogenic risk for both children and adults. Then, pesticides with HQ> 1 were identified.

$$\mathbf{HQ} = {}^{CDI}/_{RfD} \tag{30}$$

Where

$$CDI = {}^{C \times IR \times EF \times ED}/_{BW \times AT}$$

(CDI: chronic daily intake (mg ingested pesticide/kg body weight/d), RfD: reference dose of contaminant (mg/kg/d), C: measured concentration of each pesticide (maximum and median), IR: ingestion rate of water (0.87 L/d for

children, 1.41 L/d for adults), EF: exposure frequency (365 d/year), ED: exposure duration (6 and 70 years for children and adults, respectively), BW: exposed person's body weight (20 kg for children, 70 kg for adults), AT: average lifespan (2190 days for children, 25550 days for adults))

On the other hand, carcinogenic risk (R) was calculated for compounds with carcinogenic concern by using Equation (31), and pesticides were compared with each other.

$$\mathbf{R} = \mathrm{CDI} \times \mathrm{SF} \times \mathrm{ADAF} \tag{31}$$

Where

SF: cancer slope factor (mg/kg/d), ADAF: adjustment factor with age dependency (10 for <2 years old, 3 for 2-16 years, 1 for > 16 years old)

Silva et al. (2015) carried out a study of aquatic risk assessment in Mediterranean river basins by analyzing priority and potential river basin specific pesticides. In order to detect risk posed in surface waters of Portuguese, frequency of exceedance of annual average-based quality standards (AA-QS) and frequency of exceedance of maximum allowable concentration-based quality standards (MAC-QS) were calculated for each pesticide, respectively by using following Equation (32):

$$\textbf{Frequency of exceedance of AA-QS or MAC-QS} = \sum(^{n}/_{N}) \times 100 \tag{32}$$

Where

n: number of samples (sites for AA-QS) with measured water concentration / (AA-QS or MAC-QS) > 1 for related pesticide, N: total number of samples (sites for AA-QS) with analytical measurements

For the derivation of water quality standards (AA-QS and MAC-QS) in accordance with the Water Framework Directive, depending on quality and

quantity of the available data, probabilistic (using species sensitivity distributions) or deterministic approach (using assessment factors) was used, and some values were directly taken from the WFD.

Agency for Toxic Substances and Disease Registry (ATSDR, 2015) did prioritization study in order to determine Priority List of Hazardous Substances (Substance Priority List) as a requirement of The Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) by scoring 848 substances based on three criteria. Necessary information was collected/compiled via ATSDR database and site document.

Main 3 criteria:

1) Occurrence Frequency at National Priorities List (NPL) sites or facilities

The following Equation (33) is used to calculate the score for substances which are observed at least 3 NPL sites:

$$\textbf{NPL frequency score} = \left(\text{Frequency of substances} \,/_{\text{maximum frequency}}\right) \times 600 \tag{33}$$

Where maximum frequency: 1274 (number of NPL sites)

2) Toxicity

Reportable Quantity (RQ) values determined by US EPA are used. There are 5 RQ categories (1, 10, 100, 1000 and 5000 pounds) that are based on the evaluation of carcinogenicity, ignitability, reactivity, acute, chronic and aquatic toxicities along with adjustments for potential biodegradation, hydrolysis and photolysis. In case of lack of RQ data, Toxicity/Environmental Score (TES) is calculated via data/information from several databases from by using RQ approach. Some assumptions are done during the determination of TES. For ignitable and reactive substances, TES value is taken 10. If aquatic toxicity data is available, 75% of maximum value is assigned as TES value. Depending on cancer

classification groups determined by US EPA and IARC (International Agency for Research on Cancer); 1, 10 and 100 TES values are assigned for Class A, B and C respectively. For radionuclides, depending on RQ value identified by considering the magnitude of radioactivity unit (curie), TES values are assigned. (<0.1, 1, 10,100, 1000 curie receives TES of 1, 10, 100, 1000 and 5000 respectively). If no data is available, TES values are assigned by regarding structurally similar compounds with known RQ values. Table 41 shows toxicity scores which correspond to obtained RQ or TES.

Table 41. Toxicity Scores (ATSDR, 2015)

RQ or TES	**Ordinal Rank**	**Cumulative Ordinal Rank (COR)**	**$(2/3)^{COR}$**	**Toxicity Score $(2/3)^{COR}$x 600**
1	0	0	1.0000	600
10	1	1	0.6667	400
100	2	3	0.2963	178
1000	3	6	0.0878	53
5000	4	10	0.0173	10

*If TES> 5000(using RQ methodology, total score gets 0 due to deficiency of known toxicity)
**Lowest RQ (obtained from determination of each criterion) belonging to a substance is selected

3) Exposure Potential for Human

Concentration of substances in environmental compartments and exposure status of populations are considered.

- Concentration of substances

Source contribution (SC) value and score are found by using following Equations (34) and (35):

$$\mathbf{SC} = \frac{(C_a A_a) + (C_w A_w) + (C_s A_s)}{\text{RQ or TES}} \quad (34)$$

Where

C: geometric mean of maximum concentrations in specific environmental compartment for a substance (a: air (mg/m^3), w: water (mg/L), s: soil (mg/kg)), A: theoretical daily dose (A_a: 15 m^3/d, A_w: 1 L/day, A_s: 200 mg/day)

$$\textbf{SC score} = \frac{(\log \text{SC for a substance} - \log \text{min SC threshold})}{\log \text{max SC threshold}} \times 300 \qquad (35)$$

Where min SC threshold: $3.77E^{-8}$, SC Geometric mean (GM): $2.91E^{-4}$, max SC threshold: $2.24E^{0}$

If SC value is lower than the minimum threshold (GM-2 GSD), the score is taken 0 and if SC value is higher than the maximum threshold (GM + 2GSD), the score is taken 300 (GSD: geometric standard deviation).

- Exposure status

Substances are evaluated under three categories with regard to exposure counts in ATSDR site document and exposure type/probability as shown in Table 42. Exposure score is found by using Equation (36).

Table 42. Exposure Categories (ATSDR, 2015)

Exposure Categories	Point Range (Max and Min)
Category 1- Exposure to pollutant	300-200
Category 2- Exposure to medium	200-100
Category 3- Potential Exposure to medium	100-1

$$\textbf{Exposure score} = \left(\text{Exposure count of a substance} \,/_{\text{Maximum exposure count}}\right) \times (\text{Max allowed points- Min allowed points}) + \text{Min allowed points} \qquad (36)$$

Finally, the total score is obtained by summing scores for three criteria as indicated in following Equation (37):

Total score (Max 1800 points) = **NPL frequency score** (600 points) + **Toxicity score (**600 points) + **Exposure Potential for Human score** (300 for concentration and 300 for exposure) (37)

Joint Research Center (JRC, 2015) carried out a prioritization study in order to select substances/chemicals which pose a risk to the aquatic environment and human health at EU level for the "First Watch List" within the scope of Environmental Quality Standards Directive. Chemicals with no or inadequate monitoring data and hazard information were compiled from different sources and determined as candidate substances for the ranking process. Moreover, analytical methods for the detection of substances and any prohibition of usage/production of substances were also considered for the selection. Substances were ranked depending on the certain criteria for each compartment and different receptors according to risk quotient (RQ= PEC/ PNEC) that is the ratio between predicted environmental concentrations (PEC) and predicted no effect concentrations (PNEC). RQ for water phase and human health resulting from consumption of drinking water was calculated for all substances. Additionally, for chemicals with log (K_{ow}) $\geq$ 3 and chemicals with BCF $\geq$ 100 and not readily biodegradability, RQ was calculated for sediment phase and biota phase resulting from secondary poisoning and consumption of fishery products, respectively. The highest RQ value was taken into consideration for each substance by regarding the worst-case scenario. Following Figure 2 summarizes the procedure applied.

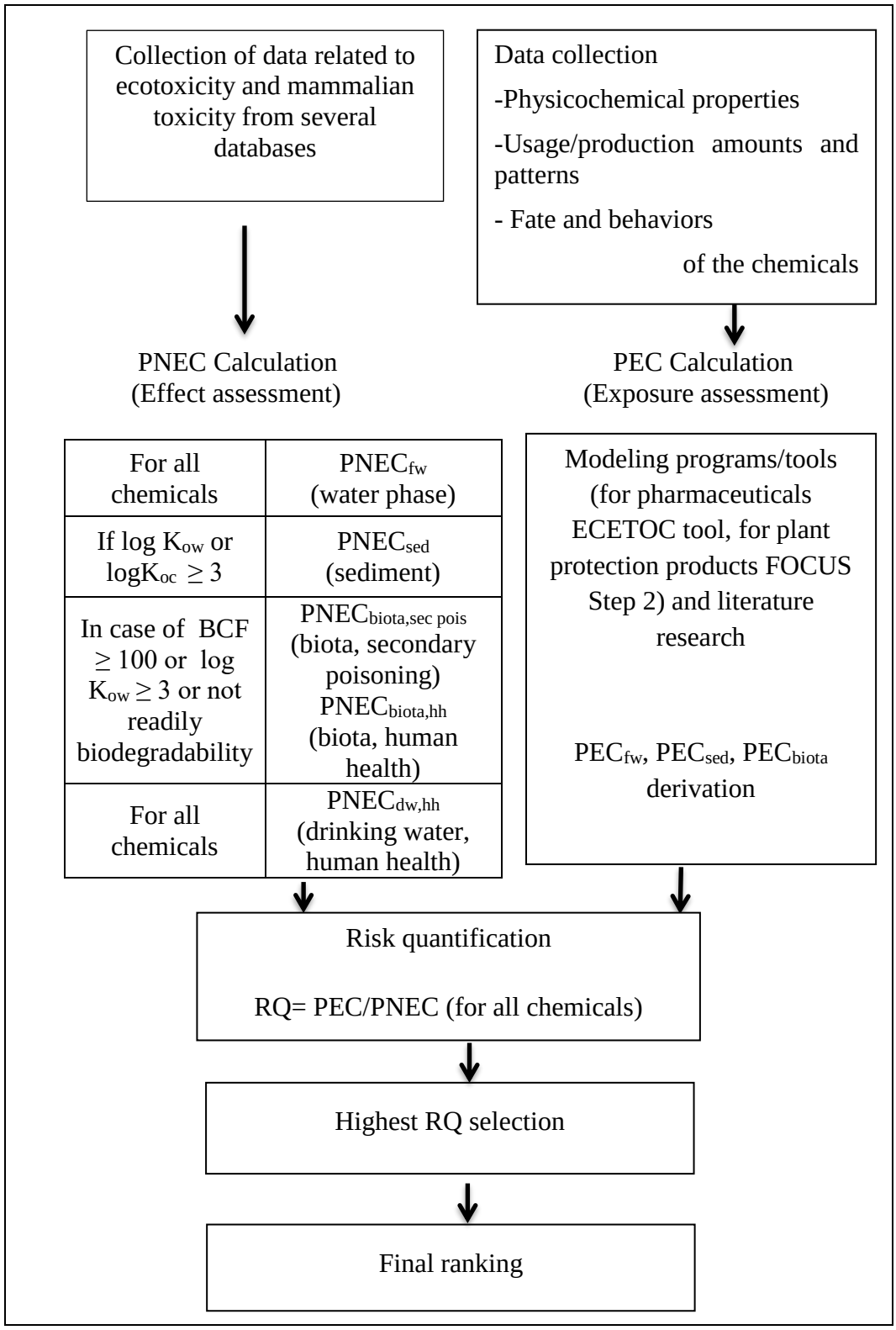

Figure 2. Summary of the Risk Assessment (JRC, 2015)

In effect assessment part, during calculation of $PNEC_{fw}$ for water phase (mg/L), aquatic toxicity data is divided by proper assessment factor as explained in Technical Guidance Document (No.27) for deriving EQS. For $PNEC_{sed}$ calculations, following Equations (38) and (39) (equilibrium partition method) are used, and necessary values are obtained from that document.

$$\mathbf{PNEC_{sed\text{-}ww}\,(mg/kg)} = \left({}^{K_{sed\text{-}water}}/_{RHO_{sed}}\right) \times PNEC_{fw} \times 1000 \qquad (38)$$

$$\mathbf{PNEC_{sed}} = CONV_{sed} \times PNEC_{sed\text{-}ww} \text{ (dry weight conversion)} \qquad (39)$$

Where

$K_{sed\text{-}water} = Fair_{sed} \times K_{air\text{-}water} + Fwater_{sed} + Fsolid_{sed} \times (Kp_{sed} / 1000) \times RHO_{solid}$

$Kp_{sed} = F_{oc} \times K_{oc}$

$CONV_{sed} = RHO_{sed} / (Fsolid_{sed} \text{ x } RHO_{solid})$

($K_{sed\text{-}water}$: sediment-water partition coefficient of a chemical (m^3/m^3), RHO_{sed}: bulk density of wet sediment (kg/m^3), 1000: m^3 to liter conversion factor, $Fwater_{sed}$: water fraction in the sediment (m^3/m^3), $Fsolid_{sed}$: solid fraction in the sediment (m^3/m^3), Kp_{sed}: partition coefficient between water and solids in the sediment (l/kg), F_{oc}: organic carbon weight fraction in sediment solids, K_{oc}: organic carbon–water partition coefficient of a chemical (l/kg) and assuming $Fair_{sed} = 0$)

During calculation of $PNEC_{biota,sec\ pois}$, NOAEL or $NOEC_{oral}$ toxicity values of related chemicals are used along with assessment factors stated in ECHA guidance and TGDs. $PNEC_{biota,hh}$ calculation is done by using acceptable/tolerable daily intake (ADI or TDI) or $NOAEL_{oral}$ values of chemicals (Equation (40)).

$$\mathbf{PNEC_{biota,hh}}\left(\frac{\mu g}{kg}\right) = \frac{0.1 \times TL \times 70}{0.115} \qquad (40)$$

Where

0.1 x TL: threshold level value of a chemical (assuming 10% included in fishery products), 70: average body weight of human, 0.115: daily fishery products consumption (kg)

$PNEC_{dw,hh}$ (mg/L) value is calculated via following Equation (41), and WHO or EU drinking water standards are also taken into consideration.

$$\mathbf{PNEC_{dw,hh}} = \frac{0.1 \times TL_{hh} \times 70}{uptake_{dw}} \quad (41)$$

Where

TL_{hh}: usually ADI or TDI value, $uptake_{dw}$: daily drinking water uptake (2 liters)

In exposure assessment part, during calculation of PEC_{fw} for fresh water, modelling tools such as ECETOC and FOCUS Step 2 are used by regarding quantities of use and usage information. PEC calculation for sediment compartment is done in a similar way to $PNEC_{sed}$ by using Equations (42) and (43).

$$\mathbf{PEC_{sed\text{-}ww}} = \left(K_{sed\text{-}water} / RHO_{sed}\right) \times PEC_{fw} \times 1000 \quad (42)$$

$$\mathbf{PEC_{sed}} = CONV_{sed} \times PEC_{sed\text{-}ww} \quad (43)$$

Where

$CONV_{sed} = RHO_{sed} / (Fsolid_{sed} \times RHO_{solid})$

$K_{sed\text{-}water} = Fair_{sed} \times K_{air\text{-}water} + Fwater_{sed} + Fsolid_{sed} \times (Kp_{sed} / 1000) \times RHO_{solid}$

Lastly, PEC for biota is calculated as follows (Equation (44)):

$$\mathbf{PEC_{biota}} = PEC_{fw} \times BCF \times BMF \quad (44)$$

Where

BCF: bioconcentration factor of a chemical, BMF: biomagnification factor

Tsaboula et al. (2016) implemented a prioritization approach based on exposure (monitoring) data, hazard information and environmental fate-behavior of pesticides in order to identify river basin specific pollutants of Pinios River Basin of Greece. According to this approach, pesticides are firstly grouped into seven categories depending on their 50 % dissipation time (DT_{50}) and hazard quotient ($HQ = MEC_{max}$ / lowest PNEC) value as indicated in Table 43.

Table 43. Classification of Pesticides for Prioritization Process

(Tsaboula et al., 2016)

Continued Exposure Long-term toxic impact ($DT_{50} \geq 2$ days) PNEC=lowest NOEC / AF	HQ > 1	Category 1	Possible candidates for river basin specific pollutants
	HQ < 1	Category 3	Low long-term risk for the environment
Acute Exposure Short-term toxic impact ($DT_{50} < 2$ days) PNEC=lowest $L(E)C_{50}$ / AF	HQ > 1	Category 5	Possible candidates for river basin specific pollutants
	HQ < 1	Category 6	Low short-term risk for the environment
LOQ > lowest PNEC		Category 2	-Insufficient analytical method (improvement is necessary) -Possible candidates for river basin specific pollutants
Low risk (HQ < 1) **but** potential impacts on human health (carcinogenicity, mutagenicity, reproductive toxicity and endocrine disruption)		Category 4	-Includes pesticides from Category 3 and 6 -Possible candidates for river basin specific pollutants
Pesticides detected below LOQ value		Category 7	Pose low risk but depending on the lowest PNEC value, they can be included into Category 2

*Where MEC_{max}: maximum measured environmental concentration, AF: assessment factor, NOEC: no observed effect concentration, $L(E)C_{50}$: lethal concentration with 50 % death of the population, PNEC: predicted no effect concentration

Then, pesticides within each of seven categories are scored by evaluating exceedance frequency of related PNEC value, exceedance extent, their spatial distribution and their PBT criteria including endocrine disruption property (First two indicators from the study done by Von der Ohe et al. (2011) with little

modification). Level of environmental risk for each pesticide is calculated by using following Equations (45), (46), (47), (48) and (49). Criteria and scores are shown in Table 44, Table 45 and Table 46.

$$\textbf{Level of environmental risk} = \text{Exceedance frequency score} + \text{Exceedance extent score} + \text{Spatial distribution score} + \text{PBT Score} \quad (45)$$

$$\textbf{Exceedance frequency score} = {}^{n}/_{N} \quad (46)$$

(in the range of 0-1)

Where

n: number of detections above PNEC, N: total number of detections above LOQ

$$\textbf{Exceedance extent} = {}^{MEC_{max}}/_{\text{lowest PNEC}} \quad (47)$$

(MEC_{max} value is used in order to take into account peak concentration level which poses greater adverse impacts to ecosystem due to heavy rainfall and irrigation events)

Table 44. Score for Exceedance Extent (Tsaboula et al., 2016)

Exceedance extent	Exceedance extent score
1-10	0.1
10-100	0.2
100-1000	0.5
>1000	1

$$\textbf{Spatial Distribution} = ({}^{s}/_{TS}) \times 100 \quad (48)$$

Where

s: number of monitoring sites with measured concentrations above LOQ, TS: total number of monitoring sites

Table 45. Score for Spatial Distribution (Tsaboula et al., 2016)

Spatial distribution	Spatial distribution score
< % 25	0.1
% 25-50	0.2
% 50-75	0.5
%75-100	1

PBT Score = (Score of persistence in water + Score of persistence in water-sediment + Bioaccumulation score + Toxicity score + Endocrine disruption score) × 0.2 (49)

Table 46. PBT Criteria and Scores (Tsaboula et al., 2016)

Criteria	Classification	Score
Persistence in water (fresh water studies)	DT_{50} > 40 d	1 (persistent)
	DT_{50} > 60 d	2 (very persistent)
Persistence in water-sediment (water-sediment studies)	DT_{50} > 100 d	1 (slow degradation)
	DT_{50} > 365 d	2 (stable)
Bioaccumulation	BCF > 100	1 (limit for concern)
	BCF > 2000	2 (bioaccumulative)
Toxicity	Long-term aquatic toxicity < 0.01 mg/L	1 (toxic to aquatic life or having impacts on human health)
		2 (toxic to aquatic life and having impacts on human health)

Table 46. PBT Criteria and Scores (Tsaboula et al., 2016) (cont'd)

Criteria	Classification	Score
	Short-term aquatic toxicity < 0.1 mg/L	
	Suspected carcinogen or carcinogen category 1A or 1B (CLP Regulation (EC)) or Mutagenic category 1A, 1B or reproductive toxicity category 1A, 1B,2 or toxicity for specific target organ as a result of repeated exposure	
Endocrine Disruption Potential (IEH and EC Annex 10 documents)	Category 2	1 (potential)
	Category 1	2 (proved at least one study)

Sangion and Gramatica (2016) prioritized a wide range of pharmaceuticals also called contaminants of emerging concern depending on their PBT properties by using computational predictive tools with two different QSAR models. Insubria-PBT Index (in QSARINS software) evaluates the number and specific type of bonds/atoms, electronic distribution and polarity of chemical structure, and this model is more conservative. On the other hand, US-EPA PBT Profiler runs different QSAR models to predict PBT properties separately and compares different estimations for each property with declared thresholds by classifying them. Consensus approach was applied for hazard assessment via two models, and 86 % agreement was found during screening/prioritization study.

Joint Research Centre (JRC, 2016) carried out a monitoring-based ranking/ prioritization study by improving method developed by Von der Ohe et al. (2011)

in order to review priority substances list under the Water Framework Directive. Substances which were evaluated but eliminated despite being at top places in modelling or monitoring-based prioritization exercises during the determination of priority substances in previous periods, substances with newly available information and new substances taking part in legislations/other documents were chosen for ranking and prioritization study. STE approach was implemented to each substance by evaluating spatial, temporal and extent of the PNEC exceedance. According to this approach, PNEC values could be calculated for each compartment (water, sediment and biota) and each receptor at risk by regarding freshwater/sediment organisms and humans.

Spatial distribution of the PNEC exceedance ($F_{spatial}$) is calculated as follows (Equation (50)), and the score is in between 0 and 1.

$$\mathbf{F_{spatial}} = \left(EXC_{95percentile} / \text{number of sampling stations}\right) \times \left(EXC_{95percentile,\ country} / \text{number of countries with measurement}\right) \quad (50)$$

Where

$EXC_{95percentile}$: number of monitoring sites where 95th percentile of measured concentrations > PNEC

$EXC_{95percentile,\ country}$: number of countries where 95th percentile of measured concentrations > PNEC

Temporal frequency of PNEC exceedance ($F_{temporal}$) takes into account peak concentrations due to mainly diffuse emission sources (pesticides, biocides, etc.). It is calculated as follows (Equation (51)), and score range is from 0 to 1.

$$\mathbf{F_{temporal}} = \sum\left(EXC_{sample} / \text{total number of analysis in specific monitoring sites}\right) / ECX_{site} \quad (51)$$

Where

EXC_{sample}: number of samples in a specific monitoring site in which related PNEC is exceeded, ECX_{site}: total number of monitoring sites where PNEC is exceeded at least once

However, a correction step is needed to compensate situation of inadequate monitoring data and sample. Firstly, all monitoring sites where PNEC is exceeded are considered, and a value (f1) is found. Secondly, another value (f2) is calculated by excluding observation stations with less than two samples in case of exceedance of PNEC. Then, **f1** value is taken if $| (f1-f2) / f1 | \leq 0.1$ or **f2** value is taken if $| (f1-f2) / f1 | > 0.1$ as $\mathbf{F_{temporal}}$.

The extent of PNEC exceedance (F_{extent}) is calculated according to the risk quotient ($RQ = EC_{95} / PNEC$) value for each substance and each monitoring site. Depending on the number of monitoring sites, EXC_{extent} values are calculated as follows, and they are normalized as shown in Table 47.

$$\text{If \# monitoring sites} \geq 20, EXC_{extent} = 95^{th} \text{ percentile } (RQ_{95percentile,site})$$

$$\text{If \# monitoring sites} < 20, EXC_{extent} = \text{maximum } (RQ_{95percentile,site})$$

Where

EC_{95}: 95^{th} percentile of measured concentrations in a specific monitoring station

Table 47. F_{extent} Value (JRC, 2016)

$\mathbf{EXC_{extent}}$	$\mathbf{F_{extent}}$ **value**
<1	0
1-2	0.04
2-5	0.07
5-10	0.11
10-20	0.18
20-50	0.28
50-100	0.41

Table 47. F_{extent} Value (JRC, 2016) (cont'd)

EXC_{extent}	**F_{extent} value**
100-500	0.56
500-1000	0.75
>1000	1

Finally, STE score for each chemical and each compartment is found by summing $F_{temporal}$, $F_{spatial}$ and F_{extent} values (Equation (52)) and STE score is converted to the risk score as shown in Table 48.

$$\textbf{Total STE score} = F_{temporal} + F_{spatial} + F_{extent} \quad (52)$$

Table 48. Risk Score (JRC, 2016)

STE score	**Risk category**	**Risk score**
≥ 2.4 and ≤ 3	Very high	1
≥ 1.8 and ≤ 2.4	High	2
≥ 1.2 and ≤ 1.8	Medium	3
≥ 0.6 and ≤ 1.2	Low	4
< 0.6	Very low	5

According to the risk ranking study carried out by Zhang et al. (2017), 14 persistent organic pollutants (POPs) in the rivers of the Bohai Region of China were relatively ranked. The median value of river concentrations of each pollutant was divided by median effect concentrations (wide range of acute and chronic toxicity data were collected but acute values were preferred) by considering each species and each endpoint (similar procedure implemented by Donnachie et al. (2014)). Due to lack of monitoring data of water phase, river concentration of each pollutant was calculated/estimated by using partition theory as a result of dividing measured sediment concentration by total organic carbon and related organic carbon-water partition coefficient.

Johnson et al. (2017) implemented a risk ranking approach for 71 different chemicals including metals, pesticides, POPs, pharmaceuticals, surfactants and nanoparticles that were observed in UK river water. As explained and applied by Donnachie et al. (2014), median river water concentrations in the UK were divided by median ecotoxicity effect concentrations (considering all available acute and chronic toxicity data) and also divided by EQS value for each chemical. Chemicals were also ranked according to precautionary risk ratio by considering 90^{th} percentile of the exposure (monitoring) data and 10^{th} percentile of the ecotoxicity data. Moreover, these results were compared by incorporating BCF and excluding either sub-lethal or lethal effects. In conclusion, it was observed that relative risk of metals was higher than pesticides and pharmaceuticals.

According to the ranking/prioritization system developed by US EPA for Clean Water Act (EPA, n.d.), chemicals that pose a hazard to the environment and human health are determined to be included or excluded in the priority pollutants list. Chemicals are ranked as a result of toxicity and exposure evaluations depending on the assigned scores that are determined by experts.

Toxicity evaluation includes the following five categories:

- Aquatic toxicity: Acute (LC_{50}), chronic (Maximum Acceptable Toxicant Concentration)
- Mammalian Toxicity: acute dermal (LD_{50}), acute oral (LD_{50}), chronic/ sub-chronic (LD_{Lo} and TD_{Lo})
- Human health: carcinogenicity, mutagenicity and teratogenicity
- Persistence in the environment: half-life, Henry's constant, K_d value, hydrolysis rate
- Bioaccumulation: BCF, BAF, $\log K_{ow}$

Exposure evaluation includes the following five categories:

- Nationwide discharge quantity (ton/year)
- Number of sites with detectable concentrations
- Detection frequency in water compartment (as a percentage)

- ❖ Detection frequency in aquatic sediments (as a percentage)
- ❖ Detection frequency in municipal or industrial effluents (as a percentage)

In order to see big picture and remark commonly used parameters during prioritization and risk assessment studies, Table 49 and Table 50 are provided as summary tables showing what parameters are used for the exposure-hazard-risk evaluations and showing how many of the studies look at the same criteria/parameters, respectively.

Table 49. Summary Table for Exposure, Hazard and Risk Assessments

<table>
<tr><th>To calculate exposure</th><th>To calculate hazard/toxicity</th><th>To calculate risk</th></tr>
<tr><td rowspan="4">Modelling-based exposure
• Fugacity models
• Amount of usage/production data (Predicted environmental concentrations) or emission data
• Modelling tools/software</td><td>Aquatic toxicity (Acute or chronic toxicity endpoints, PNEC values)</td><td rowspan="4">Extent of exceedance of the lowest PNEC or EQS value (Risk quotient values)</td></tr>
<tr><td>Human toxicity (ADI, RfD, cancer slope factors, risk phrases)</td></tr>
<tr><td>CMR effects</td></tr>
<tr><td>ED effects</td></tr>
<tr><td rowspan="4">Monitoring-based exposure
• Measured environmental concentrations (MEC_{95}, mean or median values)
• Spatial and temporal distributions (Concentrations at monitoring points > LOQ or LOD, observation frequency above LOQ or LOD)</td><td>Bioaccumulation potential (BCF, BAF, log K_{ow})</td><td rowspan="4">Frequency of exceedance of the lowest PNEC or EQS value</td></tr>
<tr><td>Persistency (Half-lives in water, soil and air, biodegradability)</td></tr>
<tr><td>Volatilization potential (Vapor pressure, Henry’s law constant)</td></tr>
<tr><td>Long-range air transport potential (Half-life in air)</td></tr>
</table>

Table 50. Summary Table for Studies in the Literature Review Part

Studies \ **Criteria***	Monitoring data	Usage data/ Models	P	B	Aquatic toxicity	Human toxicity	CMR	ED
OSPAR Commission, 2000	+	+	+	+	+	+	+	+
Guiner et al., 2001	-	+	+	-	-	+	C	-
Lerche et al., 2004	-	+	-	-	+	+	+	-
IEH, 2004	-	+	+	+	-	+	+	-
Alister&Kogan, 2006	-	+	+	+	+	+	-	-
Juraske et al., 2007	-	+	+	-	+	+	-	-
Environment Agency, 2007	+	+	+	+	+	+	-	+
Arnot&Mackay, 2008	-	+	+	+	+	+	-	-
James et al., 2009	+	-	-	-	+	+	-	-
Götz et al., 2010	+	+	+	-	-	-	-	-
Murray et al., 2010	+	-	-	-	-	+	-	-
Kumar& Xagoraraki, 2010	+	-	+	+	+	+	+	+
Neuparth, 2011	-	+	+	+	+	+	C	-
Von Der Ohe, 2011	+	-	-	-	+	+	-	-
Daginnus, 2011	-	+	+	+	+	+	+	+
ACC, 2011	-	+	+	+	+	+	+	-

Table 50. Summary Table for Studies in the Literature Review Part (cont'd)

Criteria* / **Studies**	Monitoring data	Usage data/ Models	P	B	Aquatic toxicity	Human toxicity	CMR	ED
Slobodnik, 2012	+	+	-	-	+	-	-	-
Fabrega et al., 2013	+	-	+	+	+	-	-	-
Sugeng et al., 2013	-	+	+	-	-	+	C,R	+
Dabrowski et al., 2014	-	+	+	-	-	+	+	+
Narita et al., 2014	-	+	+	-	-	+	-	-
Kuzmanovic et al., 2014	+	-	-	-	+	-	-	-
Caldwell et al., 2014	-	+	-	-	-	+	-	-
Donnachie et al., 2014	+	-	-	+	+	-	-	-
Kuzmanovic et al., 2015	+	-	-	-	+	-	-	-
Teklu et al., 2015	-	+	-	-	+	+	-	-
Papadakis et al., 2015	+	-	-	-	+	+	C	-
Silva et al., 2015	+	-	-	-	+	+	-	-
ATSDR, 2015	+	+	-	-	+	+	C	-
JRC, 2015	-	+	+	+	+	+	-	-
Tsaboula et al., 2016	+	-	+	+	+	+	+	+
Sang& Gramatica, 2016	-	+**	-	-	-	-	-	-
JRC, 2016	+	-	-	-	+	+	-	-

Table 50. Summary Table for Studies in the Literature Review Part (cont'd)

Criteria* / Studies	Monitoring data	Usage data/ Models	P	B	Aquatic toxicity	Human toxicity	CMR	ED
Johnson et al., 2017	+	-	-	+	+	-	-	-
US EPA, n.d.	+	+	+	+	+	+	+	-

*It is based on parameters that were directly used/stated in the prioritization studies.
(P:Persistency, B: Bioaccummulation, CMR: Carcinogenicity-Mutagenicity-Reproductive toxicity, ED: Endocrine disruption)
**QSAR models were used for PBT assessments of the substances.

In addition, list of the definitions of terms that were mostly used throughout the thesis is summarized in Table 51.

Table 51. List of Definitions of the Mostly Used Terms

Terms	Definitions
MEC_{95} (95^{th} percentile of MEC)	It means that 95 % of the maximum environmental concentration data are below that value (Dulio & Von der Ohe, 2013).
LOD	Limit of detection is the lowest concentration of an analyte that can be detected in a sample (Shrivastava & Gupta, 2011).
LOQ	Limit of quantification is the lowest concentration of an analyte that can be detected with acceptable accuracy (Shrivastava & Gupta, 2011). It might be equivalent to the LOD or it might be much higher concentration (Armbruster & Pry, 2008).
PNEC	According to EU TGD on risk assessment (2003), PNEC is the concentration value below which detrimental effects on living organisms do not most probably occur.
ADI*	Acceptable daily intake represents maximum amount of a chemical that could be consumed without any observed adverse effects.

Table 51. List of Definitions of the Mostly Used Terms (cont'd)

Terms	Definitions
RfD**	Reference dose is the no observed adverse effect level, obtained by dividing long-term feeding studies by an uncertainty factor.
BCF***	Bioconcentration factor is the ratio between amount of a chemical in an aquatic organism (mostly fish) and amount of a chemical in the water at equilibrium.
K_{ow}***	Octanol-water partition coefficient represents ratio of a chemical's concentrations between octanol and water phases. It measures lipophilicity of the chemicals.
Fugacity	It represents escaping tendency of a chemical from particular compartment (Mackay, 2001).
CMR effects	They represent carcinogenic, mutagenic and reproductive toxic effects; that cause cancer, DNA alteration and damage on reproductive system (Dulio & Von der Ohe, 2013).
ED effects****	Endocrine disruptors interfere with endocrine system and lead to adverse neurological, developmental, reproductive and immune effects on human health and wildlife.

*Retrieved August 2018, from https://www.sciencedirect.com/topics/pharmacology-toxicology-and-pharmaceutical-science/acceptable-daily-intake

**Retrieved August 2018, from https://www.sciencedirect.com/topics/pharmacology-toxicology-and-pharmaceutical-science/reference-dose

***Retrieved August 2018, from https://www.nap.edu/read/18872/chapter/7#61

*****Retrieved August 2018, from https://www.niehs.nih.gov/health/topics/agents/endocrine/index.cfm

2.2. The Status of Turkey about Identification of River Basin Specific Pollutants

The river basin specific pollutants of Turkey were identified as a part of three different projects carried out by the Ministry of Agriculture and Forestry. In these three projects that are introduced in the following sections, general (national) river basin specific pollutants throughout the country and EQS for these pollutants for water, sediment and biota compartments were determined.

2.2.1. TMKK (Control of Hazardous Substances Pollution) Project

It was conducted between years of 2011 and 2013 in the Konya Kapalı, Ergene and Susurluk River Basins in order to identify specific pollutants which are more likely to exist in inland waters by regarding point sources and to derive EQS. After candidate substances had been determined by taking into account literature researches, industrial activities, capacity reports of the Turkish Union of Chambers and Commodity Exchanges (TOBB) and the list of chemicals (related to substances ≥ 1 ton, which are used or imported) provided by the Ministry of Environment and Urbanization; prioritization processes were implemented by using the COMMPS (Klein et al., 1999) and Total Hazard Value Score (THVS) (Daginnus et al., 2011) methods. The modelling-based approach was used in the COMMPS procedure and only hazard assessment (neglecting exposure evaluation due to lack of information about usage amount of substances) was done in the THVS procedure. As a result, 147 substances were identified as candidate specific pollutants (TMKK, 2013).

2.2.2. KIYITEMA (Determination of Hazardous Substances in Coastal and Transitional Waters and Ecological Coastal Dynamics) Project

It was conducted between years of 2012 and 2014 in Izmir, Izmit, Iskenderun Bays and Samsun Harbor in order to determine specific pollutants originated from point sources in coastal and transitional waters and to derive EQS. During sectorial inventory studies; industrial activities, capacity reports of the Turkish Union of Chambers and Commodity Exchanges (TOBB), Best Available Techniques Reference Documents (BREFs) related to existing sectors, the list of chemicals (related to substances ≥ 1 ton, which are used or imported) provided by the Ministry of Environment and Urbanization, national and international legislations, specific pollutants determined by the European Union (EU) were considered. After screening (by risk phrases, PBT properties and expert opinions) and prioritization processes (by COMMPS and THVS) had been applied, 138 substances were identified as candidate specific pollutants (KIYITEMA, 2014).

2.2.3. BIKOP (Determination of Water Pollution Resulting from Usage of Plant Protection Products and Determination of Environmental Quality Standards on the Basis of Substance or Substance Group) Project

It was conducted between the years of 2012 and 2014 in the Seyhan, Ceyhan, Buyuk Menderes, Firat-Dicle River Basins and Provinces of Amasya, Manisa and Sakarya in order to identify specific pollutants originated from diffuse sources. The lists (related to plant protection products which were used or still using) provided by the Ministry of Agriculture and Forestry were taken into consideration during the determination of candidate substances. As a result of the prioritization (by the COMMPS and THVS methods) and monitoring studies, 293 substances were determined as candidate specific pollutants (BIKOP, 2014).

2.2.4. Preparation of the National List of Specific Pollutants

Specific pollutants identified in TMKK and KIYITEMA projects were revised by evaluating industrial processes that substances take part, the capability of analytical methods (LOD, LOQ values), monitoring studies, the applicability of EQS values, PBT properties of substances. Along with BIKOP project's outcome and expert judgement, national specific pollutants of Turkey were identified (Siltu, 2015). National specific pollutants and their EQS take place in SWQR, whose target is to determine biological, chemical, physicochemical and hydromorphological qualities of all over-surface waters by monitoring studies and to specify procedures and principles in order to achieve good water status by classifying water bodies.

2.3. The Status of Europe about Identification of River Basin Specific Pollutants

Studies done by the member states of EU about the determination of specific pollutants were reported by Piha et al. (2010). According to that report, the majority of the countries implemented a two-stage selection approach, which consists of the formation of inventory of chemicals and identification of specific

pollutants from the candidate list. However, it was observed that there is no harmony between the methods applied by those member states. Different procedures like usage of emission data, production data, monitoring data, hazard (toxicity) data or application of the COMMPS method or utilization of Common Implementation Strategy (CIS) Guidance Document No.3 have been performed.

Number of river basin specific pollutants determined by some European countries were compiled and summarized in Table 52. When statuses of Turkey and Europe are compared in terms of number of river basin specific pollutants determined, it is clearly seen that much more pollutants must be periodically monitored in order to protect quality of the receiving water bodies in Turkey to achieve good ecological water status.

Table 52. Number of River Basin Specific Pollutants of Europe
(Johnson, 2012; KIYITEMA, 2014)

European Countries	**Number of river basin specific pollutants**
Austria	33
Belgium	116
Bulgaria	18
Cyprus	3
Czech Republic	86
Denmark	25
Estonia (WRC & EC, 2015)	13
Finland	13
France	10
Germany (Federal Environment Agency, 2013)	172
Greece (EC, 2015)	60

Table 52. Number of River Basin Specific Pollutants of Europe (cont'd)

(Johnson, 2012; KIYITEMA, 2014)

European Countries	**Number of river basin specific pollutants**
Hungary (WRC & EC, 2015)	4
Ireland	18
Italy	51
Latvia	11
Lithuania	6
Luxemburg	55
Malta	8
Netherlands	151
Norway	20
Poland	20
Romania	105
Slovakia	25
Slovenia	37
Spain	16
Sweden	29
United Kingdom	18

CHAPTER 3

METHODOLOGY

Prioritization methods suggested by the EU Commission and prioritization studies in the literature were inclusively reviewed. Since the COMMPS and NORMAN prioritization methods are more comprehensive and detailed in terms of exposure, hazard and risk assessments, they were preferred for the determination of specific pollutants in the Yesilirmak River Basin.

The prioritization methodology adopted in this thesis study involves the application of the COMMPS and NORMAN prioritization methods separately to the candidate substances by using 1.5-year surface water quality monitoring data (August 2016-January 2018). Over 300 samples that were collected from 42 monitoring stations within 1.5-year were included in this study. Eight monitoring data sets (August 2016, October 2016, February 2017, April 2017, June 2017, August 2017, December 2017 and January 2018) were analyzed and reported by TUBITAK MAM. Analyses were done based on WFD-Guidance Document No.19 (Guidance on Surface Water Chemical Monitoring under the Water Framework Directive) internationally accepted standard methods (GC/MS, LC/MS, GC/ECD etc.). Physicochemical and toxicological properties of the candidate substances were compiled and stored along with the set of monitoring data and monitoring stations in an Excel file to be submitted via form of CD. Then, the candidate substances were scored and ranked by using these two methods. Due to the difference in the ranking pattern of substances, it was decided that COMMPS and NORMAN scores were combined for each substance by using weighting factor approach in order to obtain a single ranking score and list.

3.1. Forming List of the Candidate Substances

During the formation of the candidate substance list for the ranking/prioritization process, point and diffuse pollution sources in the Yesilirmak River Basin were investigated deeply by regarding industrial and agricultural activities in order to find extra chemicals that are not included in national (generic) 250 specific pollutants of Turkey. Most of the probable chemicals that are expected to be found in the river basin have already eliminated during the preparation of national specific pollutants list due to their physicochemical and toxicological properties. Therefore, only 250 national specific pollutants of Turkey (expressed clearly in SWQR and also shown in APPENDIX A-Table 78 along with measured concentrations in the basin) were decided to be used as a candidate substances for the identification of the Yesilirmak River Basin specific pollutants. After methods to be applied and candidate substances had been determined, physicochemical and toxicological information along with monitoring data of the substances were compiled by means of Excel program by setting the appropriate format.

3.2. COMMPS Prioritization Method

COMMPS is the abbreviation for Combined Monitoring-based and Modelling-based Priority Setting Scheme, which integrates relative risk-based ranking approach and final expert judgment (Klein et al., 1999). During the determination of priority substances in the context of the EU Water Framework Directive, this procedure was applied for chemicals which take part in 76/464/EEC Council Directive, Third North Sea Conference, 793/93/EEC Council Regulation, 91/414/EEC Council Directive, OSPAR list, HELCOM list and the list of monitoring substances identified by the Member States.

The COMMPS method basically consists of the following steps:

- Identification of the candidate substances for the ranking process
- Exposure score calculation either using monitoring data or modelling data
- Effect score calculation which is based on experimental toxicity data

- Risk-based score calculation by combining exposure and effect scores for each chemical either for water phase or sediment phase
- Determination of priority/specific substances by screening and judgment

This procedure is summarized briefly in Figure 3 and the risk-based priority score is calculated by using Equation (53):

$$\mathbf{I\_prio} = \mathbf{I\_exp} \times \mathbf{I\_eff} \tag{53}$$

Where

I_prio: priority index/score (0-100)

I_exp: exposure index/score (0-10)

I_eff: effect index/score (0-10)

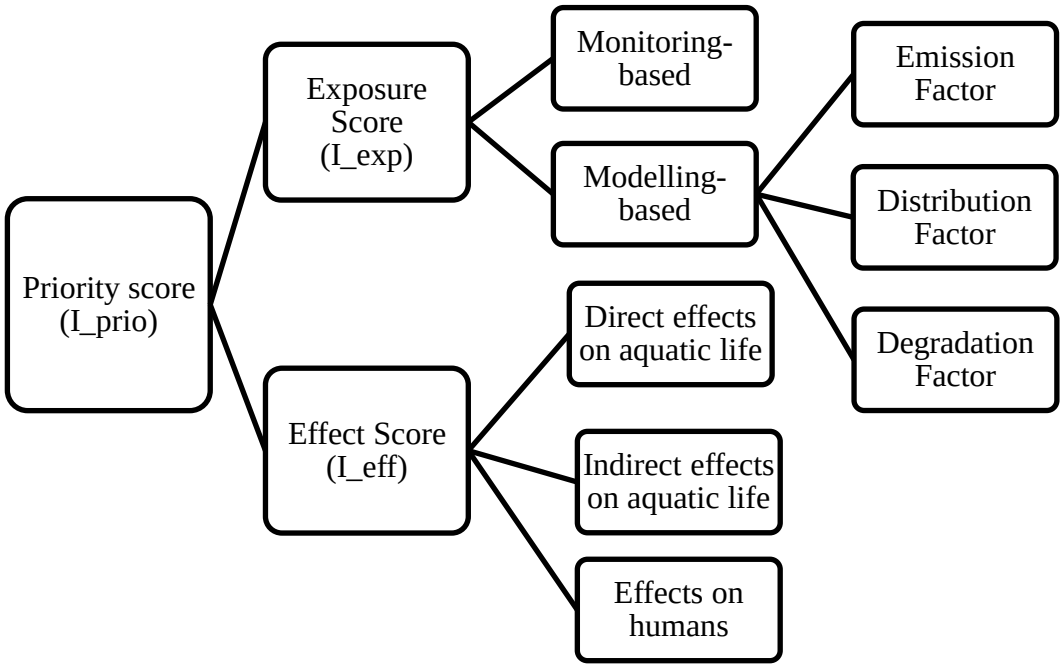

Figure 3. Short Representation of the COMMPS Procedure (Klein et al., 1999)

3.2.1. Exposure Score

Exposure score can be calculated either modeling-based or monitoring-based depending on the available data quality and quantity.

3.2.1.1. Modelling-Based Exposure Score

Modelling-based exposure score is calculated by using EURAM algorithms for aquatic phase. This model contains three factors which are emission, distribution and degradation factors, and calculated by following Equations (54) and (55).

$$\mathbf{I\_exp} = 1.37\,(\log(EEXV) + 1.301) \tag{54}$$

$$EEXV = \text{Emission} \times \text{Distribution} \times \text{Degradation} \tag{55}$$

The range of this score is in between 0 and 10 as a result of normalization.

- Emission

Annual usage amount (T_i, ton) and major usage category of chemicals are taken into consideration. The following Equation (56) and Table 53 are used for calculation of the emission factor.

$$\mathbf{Emission} = 0.01 \times T_1 + 0.1 \times T_2 + 0.2 \times T_3 + 1.0 \times T_4 \tag{56}$$

Table 53. Major Usage Categories and Fractions for Emission Factor Calculation (Klein et al., 1999)

Major usage category	Closed system usage	Usage ending up with matrix inclusion	Non dispersive usage	Dispersive usage	Default value
Fraction	0.01	0.1	0.2	1.0	1.0

- Distribution

Distribution factor indicates a fraction of a chemical that partitions into the aquatic environment at equilibrium. For each environmental compartment, fugacity, fugacity capacity and concentration of the chemical are calculated through Mackay Level I model which is summarized in Table 54 and Table 55.

Table 54. Mackay Level I Model (Mackay et al., 1996; Mackay, 2001)

	Model
Fugacity Capacity (Z) ($mol/m^3 \cdot Pa$) Affinity of a chemical for each environmental compartment	$Z_{air} = 1 / RT$
	$Z_{water} = Z_{air} / K_{aw} = 1/ H = S / V_p$
	$Z_{soil} = (Z_{water} \times \rho_i \times f_{oc} \times K_{oc}) / 1000$
	$Z_{sediment} = (Z_{water} \times \rho_i \times f_{oc} \times K_{oc}) / 1000$
	$Z_{ss} = (Z_{water} \times \rho_i \times f_{oc} \times K_{oc}) / 1000$
	$Z_{fish} = (Z_{water} \times \rho_i \times L \times K_{ow}) / 1000$
Fugacity (f) (Pa) Escaping tendency of a chemical from particular compartment	$f = M / \Sigma (V_i \times Z_i)$ M: 10^8/ Molecular weight of a chemical
Concentration in each phase (C) (mol/m^3)	$C_i = f \times Z_i$

*R: gas constant (8.314 J/mol K), T: temperature (K), S: water solubility (mol/m^3), V_p: vapor pressure (Pa), ρ_i: density of i phase (kg/m^3), V_i: volume of i phase, foc_i: organic carbon mass fraction for i phase, L: fish lipid content (0.10), $K_{oc} = 0.41 \times K_{ow}$

Table 55. Mackay Level I Model Environmental Properties (Mackay et al., 1996; Mackay, 2001)

Compartment	**Volume (m^3)**	**Depth (m)**	**Area (m^2)**	**Organic carbon fraction(f_{oc})**	**Density (kg/m^3)**
Air (1)	10^{14}	1000	10×10^{10}	-	1.2
Water (2)	2×10^{11}	20	10×10^9	-	1000
Soil (3)	9×10^9	0.1	90×10^9	0.02	2400
Sediment (4)	10^8	0.01	10×10^9	0.04	2400
SS (5)	10^6	-	-	0.2	1500
Fish (Biota) (6)	2×10^5	-	-	-	1000

Since calculations related to plant protection products and inorganic metal substances are not applicable by using Mackay model due to their physicochemical properties, only monitoring-based ranking approach must be preferred for them.

- Degradation

Degradation factor is based on the biodegradability of a substance in the aquatic compartment. It is calculated by using information in Table 56.

Table 56. Degradation Factor (Klein et al., 1999)

Biodegradability	Biodegrade readily	Biodegrade inherently	Persistent	Default value
Factor	0.1	0.5	1.0	1.0

3.2.1.2 Monitoring-Based Exposure Score

In order to calculate monitoring-based exposure score, firstly arithmetic mean of a substance's concentrations at each monitoring station is computed. Then, the 90th percentile of them is taken by regarding concentrations belonging to the same substances at the entire monitoring points. This value is denoted by $C_{i.}$ The maximum score is adjusted to 10. The score is calculated for each substance as follows (Equation (57)):

$$\mathbf{I\_exp\,(substance\ i)} = \frac{\log\left(C_i \;/\; (C_{min} \times 10^{-1})\right)}{\log\left(C_{max} \;/\; (C_{min} \times 10^{-1})\right)} \times 10 \qquad (57)$$

If the number of monitoring points where detection/quantification of a substance occurs is less than 10, the maximum arithmetic mean of a substance's concentrations is used instead of the 90th percentile approach.

Minimum and maximum concentration values are shown in Table 57.

Table 57. C_{min} and C_{max} Values for Exposure Score Calculation (Klein et al., 1999)

Values	Organic substances (in water phase) (µg/L)	Organic substances (in water phase-maximum possibility) (µg/L)	Metals (in water phase) (µg/L)	Organic substances (in sediment) (µg/kg)	Metals (in sediment) (mg/kg)
C_{max}	100	100	200	10000	2000
C_{min}	0.0001	0.0001	0.2	0.01	6

Exposure score for metals and inorganic metal compounds can differ substantially depending on either using total (particle bound + dissolved) or dissolved fraction (filtered part). Because speciation has a great impact on bioavailability, using the dissolved fraction of metal compounds is preferred by experts for the exposure assessment.

If necessary data are available for the calculations of both monitoring-based and modelling-based exposure scores, correlation graphs for all chemicals but metals are drawn and by the help of experts, more accurate and logical approach can be used.

3.2.2. Effect Score

Effect score combines

- direct effects of a chemical on aquatic life (EFS_d)
- indirect effects of a chemical on aquatic life (EFS_i)
- indirect effects of a chemical on humans through consumption of contaminated food or water by considering several endpoints related to acute and chronic toxicity (EFS_h)

It is based on the EURAM model and range of the effect score is in between 0 and 10. It is calculated as follows (Equation (58)):

$$\mathbf{I\_eff} = EFS_d + EFS_i + EFS_h \quad (58)$$

3.2.2.1. Direct Aquatic Effects (EFS_d)

Direct aquatic effect score is based on predicted no effect concentration (PNEC) value of a chemical. For calculation of PNEC value for each chemical, acute ($L(E)C_{50}$) or chronic toxicity data (NOEC) of a chemical is divided by assessment factor as stated in the European Commission Technical Guidance Documents on Risk Assessment (EU Commission, 2011). Table 58 indicates appropriate assessment factors to calculate $PNEC_i$ (for each substance) depending on availability of experimental toxicity tests for three taxonomic groups which are fish, invertebrates and plants (algae).

Table 58. Assessment Factors for PNEC Calculation (Klein et al., 1999)

Test Type	**Number of taxonomic groups having toxicity test**	**Assessment Factor (AF)**
Acute ($L(E)C_{50}$)	1	1000
	2	1000
	3	1000
Chronic (NOEC)	1 (Fish or invertebrates)	100
	2	50
	3	10

Due to the adoption of a conservative approach, the lowest chronic or acute toxicity data belonging to the highest hierarchical level is chosen. In case both chronic and acute data are available, preferably chronic data is used for the calculation of PNEC.

Direct aquatic effect score is calculated via Equation (59).

$$\mathbf{EFS_d\,(substance\ i)} = \frac{\log\left(PNEC_i\ /\ (10\ \times PNEC_{max})\right)}{\log\left(PNEC_{min}\ /\ (10\ \times PNEC_{max})\right)} \times WF \qquad (59)$$

Where

WF: Weighting factor (8 for metals, 5 for organic chemicals)

The range of EFS_d is in between 0 and 8 for metals, and 0 and 5 for organic substances. Maximum and minimum PNEC values are given in Table 59 to be used in the calculation of direct effect score.

Table 59. Limit Values of PNECs for Direct Effect Score Calculation (Klein et al., 1999)

Values	Organic chemicals (for water phase) (mg/L)	Organic chemicals (for sediment) (mg/kg)	Metals (for water phase) (mg/L)
$PNEC_{max}$	1	10	0.1
$PNEC_{min}$	0.000001	0.000001	0.000001

If acute or chronic toxicity tests are not available in the literature for a substance, PNEC value is taken as 0.00001 mg/L.

For metals, background concentrations must be determined due to issues of bioavailability (total or dissolved form) and essentiality/toxicity for organisms. If PNEC value is lower than the background concentration for a metal, background concentration is used for the calculation for the related metal. Different options can also be used for comparisons.

3.2.2.2. Indirect Aquatic Effects (EFS_i)

In order to calculate indirect aquatic effect score, bioconcentration factor (BCF), octanol-water partition coefficient (log K_{ow}) and/or molecular weight of a

substance are evaluated. In case both BCF and log K_{ow} are available, BCF of a substance is preferred. The scores of indirect aquatic effect are shown in Table 60.

Table 60. Indirect Aquatic Effect Scores (EFS_i) (Klein et al., 1999)

Log (K_{ow})	< 3 or	3 ≤ < 4 and	4 ≤ < 5 and	≥ 5 and	no log K_{ow} and
MW	> 700	< 700	< 700	< 700	< 700
BCF	< 100	100 < < 1000	1000< <10000	> 10000	no BCF
EFS_i	0	1	2	3	3

3.2.2.3. Effects on Humans (EFS_h)

This score is based on carcinogenic, mutagenic, reproductive effects of a chemical along with chronic effect as a result of oral uptake. As a guidance, risk phrases which take part in "Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures" can be regarded. The scoring procedure is shown in Table 61.

Table 61. EFS_h Score Depending on Risk Phrases (Klein et al., 1999)

Carcinogen	R45	R40	-	-	-	-
Mutagen	R46	R40	No test	-	-	-
Reproductive effects	R47, R60 or R61	R62, R63 or R64	No test	No test	-	-
Chronic effect by oral uptake	-	-	R23 -R28 with* R48	R20- R22 with* R48	R33	-
EFS_h	2	1.8	1.4	1.2	1	0

*any combinations of R48 with those R phrases

In aquatic phase, for organic substances total effect score equals to the summation of the direct, indirect aquatic effect scores and human effect score (EFS_d (5) + EFS_i (3) + EFS_h (2)). On the other hand, for metals only direct aquatic effects and human effects are considered (EFS_d (8) + EFS_h (2)). Indirect aquatic effects are not determined since the fate of metals is difficult to predict. BCF and K_{ow} parameters are not applicable for metals due to

- the ability of organisms to manage accumulation and excretion of metals
- the necessity of several metals to different organisms
- the existence of metal diversity and speciation under the natural condition

3.3. Procedure Followed and Assumptions Made for the Application of the COMMPS Method

For monitoring-based exposure score, after average concentrations of a candidate substance at each monitoring point had been found by using the 1.5-year monitoring data, 90^{th} percentile of them was calculated for each candidate substance. As stated in the COMMPS procedure by using related formula (Equation (57)), exposure score was found for each substance.

For the calculation of effect score, direct aquatic effect score, indirect aquatic effect score and effect on humans score were combined (summed) for each substance. Direct aquatic effect score was calculated via formula shown in the procedure (Equation (59)) by founding PNEC value which is based on the lowest chronic toxicity data (if not available the lowest acute toxicity data) belonging to 3 trophic levels (fish, daphnia and algae). For the calculation of indirect aquatic effect score, corresponding scores as stated in the procedure (Table 60) were given depending on the magnitude of BCF value (K_{ow} value was used if BCF is not available). Effects on humans score was calculated as a result of the evaluation of the risk phrases of each substance (Table 61). As the last step, exposure and effect scores were multiplied as indicated in Equation (53). According to their COMMPS scores which are in between 0 and 100, candidate substances were ranked from highest to lowest.

Main assumptions made and data selections are summarized as follows:

- Necessary data related to physicochemical and toxicological properties of chemicals/pollutants were taken from reliable databases such as University of Hertfordshire, PubChem, TOXNET, EPI Suite and also from related Legislation/Directives/Regulations and scientific documents/material safety data sheets obtained by the literature search as well as a document supplied by TUBITAK MAM.

- Metalloids such as boron, silicon, arsenic and antimony were also involved in the prioritization study (excluding other inorganics and mixture of total petroleum hydrocarbons).

- Monitoring-based exposure assessment was performed by using 8-period monitoring data obtained from 42 monitoring stations (shown in APPENDIX B-Table 79 and Figure 8) within 1.5 years. In case there was a reported substance's concentration value that was lower than the corresponding LOD value, it was disregarded. During calculation of exposure score, if concentration of a substance was detected but not quantified (< LOD), half of the LOD value was used for related monitoring stations instead of taking 0 or excluding those monitoring points. In this manner, it was aimed to include all substances in the ranking/prioritization procedure. In case concentration of a substance exceeds maximum limit concentration value (C_{max}) which is stated in the procedure (Table 57), the highest score of 10 was assigned for that substance as exposure score. Otherwise, exposure score would be beyond the maximum score of 10.

- Natural background concentration data for metals (as shown in Table 62) in the Yesilirmak River Basin were taken from studies carried out by METU Project Group as a part of TUBITAK Project numbered 115Y013. The 5^{th} percentile monitoring data approach was used by excluding points where concentration is lower than the LOD value instead of taking them as LOD/2.

In case background concentrations were greater than the related PNEC values, background concentrations were used for the calculations instead of the PNEC values.

- During calculation of direct aquatic effect score, for the determination of PNEC, the lowest chronic toxicity values were preferred depending on the availability of data as indicated in the method. To be on the safe side, PNEC values were also compared with EQS value in SWQR. It was tried to provide that all calculated PNEC values were below (or very close to) related EQS for each substance by making minor changes in the choice of assessment factor and toxicity data belonging to different trophic level or using EQS values. In case calculated PNEC value for a substance was smaller than $PNEC_{min}$ which is stated in the procedure (Table 59) since direct aquatic effect score (calculated by using Equation (59)) would be beyond the maximum score of 5 (for organics) or 8 (for metals), the highest score was assigned as the direct aquatic score for that substance.

Table 62. Natural Background Concentrations of Metals and Metalloids in the Yesilirmak River Basin

Substances	**Natural background concentrations (µg/L)**
Aluminium	45.87
Antimony	0.1961
Arsenic	1.026
Copper	11.390
Barium	31.338
Beryllium	0.0370
Boron	55.30
Zinc	3.661
Iron	59.22
Silver	0.031
Tin	12.336

Table 62. Natural Background Concentrations of Metals and Metalloids in the Yesilirmak River Basin (cont'd)

Substances	Natural background concentrations (µg/L)
Cobalt	0.0872
Chromium	0.516
Silicon	873
Titanium	8.5869
Vanadium	1.5192

3.4. NORMAN Prioritization Method

NORMAN is the abbreviation for Network of Reference Laboratories, Research Centers and Related Organizations for Monitoring of Emerging Environmental Substances. NORMAN is a research network where institutions of the member states investigate and monitor emerging environmental substances which show evidence of risk. It started working in 2005. Different institutions and organizations from almost 25 countries including most of the European countries and also Canada, USA are the members of the NORMAN association according to the updated list of current NORMAN members ("NORMAN Membership", 2018). In recent years, Namik Kemal University - Corlu Engineering Faculty from Turkey also took part in the association.

The NORMAN method enables competent authorities and water managers to determine chemical substances that pose a relatively higher risk to the environment and human health and chemical substances that are discharged into receiving bodies in significant quantities. These priority/specific substances can be identified at river basin level, national level or European level. It is provided that decision-makers can take necessary actions in terms of monitoring chemical substances and forming/revising lists of priority/specific substances by using this common framework (Dulio & Von Der Ohe, 2013).

According to the method developed by the NORMAN (Dulio & Von Der Ohe, 2013),

- Firstly, substances are classified into action categories depending on their monitoring (exposure assessments) data, limit of quantification (LOQ) and PNEC values (risk assessments) in order to obtain homogeneous groups in terms of data availability and to prevent exclusion of substances with insufficient data. Categorization is summarized in Figure 4 and Figure 5.
- Secondly, substances taking part in each action category are scored and prioritized by using exposure (based on monitoring and/or usage data), hazard and risk indicators.
- Finally, prioritization work is revised by updating data related to the substances.

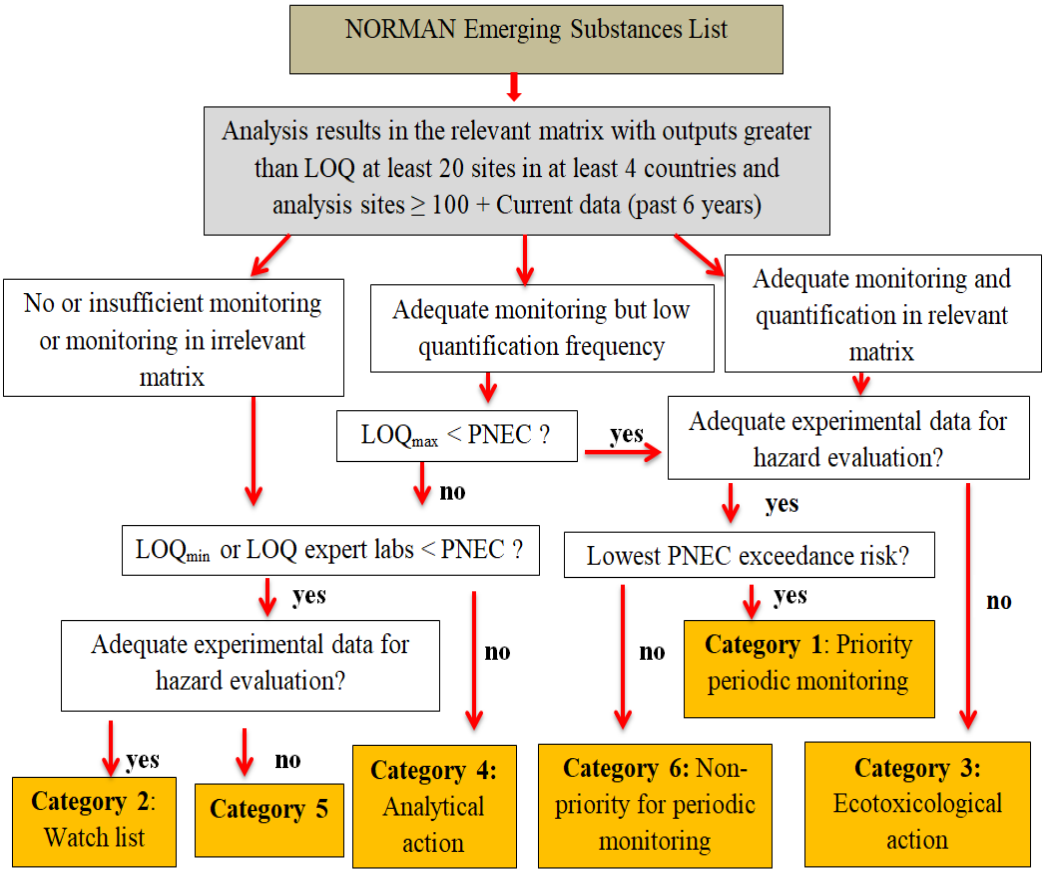

Figure 4. NORMAN Action Categories (Dulio & Von Der Ohe, 2013)

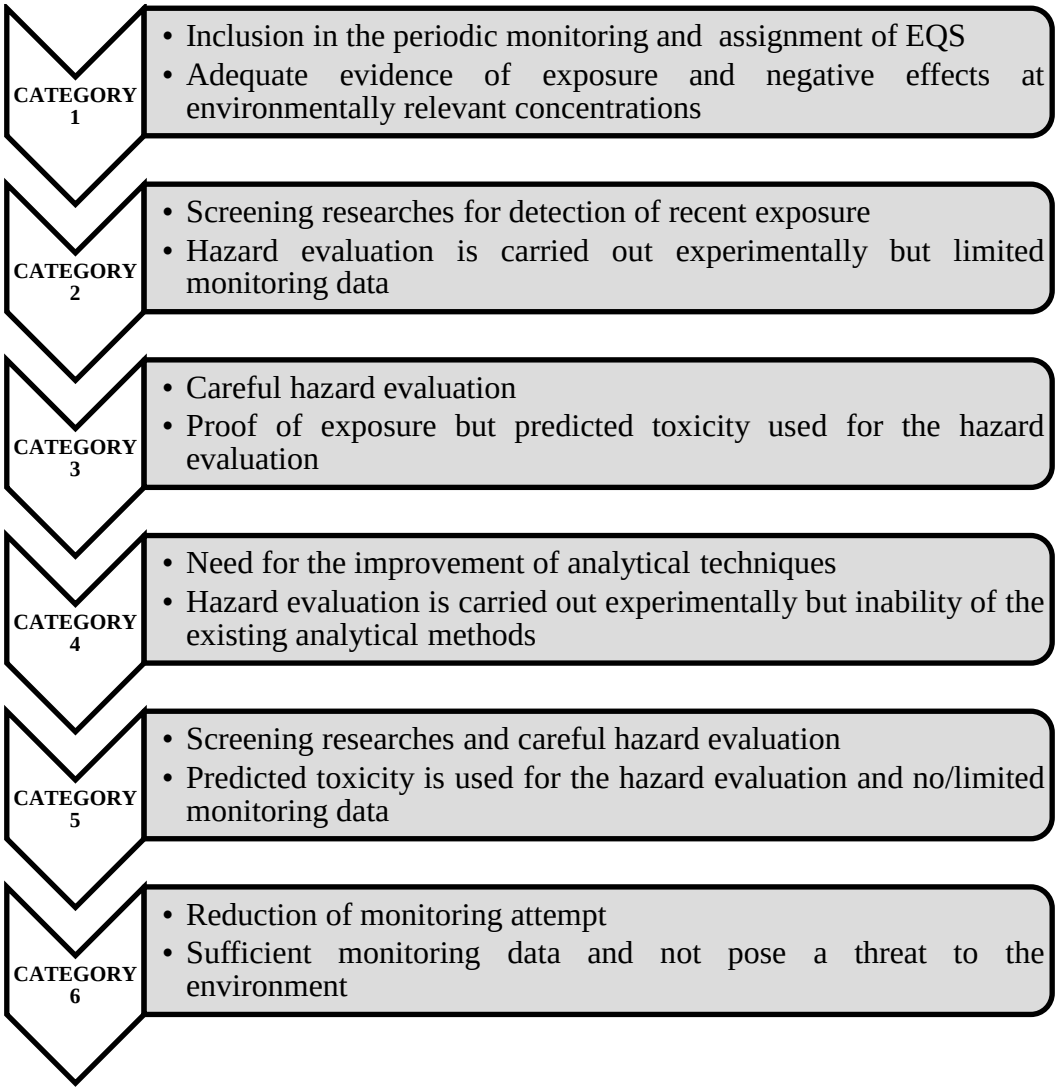

Figure 5. Details of the Action Categories in the NORMAN Method

(Dulio & Von Der Ohe, 2013)

After chemicals are classified with regard to their action category, the total score is calculated by summing the exposure, hazard and risk assessment results for each of them as indicated in Equation (60).

$$\textbf{Prioritization score (0-3)} = \textbf{Exposure score (0-1)} + \textbf{Hazard score (0-1)} + \textbf{Risk score (0-1)} \quad (60)$$

3.4.1. Exposure Assessment

Main indicators used for the exposure evaluation (shown in Table 63) are:

- Monitoring data-based indicators

A) Observation frequency above LOQ: Positive measurements are compared to the total number of observations for each substance. It gives an idea about spatial and temporal exposure.

B) Number of countries with positive observations: It represents the geographical (spatial) distribution of emerging substances and hazard potentials throughout Europe. A number of watersheds with positive measurements can also be used alternatively as an indicator for a single country.

C) Positive observation results: If substances have existed at many sites, they become a potential hazard concern.

D) Trend of concentration: Concentrations of at least 5 years are compiled. Then, 95^{th} percentile of maximum concentrations at each site is calculated for each compound and plotted with respect to years. By observing concentration trend (increasing, decreasing or staying stable), appropriate scores are given.

E) Existence in groundwater: Degree of concern is increased depending on the presence of substances in groundwater.

- Usage data-based indicators

F) Annual use/production: Chemicals which are used/produced in great quantities pose a higher risk due to the higher possibility to contaminate the environment.

G) Usage pattern: Depending on usage category, the fate of substances (chance of ending up in the environment) is affected.

Exposure score is calculated as shown in Equation (61) and (62):

$$\textbf{Exposure Score (Category 1, 3, 6)} = (EXPO\_O + EXPO\_P) / 2 \quad (61)$$

$$\textbf{Exposure Score (Category 2, 4, 5)} = EXPO\_P \quad (62)$$

Table 63. Calculation of the NORMAN Exposure Score

(Dulio & Von Der Ohe, 2013)

Indicators		Subheadings	Value	Subscores	
EXPOSURE	Observed Exposure (monitoring data)	**A)**Observation frequency above LOQ	Fraction of observations > LOQ	Rounding off to two decimal numbers	EXPO_O = (A+B+C+D+E) / 5
		B)Number of countries with positive observations	Number of countries where concentration > LOQ	Value between 0-1 0 (or no data)= 0 ≥ 1= 0.10 ≥ 2= 0.20 ≥ 5= 0.50 ≥ 10= 1	
		C)Positive observation results	Number of monitoring sites where concentration > LOQ	Value between 0-1 0 (or no data)= 0 ≥ 1= 0.10 ≥ 10= 0.20 ≥ 100=0.50 ≥ 1000=1	
		D)Trend of concentration	Trend analysis of MEC_{95} at least 5 years and 6 sites	Remarkable increasing trend=1 Increasing trend= 0.5 No pattern= 0.25 No data= 0.1 Decreasing trend= 0	
		E)Existence in groundwater		Yes= 1 No= 0	
	Predicted Exposure (usage data)	**F)**Annual use/ production	Production amount (ton)	< 1= 0.1 1-10= 0.2 10-100= 0.5 >100= 1	EXPO_P = (F+G) / 2
		G)Usage pattern		* Environmental usage=1 * Wide dispersive usage (urban wastewater and diffuse sources)= 0.75 * Non-dispersive usage (Controlled point sources)=0.50 * Unknown=0.25 * Controlled system (no direct release to the environment)= 0.1	

3.4.2. Hazard Assessment

Main indicators used for the hazard evaluation (shown in Table 64 and Table 65) are:

- Environmental hazards indicators

H) PBT/vPvB: If substances have persistent, bioaccumulative and toxic properties or they are very persistent and very bioaccumulative, they pose an extra threat to the environment. They are evaluated by checking their physicochemical and toxicological properties such as half-life for water/ sediments, bioconcentration factor (BCF) and predicted no effect concentration (PNEC) values.

I) Long-range transport of air (LRAT): Atmospheric oxidation half-life and Henry's Law constant (or air-water partition coefficient- log K_{ow}) are main parameters that are used for the evaluation of transport and deposition of substances.

J) Nonstandard endpoints: Other significant effects are also taken into consideration. These endpoints include estrogen/androgen receptor-mediated effects, effects on behavior, heart rate, enzyme activity, nervous and immune system, etc.

- Human health indicators

K) Carcinogenicity, Mutagenicity and Reproductive toxicity (CMR): European Union Classification, Labeling and Packaging Regulation (CE/2008) or other international classification techniques can be used.

For carcinogenicity evaluation and scoring, substances take part in

- ❖ Category 1 if they are known carcinogens for humans
- ❖ Category 2 if they are presumed or probable carcinogens for humans
- ❖ Category 3 if they are suspected or possible carcinogens for humans

For mutagenicity evaluation and scoring, substances take part in

- ❖ Category 1 if they are mutagenic with sufficient proof from human epidemiological searches
- ❖ Category 2 if they have positive findings from in vivo somatic or germ cell mutagenicity tests of mammals or germ cell mutagenicity tests of humans
- ❖ Category 3 if there is a possibility to promote genetic mutations in humans' germ cells

For reproductive toxicity evaluation and scoring, substances take part in

- ❖ Category 1 if they are known reproductive toxicants for humans
- ❖ Category 2 if they are presumed reproductive toxicants for humans
- ❖ Category 3 if they are suspected reproductive toxicants for humans

L) Endocrine disruption (ED): Endocrine disruption potential of substances is also taken into consideration for the hazard evaluation.

Table 64. Calculation of the NORMAN Hazard Score

(Dulio & Von Der Ohe, 2013)

		Subheadings	Value	Subscores	Hazard score
HAZARD	**Human Health and Environmental Hazards**	**H)**PBT/ vPvB	((P + B + T)+ PBT.vPvB) / 4	Shown in Table 65	**Hazard score = (H + I + J + K+ L) / 5**
		I) Long-range transport of air (LRAT)	Half-life (air) > 2 days and Vapor pressure(VP) < 1000 Pa	Half-life (air) >2 d and VP < 1000 Pa = 1 Half-life (air)≤ 2 d and/or VP ≥ 1000 Pa = 0	
		J)Nonstandard endpoints	Neurotoxicity, immunotoxicity, heart rate, etc.	Existing= 1 Under research= 0.5 Not examined= 0.25 No/ not toxic= 0	
		K)Carcinogenicity, Mutagenicity and Reproductive toxicity (CMR)	Maximum CMR score	CMR Category 1= 1 CMR Category 2= 0.75 CMR Category 3= 0.5 Under research = 0.5 Inadequate info= 0.25 Not examined= 0.25 No/ not classified= 0	
		L)Endocrine disruption (ED)		Proven = 1 Suspected= 0.5 Not examined= 0.25 No= 0	

Table 65. PBT Limit Values and Their Scores in the NORMAN Method (Dulio & Von Der Ohe, 2013)

Property	Limit values		Score
Persistence (P) **Half-life ($t_{1/2}$)** **(for water and sediments)**	vP	$t_{1/2}$ > 60 d (for fresh and marine water) or $t_{1/2}$ > 180 d (for fresh and marine sediments)	1
	P	$t_{1/2}$ > 40 d (for fresh and marine water) or $t_{1/2}$ > 120 d (for fresh and marine sediments)	1
	Suspicious P	$t_{1/2}$ > 20 d (for fresh and marine water) or $t_{1/2}$ > 60 d (for fresh and marine sediments)	0.5
	No data		0.1
	Not Persistent		0
Bioaccumulation (B) **BCF**	vB	BCF > 5000	1
	B	BCF > 2000	1
	Suspicious B	BCF > 500	0.5
	No data		0.1
	Not Bioaccumulative		0
Toxicity (T) **Lowest PNEC**	T+	Lowest PNEC < 0.01 μg/L	1
	T	Lowest PNEC < 0.1 μg/L	1
	Potential T	Lowest PNEC < 1 μg/L	0.5
	Not likely T	Lowest PNEC < 10 μg/L	0.1
	Insoluble		0.1
	No data		0.1
	Not Toxic	Lowest PNEC ≥10 μg/L	0

While the lowest PNEC values are determined by considering data availability and expert judgments, the following procedure (as shown in Figure 6) is applied.

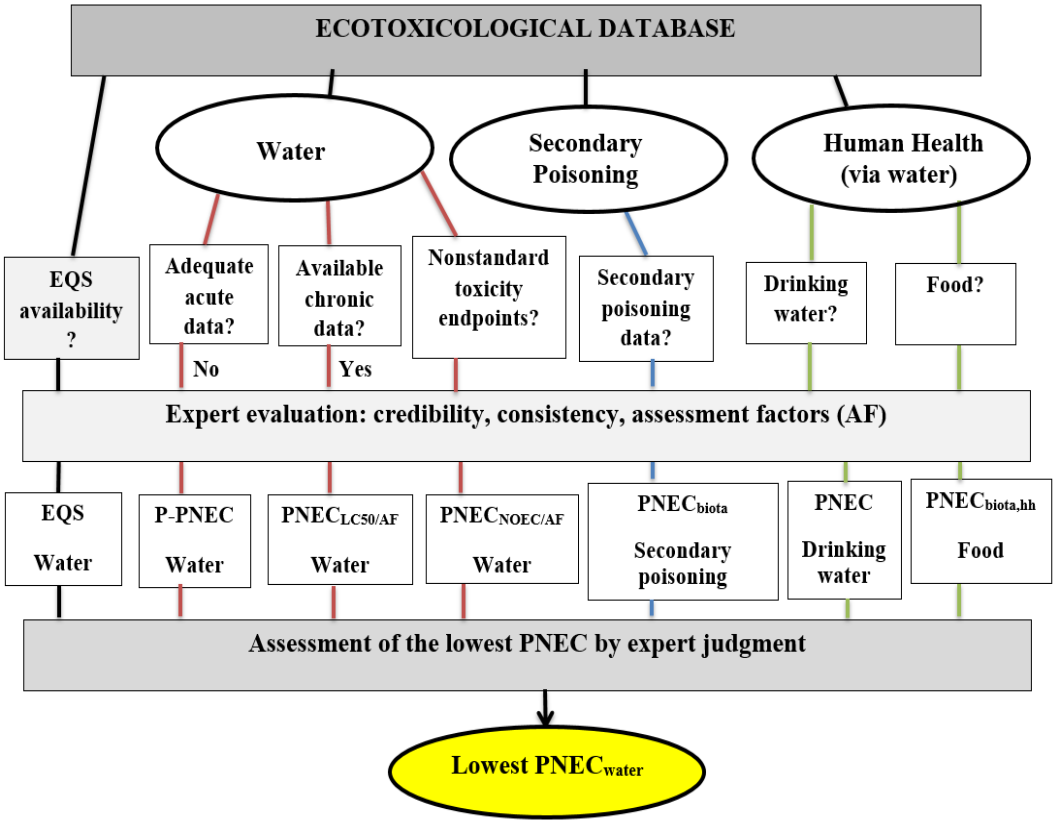

Figure 6. Choice of the Lowest PNEC Value in the NORMAN Procedure (Dulio & Von Der Ohe, 2013)

If acute experimental data are used, lowest $PNEC_{water}$ is calculated for each substance by dividing lowest LC_{50} or EC_{50} value obtained from three trophic species that are fish, invertebrates (mostly Daphnia) and algae by assessment factor of 1000. If chronic experimental data are used, dividing lowest NOEC value by assessment factor of 100 gives lowest $PNEC_{water}$ value for related substance. In order to regard indirect impacts of substances, this enhanced safety coefficient is implemented to chronic data. If PNEC value is intended to find for sediments, equilibrium partitioning approach stated in the Technical Guidance for Deriving Environmental Quality Standards (EU Commission, 2011) is applied to the lowest $PNEC_{water}$ value. For the $PNEC_{biota}$ calculation, BCF factor approach is used. In case of no data for the substances, quantitative structure-activity relationship (QSAR) model is preferred to find provisional PNEC value.

3.4.3. Risk Assessment

Main indicators used for the risk evaluation (shown in Table 66) are:

M) Exceedance frequency of the lowest PNEC (n / N): It indicates a spatial distribution of exposure. Fraction of the monitoring sites where maximum environmental concentrations at each site (MEC_{site}) are greater than the lowest PNEC is found for each substance. (n is the number of monitoring sites where MEC_{site} / lowest PNEC >1 and N is the total number of monitoring sites where analytical measurements/observations are done for a substance).

N) Exceedance degree/extent of the lowest PNEC (MEC_{95} / lowest PNEC): It indicates the severity of exposure. Depending on the magnitude of the ratio, the corresponding score is assigned for each substance. MEC_{95} represents 95^{th} percentile of all MEC_{site} values.

It requires at least 20 monitoring sites with analytical measurements above LOQ. If numbers of monitoring sites where concentrations cannot be quantified are less than 20, maximum environmental concentration among all sites ($MEC_{site\text{-}max}$) is used for related compound instead of MEC_{95} approach.

Table 66. Calculation of the NORMAN Risk Score (Dulio &Von Der Ohe, 2013)

Indicators		**Subheadings**	**Value**	**Subscores**	**Risk Score**
RISK	**Frequency of exceedance**	**M)**Exceedance frequency of the lowest PNEC	n / N	Rounding off to two decimal numbers	**Risk Score = (M + N) / 2**
	Degree/ Extent of exceedance	**N)** Exceedance degree of the lowest PNEC	MEC_{95} / lowest PNEC	* ratio < 1= 0 * ratio ≤ 10= 0.1 * 10< ratio ≤100 = 0.25 * 100< ratio ≤ 1000 = 0.5 * ratio> 1000 =1	

*For Category (1, 3 and 6) = MEC_{95} (recent data), For Category (2, 4 and 5) = MEC_{95} (all data from all years)

**Total prioritization score (0-3) = Exposure score (0-1) + Hazard score (0-1) + Risk score (0-1)

3.5. Procedure Followed and Assumptions Made for the Application of the NORMAN Method

For the calculation of observed exposure score which was based on the 1.5- year monitoring data, three criteria were evaluated. These are observation frequency above LOD, number of European countries where the substance is a specific pollutant and positive observation results (evaluating all measurements regardless of particular monitoring stations). Depending on the values, corresponding scores were given as stated in the procedure (see Table 63). Average of these three scores was assigned as exposure score for each substance.

For the hazard score, candidate substances were evaluated by considering their PBT properties (water half-life, BCF and PNEC values), LRAT (air half-life and vapor pressure), nonstandard toxicity endpoints, CMR and ED properties. Corresponding scores were given as stated in the procedure (see Table 64 and Table 65) depending on the magnitude of the values. Average of these five criteria was taken as hazard score for each substance.

For the calculation of risk score, frequency and extent of exceedance of the lowest PNEC value were assessed. Frequency of exceedance was calculated by finding the fraction of monitoring points where MEC_{site} values exceeded the lowest PNEC as a result of the evaluation of each monitoring point. On the other hand, extent of exceedance was calculated dividing 95^{th} percentile of MEC values (or $MEC_{site\text{-}max}$ value depending on numbers of monitoring sites where concentrations were quantified) by the lowest PNEC value (obtained by using assessment factor approach as a result of consideration of both acute and chronic toxicity data for 3 trophic species depending on data availability) for each substance. After corresponding scores were given as stated in the procedure (see Table 66), average of these two criteria was assigned as risk score.

As the last step, exposure, hazard and risk scores were summed up for each substance (Equation (60)). According to their NORMAN scores which are in between 0 and 3, candidate substances were ranked from highest to lowest.

Main assumptions made and data selections are summarized as follows:

- Necessary data related to physicochemical and toxicological properties of chemicals/pollutants were taken from reliable databases such as University of Hertfordshire, PubChem, TOXNET, EPI Suite and also from related Legislation/Directives/Regulations and scientific documents/material safety data sheets obtained by the literature search as well as a document supplied by TUBITAK MAM.

- Metals and metalloids were also included in the prioritization study by making conservative assumptions although they are not explained explicitly in the procedure (other inorganics and mixture of total petroleum hydrocarbons were excluded). Since it is hard to determine the fate and behaviors of metals/metalloids due to complex formation/speciation, and also persistency-bioaccumulation evaluations are not applicable for metals/metalloids, a score of 0.1 (uncertainty score) was used for those evaluations.

- Natural background concentration data for metals and metalloids in the Yesilirmak River Basin (see Table 62) were taken from studies carried out by the METU Project Group as a part of the TUBITAK Project (115Y013). The 5^{th} percentile monitoring data approach was used by excluding points where concentration is lower than the LOD value instead of taking them as LOD/2. In case background concentrations were greater than the PNEC values, background concentrations were used for the calculations instead of the PNEC values.

- Monitoring-based exposure assessment was performed by using 8-period monitoring data obtained from 42 monitoring stations (shown in APPENDIX B-Table 79 and Figure 8) within 1.5 years. In case there was a reported substance's concentration value that was lower than the corresponding LOD value, it was disregarded. During calculation of the exposure score, if concentration of a substance was detected but not quantified (< LOD), half of

the LOD value was used for related monitoring stations instead of taking 0 or excluding those monitoring points. In this manner, it was aimed to include all substances in the ranking/prioritization procedure. However, this caused an overestimation of the score for substances whose lowest PNEC values are smaller than half of the LOD value in the risk assessment part (see Table 66). Therefore, related non-quantified substances in any of the monitoring periods were indicated in bold fonts in the scoring and ranking procedure.

- Predicted exposure was not calculated for substances due to lack of usage data. Only the assessment of observed exposure based on monitoring data was done regardless of the category that substance belongs to. In observed exposure part, two indicators/criteria which are "concentration trend" and "observation of substances in groundwater" were excluded because of data deficiencies. In addition, instead of the evaluation of "number of countries with positive observations" criterion, "number of European countries where the substance is a specific pollutant" criterion was used due to difficulties in terms of data access.

- During hazard assessment, for persistency analysis, half-life values (for freshwater especially river) of substances were assigned by taking into account abiotic degradations (volatilization, hydrolysis and photolysis etc.) and attenuation effect due to adsorption to suspended solids and sediments. For toxicity analysis in case the lowest PNEC value (obtained by using both acute and chronic ecotoxicity data for aquatic ecosystem with appropriate assessment factors and choosing the lowest PNEC value among them) was greater than EQS, EQS value was preferred/used for that substance. Moreover, for the determination of CMR Category, if the category of a substance was not expressed explicitly in the literature, an evaluation was made depending on the availability of evidence assuming that it was included in Category 2 or Category 3 for substances with probable/possible/potential/suspected carcinogenicity and/or mutagenicity and/or effects on reproduction.

3.6. Weighting Factor Approach

Since the COMMPS and NORMAN prioritization methods use different algorithms and different evaluation criteria, it is expected that different ranking trends/patterns are obtained. Therefore, there is a need to combine these two different scores in order to obtain a single ranking list. For this purpose, consolidated methodologies related to multiple attribute/criteria decision making (MADM) reported by Maggino and Ruviglioni (2009) were reviewed and considered. Then, a similar approach used by Siltu (2015) was chosen to be applied with significant modifications.

In this approach, in order to obtain weighting factors, the two methods were compared and graded under three main headings which are:

- Scope/Extent of the assessments (in terms of exposure, hazard and risk)
- Protectiveness of the methods
- Applicability of the methods.

CHAPTER 4

RESULTS AND DISCUSSION

In this chapter, ranking results of the COMMPS and NORMAN prioritization methods are listed by giving examples of how calculations are done. The final ranking is carried out by means of weighting factor approach as a result of the combination of the COMMPS and NORMAN scores for each candidate substances. In the end, proposed specific pollutants for the Yesilirmak River Basin are provided with the reason.

4.1. Ranking Results of the COMMPS Prioritization Method

In this part, calculation of the COMMPS scores and ranking of the chemicals by the COMMPS method are explained.

4.1.1. Calculations of the COMMPS Scores

COMMPS prioritization method was applied to 250 national specific pollutants of Turkey by using 1.5-year monitoring data in the Yesilirmak River Basin. As an example, calculations of the scores for arsenic and permethrin are given below.

For arsenic

- Calculation of the COMMPS score for arsenic (0-100):

Necessary data which were used in the calculation procedure for As by the COMMPS method are summarized in Table 67.

Table 67. COMMPS Data for As

Parameter	Value	Parameter	Value	Parameter	Value
C_i (µg/L)	23.314	C_{min} (µg/L)	0.2	C_{max} (µg/L)	200
$PNEC_{min}$ (mg/L)	0.000001	$PNEC_{max}$ (mg/L)	0.1	LC_{50} (Fish)- 96 h (mg/L)	1.57
LC_{50} /EC_{50} (Daphnia)-48 h (mg/L)	5.26	LC_{50} (Algae)- 72/96 h (mg/L)	no data	NOEC (Fish)- 21 d (mg/L)	0.01
NOEC (Daphnia)- 21 d (mg/L)	no data	NOEC (Algae)- 72 h (mg/L)	no data	AF	100
WF	8	$PNEC_i$ (mg/L)	0.0001	Log K_{ow}	-
MW	75	BCF	-	Risk phrases	R: 22, 23/25, 36/38, 45, 50/53

*Since indirect aquatic effect score is not applicable for metals, BCF and Log K_{ow} parameters are not used.

**Background concentration for As is 0.001026 mg/L in the basin as shown in Table 62.

***This table was filled out by obtaining necessary parameters for the application of the method from reliable databases and documents and by using monitoring data/results.

****C_{min}, C_{max}, $PNEC_{min}$ and $PNEC_{max}$ values come from Table 57 and Table 59.

Calculations were done by using Equations (53), (57), (58) and (59) as stated in the procedure that are explained in Chapter 3.

$$\mathbf{I\_prio} = \mathbf{I\_exp} \times \mathbf{I\_eff} \tag{53}$$

$$\mathbf{I\_exp\,(substance\ i)} = \frac{\log\,(C_i\ /\ (C_{min} \times 10^{-1}))}{\log\,(C_{max}\ /\ (C_{min} \times 10^{-1}))} \times 10 \tag{57}$$

Where

C_i = 23.314 µg/L (Calculated by means of Excel program which were submitted via CD also shown in APPENDIX A-Table 78)

C_{max}= 200 µg/L, C_{min}= 0.2 µg/L

$$\textbf{I\_exp (for arsenic)} = \frac{\log\,(23.314\ /\ (0.2 \times 10^{-1}))}{\log\,(200\ /\ (0.2 \times 10^{-1}))} \times 10 = 7.6665$$

$$\textbf{I\_eff} = EFS_d + EFS_h \quad (EFS_i \text{ not applicable for metals}) \qquad (58)$$

$$\textbf{EFS}_\textbf{d}\textbf{ (substance i)} = \frac{\log\,(PNEC_i\ /\ (10 \times PNEC_{max}))}{\log\,(PNEC_{min}\ /\ (10 \times PNEC_{max}))} \times WF \qquad (59)$$

Where

$PNEC_i = {}^{NOEC,\ fish}/_{AF} = {}^{0.01}/_{100} = 0.0001$ mg/L

(Lowest chronic data among three trophic levels was preferred according to the method. Fish data was used with appropriate AF by considering the availability of the data for the species)

However, since background concentration, which is 0.001026 mg/L, is greater than PNEC value, background concentration value was used instead of PNEC value.

$PNEC_{max}$= 0.1 mg/L

$PNEC_{min}$= 0.000001 mg/L

WF= 8 (for metals)

$$\textbf{EFS}_\textbf{d}\textbf{ (for arsenic)} = \frac{\log\,(0.001026\ /\ (10 \times 0.1))}{\log\,(0.000001\ /\ (10 \times 0.1))} \times 8$$

EFS_d (for arsenic) = 3.9851

EFS_h (for arsenic) = 2

(As a result of the evaluation of risk phrases with risk phrases of R: 22, 23/25, 36/38, 45, 50/53 as shown in Table 61)

I_eff (for arsenic) = 3.9851 + 2 = 5.9851

I_prio (for arsenic) = 7.6665 × 5.9851 = 45.885

For permethrin

- Calculation of the COMMPS score for permethrin (0-100):

Necessary data which were used in the calculation procedure for permethrin by the COMMPS method are summarized in Table 68.

Table 68. COMMPS Data for Permethrin

Parameter	Value	Parameter	Value	Parameter	Value
C_i (µg/L)	0.072	C_{min} (µg/L)	0.0001	C_{max} (µg/L)	100
$PNEC_{min}$ (mg/L)	0.000001	$PNEC_{max}$ (mg/L)	1	LC_{50} (Fish)- 96 h (mg/L)	0.0125
LC_{50} /EC_{50} (Daphnia)-48 h (mg/L)	0.0006	LC_{50} (Algae)- 72/96 h (mg/L)	0.12	NOEC (Fish)- 21 d (mg/L)	0.00012
NOEC (Daphnia)- 21 d (mg/L)	no data	NOEC (Algae)- 72 h (mg/L)	0.0009	AF	50
WF	5	$PNEC_i$ (mg/L)	$2.4x10^{-6}$	Log K_{ow}	6.5
MW	391.3	BCF	560	Risk phrases	R:20/22, 33,40, 42, 43, 50/53

*This table was filled out by obtaining necessary parameters for the application of the method from reliable databases and documents and by using monitoring data/results.
**C_{min}, C_{max}, $PNEC_{min}$ and $PNEC_{max}$ values come from Table 57 and Table 59.

Calculations were done by using Equations (53), (57), (58) and (59) as stated in the procedure that are explained in Chapter 3.

$$\mathbf{I\_prio} = \mathbf{I\_exp} \times \mathbf{I\_eff} \quad (53)$$

$$\mathbf{I\_exp\,(substance\ i)} = \frac{\log\,(C_i\ /\ (C_{min} \times 10^{-1}))}{\log\,(C_{max}\ /\ (C_{min} \times 10^{-1}))} \times 10 \quad (57)$$

Where

C_i = 0.072 µg/L (Calculated by means of Excel program which were submitted via CD, also shown in APPENDIX A-Table 78)

C_{max}= 100 µg/L, C_{min}= 0.0001 µg/L

$$\textbf{I\_ exp (for permethrin)} = \frac{\log\ (0.072\ /\ (0.0001\ \times 10^{-1}))}{\log\ (100\ /\ (0.0001 \times 10^{-1}))} \times 10 = 5.51$$

$$\textbf{I\_eff} = EFS_d\ +\ EFS_i\ +\ EFS_h \qquad (58)$$

$$\textbf{EFS}_\textbf{d}\textbf{ (substance i)} = \frac{\log (PNEC_i\ /\ (10\ \times\ PNEC_{max}))}{\log (PNEC_{min}\ /\ (10\ \times\ PNEC_{max}))} \times\ WF \qquad (59)$$

Where

$PNEC_i = {}^{NOEC,\ fish}/_{AF} =\ {}^{0.00012}/_{50} = 0.0000024$ mg/L

(Lowest chronic data was preferred according to the method)

$PNEC_{max}$= 1 mg/L

$PNEC_{min}$= 0.000001 mg/L

WF= 5 (for organics)

$$\textbf{EFS}_\textbf{d}\textbf{ (for permethrin)}\ =\ \frac{\log\ (\ 0.0000024\ /(10\ \times 1\ ))}{\log\ (0.000001\ /(10 \times 1))} \times 5\ =\ 4.728$$

EFS_i (for permethrin) = 1 (as shown in Table 60 with BCF value of 560)

EFS_h (for permethrin) = 1.8

(As a result of the evaluation of risk phrases with risk phrases of R: 20/22, 33, 40, 42, 43, 50/53 as shown in Table 61)

I_eff (for permethrin) = 4.728 + 1 +1.8 = 7.528

I_prio (for permethrin) = $5.51 \times 7.528 \approx 41.48$

4.1.2. Ranking of the Chemicals by the COMMPS Method

Ranking results of top 50 candidate substances are shown in Table 69. The complete list of COMMPS ranking results is given in APPENDIX C-Table 80.

Table 69. Ranking Results Obtained by Using COMMPS Method

RANK	***CHEMICAL NAME***	***EXPOSURE SCORE***	***EFFECT SCORE***	***COMMPS SCORE****
1	Fenarimol	9.422	6.482	61.076
2	Perylene	4.743	9.770	46.337
3	Arsenic	7.666	5.985	45.885
4	2-Chloronaphthalene	7.054	6.504	45.874
5	Antimony	7.547	6.041	45.589
6	Ethalfluralin	6.132	7.104	43.557
7	**Tris(nonylphenyl) phosphite; TNPP**	6.964	6.031	42.000
8	Permethrin	5.509	7.528	41.477
9	Fenthion	5.518	7.400	40.833
10	Fenpropimorph	6.333	6.371	40.351
11	**2-Amino-4-chlorophenol**	5.284	7.628	40.306
12	Prothiofos	5.505	7.181	39.530
13	Chromium	6.192	6.119	37.892
14	Polychlorinated biphenyls (PCBs)	4.312	8.571	36.958
15	DDT (Total)	3.761	9.776	36.765
16	**Butralin**	4.854	7.571	36.753
17	Tridecane	5.357	6.786	36.355
18	**2.4-D. isooctyl ester**	5.714	6.356	36.322
19	Metam Potassium	5.437	6.671	36.274
20	**Tolfenpyrad**	4.854	7.355	35.702
21	4.4'-DDD	3.853	9.118	35.135
22	**Clofibric acid**	6.964	5.031	35.035
23	Chlorobenzilate	6.475	5.286	34.226
24	**4.5-dichloro-2-octyl-2H-isothiazol-3-on; DCOIT**	4.854	7.000	33.979

Table 69. Ranking Results Obtained by Using COMMPS Method (cont'd)

RANK	***CHEMICAL NAME***	***EXPOSURE SCORE***	***EFFECT SCORE***	***COMMPS SCORE****
25	**Pyridaben**	4.854	7.000	33.979
26	**Quinalphos**	4.854	7.000	33.979
27	**Oxadiazon**	4.854	6.910	33.544
28	**Fenitrothion**	6.283	5.329	33.480
29	**Dieldrin**	3.426	9.743	33.377
30	Atrazine-desethyl (Deethylatrazine)	6.196	5.371	33.281
31	Diflubenzuron	5.528	6.000	33.169
32	Chlorothalonil	5.432	6.031	32.760
33	**Musk xylene**	5.284	6.123	32.354
34	**17 alpha Ethinyl Estradiol**	5.284	6.072	32.087
35	Carbendazim	5.379	5.945	31.980
36	Benzo[*e*]pyrene	3.551	9.000	31.963
37	**Fenbutatin oxide**	5.284	5.997	31.687
38	**Pyriproxyfen**	4.286	7.136	30.583
39	**Triclosan**	5.284	5.786	30.577
40	**2.3.4.5.6-Pentachlorotoluene**	5.284	5.776	30.520
41	Cyfluthrin	5.052	6.000	30.310
42	**Dibutyltin oxide**	3.856	7.857	30.295
43	PCB 153	3.410	8.785	29.956
44	Zinc	9.218	3.249	29.945
45	**Prochloraz**	4.854	6.156	29.884
46	Dioctyl Phthalate	5.700	5.214	29.718
47	Captan	5.298	5.511	29.201
48	**Propetamphos**	4.854	6.000	29.125
49	**Triflumuron**	4.854	6.000	29.125
50	**4-Aminoazobenzene**	5.284	5.463	28.866

*COMMPS score= Exposure score x Effect score

**Chemicals which were detected but not quantified in any of the monitoring periods are indicated in bold font. They were included in the ranking/prioritization procedure by taking their concentrations as LOD/ 2.

***Mixtures and inorganics other than metals-metalloids were not included in the ranking/ prioritization process.

The results showed that organic chemicals such as pesticides and industrial chemicals ranked at the top places comparing to metals. Only four metals, which are As, Sb, Cr and Zn, were found in the top 50. Especially, chlorinated organics (organochlorides) were drawn the attention.

Since priority score is obtained by combining exposure and hazard assessments, hazardous chemicals posing a threat to the environment and human health and being observed at relatively high concentrations are expected to be at the top in the ranking. Besides, it was observed that even if some chemicals were not quantified in any of the monitoring periods, they ranked at the top places. It resulted from the relatively high values of the related LOD and toxicity. Because half of the related LOD values were taken as concentration values for non-quantified chemicals to be on the safe (conservative) side; this caused uncertainty and affected the ranking procedure. In addition, hazard (toxicity) evaluation had significant contribution to the ranking of these non-quantified dangerous substances. Another discussion can be made for very hydrophobic organic chemicals ($\log K_{ow} > 3$ or 5). Since they prefer sediment phase due to low solubility values in the water, risk assessment of those substances may be underestimated. A sediment phase prioritization procedure could be more relevant for those substances via sediment monitoring data and $PNEC_{sed}$ values which are obtained by converting $PNEC_{fw}$ values through equilibrium partitioning approach.

4.2. Ranking Results of the NORMAN Prioritization Method

In this part, calculation of the NORMAN scores and ranking of the chemicals by the NORMAN method are explained.

4.2.1. Calculations of the NORMAN Scores

NORMAN prioritization method was applied to 250 national specific pollutants of Turkey by using 1.5-year monitoring data in the Yesilirmak River Basin. As an example, calculations of the scores for arsenic and permethrin are given below.

For arsenic

- Calculation of the NORMAN score for arsenic (0-3):

Necessary data which were used in the calculation procedure for As by the NORMAN method are summarized in Table 70.

Table 70. NORMAN Data for As

Parameter	Value	Parameter	Value	Parameter	Value
Number of monitoring points	42	Number of measurements	321	Number of positive observations	321
Half-life (water)	no data	BCF	no data	EQS (µg/L)	53
LC_{50} (Fish)-96 h (mg/L)	1.57	LC_{50} /EC_{50} (Daphnia)-48 h (mg/L)	5.26	LC_{50} (Algae)-72/96 h (mg/L)	no data
NOEC (Fish)- 21 d (mg/L)	0.01	NOEC (Daphnia)- 21 d (mg/L)	no data	NOEC (Algae)- 72 h (mg/L)	no data
AF	100	Lowest PNEC (µg/L)*	0.1	V_p	so small
Half-life (air)	no data	Other toxicities	yes	CMR Category	Category 1
ED	yes	MEC_{95} (µg/L)	51.289	Background C (µg/L)*	1.026

*Since background c is greater than the lowest PNEC, background concentration value was used instead of PNEC value for the calculations.
**This table was filled out by obtaining necessary parameters for the application of the method from reliable databases and documents and by using monitoring data/results.
***EQS value is available in SWQR.

Calculations were done in accordance with information in the procedure that are explained in Chapter 3.

$$\textbf{Prioritization score} = \textbf{Exposure score} + \textbf{Hazard score} + \textbf{Risk score} \quad (60)$$

$$\textbf{Exposure Score} = \frac{A + B + C}{3} \qquad \text{(see Table 63)}$$

Where

A= Observation frequency above LOD (321 detections out of 321 measurements, 321/ 321=1, which corresponds to the score of 1)

B = Number of European countries where the substance is a specific pollutant (17 countries, which corresponds to the score of 1)
(Instead of "number of countries with positive observations" criterion, this one was used, and same evaluation criteria were applied)

C = Positive observation results (the substance was observed 321 times, which corresponds to the score of 0.5)

$$\textbf{Exposure Score (for arsenic)} = \frac{1 + 1 + 0.5}{3} = 0.833$$

$$\textbf{Hazard score} = \frac{H + I + J + K + L}{5} \qquad \text{(see Table 64 and Table 65)}$$

Where

$$H = \frac{(P + B + T) + PBT.vPvB}{4} = \frac{(0.1 + 0.1 + 0.1) + 0}{4} = 0.075$$

(Depending on physicochemical and toxicological profiles, corresponding scores were assigned according to the scoring procedure in hazard assessment in the NORMAN method)

I= Long-range transport of air (LRAT) (score of 0 was assigned by considering solubility and air half-life values)

J= Nonstandard endpoints (Score of 1 was assigned due to the existence of health effects such as negative impacts of cardiovascular system and cognitive development)

K= CMR Properties (Score of 1 was assigned due to classification of Category 1)

L= Endocrine disruption (Score of 1 was assigned since it is an endocrine disrupting chemical)

$$\textbf{Hazard score (for arsenic)} = \frac{0.075 + 0 + 1 + 1 + 1}{5} = 0.615$$

$$\textbf{Risk score} = \frac{M + N}{2} \qquad \text{(see Table 66)}$$

Where

M= Frequency of exceedance of the lowest PNEC = $^{n}/_{N} = {}^{42}/_{42} = 1$

(MEC_{site} values of the chemical exceeded the lowest PNEC value at every monitoring station. This corresponds to the score of 1)

N= Extent of exceedance of the lowest PNEC = $^{MEC_{95}}/_{\text{lowest PNEC}}$= $^{51.289}/_{1.026}$ = 49.99

(This corresponds to score of 0.25. MEC_{site} and MEC_{95} values were calculated for each candidate substance by means of Excel program that submitted via CD)

Where lowest PNEC = $^{\text{NOEC, fish}}/_{AF} = {}^{0.01}/_{100}$ = 0.0001 mg/L= 0.1 µg/L

However, since background concentration, which is 1.026 µg/L, is greater than the lowest PNEC value, background concentration value was used instead of PNEC value.

$$\textbf{Risk score(for arsenic)} = \frac{1 + 0.25}{2} = 0.625$$

$$\textbf{Prioritization score (for arsenic)} = 0.833 + 0.615 + 0.625 = 2.073$$

<u>For permethrin</u>

- Calculation of the NORMAN score for permethrin (0-3):

Necessary data which were used in the calculation procedure for permethrin by the NORMAN method are summarized in Table 71.

Table 71. NORMAN Data for Permethrin

Parameter	Value	Parameter	Value	Parameter	Value
Number of monitoring points	42	Number of measurements	321	Number of positive observations	2
Half-life (water)	39 d	BCF	560	EQS (µg/L)	0.12
LC_{50} (Fish)- 96 h (mg/L)	0.0125	LC_{50} /EC_{50} (Daphnia)-48 h (mg/L)	0.0006	LC_{50} (Algae)- 72/96 h (mg/L)	0.12
NOEC (Fish)- 21 d (mg/L)	0.00012	NOEC (Daphnia)- 21 d (mg/L)	no data	NOEC (Algae)- 72 h (mg/L)	0.0009
AF	1000	Lowest PNEC (µg/L)	0.0006	V_p	so small
Half-life (air)	17 h	Other toxicities	yes	CMR Category	Category 2
ED	yes	MEC_{95} (µg/L)	0.53996		

*This table was filled out by obtaining necessary parameters for the application of the method from reliable databases and documents and by using monitoring data/results.
**EQS value is available in SWQR.

Calculations were done in accordance with information in the procedure that are explained in Chapter 3.

$$\textbf{Prioritization score} = \textbf{Exposure score} + \textbf{Hazard score} + \textbf{Risk score} \quad (60)$$

$$\textbf{Exposure Score} = \frac{A + B + C}{3} \quad \text{(see Table 63)}$$

Where

A= Observation frequency above LOD (2 detections out of 321 measurements, 2/ 321=0.01, which corresponds to the score of 0.01)

B = Number of European countries where the substance is a specific pollutant (1 country, which corresponds to the score of 0.1)
(Instead of "number of countries with positive observations" criterion, this one was used, and same evaluation criteria were applied)

C = Positive observation results (the substance was observed 2 times, which corresponds to the score of 0.1)

$$\textbf{Exposure Score (for permethrin)} = \frac{0.01 + 0.1 + 0.1}{3} = 0.07$$

$$\textbf{Hazard score} = \frac{H + I + J + K + L}{5} \qquad \text{(see Table 64 and Table 65)}$$

Where

$$H = \frac{(P + B + T) + PBT.vPvB}{4} = \frac{(0.5 + 0.5 + 1) + 0}{4} = 0.5$$

(Depending on physicochemical and toxicological profiles, corresponding scores were assigned according to the scoring procedure in hazard assessment in the NORMAN method)

I= Long-range transport of air (LRAT) (score of 0 was assigned by considering solubility and air half-life values)

J= Nonstandard endpoints (Score of 1 was assigned due to the existence of health effects)

K= CMR Properties (Score of 0.75 was assigned due to the classification of Category 2)

L= Endocrine disruption (Score of 1 was assigned since it is an endocrine disrupting chemical)

$$\textbf{Hazard score (for permethrin)} = \frac{0.5 + 0 + 1 + 0.75 + 1}{5} = 0.65$$

$$\textbf{Risk score} = \frac{M + N}{2} \qquad \text{(see Table 66)}$$

Where

M= Frequency of exceedance of the lowest PNEC = $^{n}/_{N} = {}^{42}/_{42} = 1$

(MEC_{site} values of the chemical exceeded the lowest PNEC value at every monitoring station. This corresponds to the score of 1)

N= Extent of exceedance of the lowest PNEC = $^{MEC_{95}}/_{\text{lowest PNEC}} =$ $^{0.53996}/_{0.0006} = 899.93$

(This corresponds to score of 0.5. MEC_{site} and MEC_{95} values were calculated for each candidate substance by means of Excel program that submitted via CD)

Where lowest PNEC = $^{L(E)C_{50}}/_{AF} = {}^{0.0006}/_{1000} = 0.0000006$ mg/L = 0.0006 µg/L

Risk score (for permethrin) $= \frac{1 + 0.5}{2} = 0.75$

Prioritization score (for permethrin) $= 0.07 + 0.65 + 0.75 \approx 1.47$

4.2.2. Ranking of the Chemicals by the NORMAN Method

Ranking results of top 50 candidate substances are shown in Table 72. The complete list of NORMAN ranking results is given in APPENDIX D-Table 81.

Table 72. Ranking Results Obtained by Using NORMAN Method

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
1	Arsenic	0.833	0.615	0.625	2.073
2	Zinc	0.833	0.465	0.750	2.048
3	Chromium	0.833	0.435	0.625	1.893

Table 72. Ranking Results Obtained by Using NORMAN Method (cont'd)

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
4	Cobalt	0.667	0.460	0.750	1.877
5	Aluminium	0.667	0.355	0.750	1.772
6	Copper	0.833	0.310	0.625	1.768
7	Silver	0.664	0.410	0.625	1.699
8	DDT (Total)	0.106	0.950	0.625	1.681
9	Iron	0.667	0.210	0.750	1.627
10	Endrin	0.101	0.900	0.625	1.626
11	Antimony	0.659	0.385	0.565	1.610
12	Vanadium	0.667	0.310	0.625	1.602
13	Barium	0.667	0.360	0.550	1.577
14	Diflubenzuron	0.088	0.450	1.000	1.538
15	Cyfluthrin	0.083	0.400	1.000	1.483
16	Permethrin	0.069	0.650	0.750	1.469
17	Perylene	0.102	0.600	0.750	1.452
18	**Fenitrothion**	0.167	0.500	0.750	1.417
19	Fenthion	0.204	0.575	0.625	1.404
20	Acetochlor	0.127	0.650	0.625	1.402
21	**Malathion**	0.167	0.600	0.625	1.392
22	Chlorobenzilate	0.035	0.725	0.625	1.385
23	**Dieldrin**	0.067	0.750	0.550	1.367
24	PCB 28	0.156	0.950	0.252	1.359
25	Diazinon	0.101	0.625	0.625	1.351
26	Boron	0.667	0.160	0.514	1.341
27	PCB 138	0.145	0.950	0.196	1.291
28	Silicon	0.500	0.160	0.625	1.285
29	Pendimethalin	0.101	0.525	0.625	1.251
30	Diflufenican	0.071	0.425	0.750	1.246
31	Prothiofos	0.085	0.410	0.750	1.245
32	PCB 180	0.108	0.950	0.185	1.243
33	Carbofuran	0.034	0.575	0.625	1.234
34	**Triclosan**	0.033	0.575	0.625	1.233
35	PCB 153	0.145	0.950	0.110	1.204

Table 72. Ranking Results Obtained by Using NORMAN Method (cont'd)

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
36	Polychlorinated biphenyls (PCBs)	0.201	1.000	0.000	1.201
37	Atrazine-desethyl (Deethylatrazine)	0.147	0.500	0.550	1.197
38	**Prometryn**	0.067	0.500	0.625	1.192
39	**Terbuthylazine**	0.167	0.450	0.550	1.167
40	**Methomyl**	0.000	0.605	0.550	1.155
41	**Quinalphos**	0.000	0.530	0.625	1.155
42	**Fenbutatin oxide**	0.000	0.525	0.625	1.150
43	PCB 52	0.109	0.950	0.086	1.145
44	Fenpropathrin	0.034	0.350	0.750	1.134
45	4.4'-DDE	0.102	0.950	0.074	1.126
46	**Pirimicarb**	0.067	0.500	0.550	1.117
47	Fenarimol	0.034	0.550	0.512	1.096
48	Carbendazim	0.128	0.650	0.315	1.094
49	Ethalfluralin	0.094	0.425	0.560	1.078
50	Azinphos-methyl	0.201	0.250	0.625	1.076

*NORMAN Score= ES +HS+ RS where ES: Exposure Score. HS: Hazard Score. RS: Risk Score

**Chemicals which were detected but not quantified in any of the monitoring periods are indicated in bold font. They were included in the ranking/prioritization procedure by taking their concentrations as LOD/ 2

***Mixtures and inorganics other than metals-metalloids were not included in the ranking/ prioritization process.

The results showed that metals ranked at the top places comparing to organic chemicals unlike the COMMPS method. Since exposure data which take part in both exposure and risk assessment parts are more dominant over the total score in the NORMAN method, and metals were observed almost every monitoring station with higher concentrations, metals were highlighted. Pesticides also came into prominence.

Because prioritization score is obtained by combining exposure, hazard and risk assessments; frequently detected/quantified chemicals with higher toxicity and higher environmental concentration levels (> related lowest PNEC) are expected to be at the top in the ranking.

In the NORMAN method, due to the usage of higher AF (assessment factors) for the calculation of the lowest PNEC, it was observed that there were significant differences between the lowest PNEC and EQS values. Also, due to lack of effect (toxicity) data for some species and data differences, those values were not found to be close to each other. As a conservative approach, the lowest value among them was chosen for the risk calculations. Along with this, setting concentration values as half of related LOD for non-quantified chemicals also affected risk analysis during frequency and extent of exceedance of the lowest PNEC calculations in case values of LOD/2 were greater than the lowest PNEC.

Risk assessment of hydrophobic substances might be underestimated when assessments related to only water compartment are done. Since they prefer sediment phase rather than the water due to having hydrophobic characteristics and low solubility values; choosing relevant matrix and monitoring in relevant sediment phase can avoid underestimation of risk assessment.

4.3. Final Ranking by Weighting Factor Approach

The COMMPS and NORMAN prioritization methods were separately applied by using 1.5-year monitoring data in order to identify (water phase relevant) specific pollutants of the Yesilirmak River Basin. The national 250 specific pollutants of Turkey were used as candidate substances and they were scored and ranked. The results showed that different ranking trends/patterns were obtained since the methods use different algorithms and different evaluation criteria. In top 50, 23 substances were found to be common (as shown in Table 73). In the COMMPS method, organic substances especially chlorinated ones were highlighted whereas metals and pesticides were ranked at the top places in the NORMAN method.

Therefore, the weighting factor approach was decided to be used in order to obtain a single ranking list by creating integrated score for each substance.

Table 73. Common Chemicals Found in Top 50 for the COMMPS and NORMAN Methods

Chemical Name	CAS No
Antimony	7440-36-0
Arsenic	7440-38-2
Atrazine-desethyl (Deethylatrazine)	6190-65-4
Carbendazim	10605-21-7
Chlorobenzilate	510-15-6
Chromium	7440-47-3
Cyfluthrin	68359-37-5
DDT (Total)	50-29-3
Dieldrin	60-57-1
Diflubenzuron	35367-38-5
Ethalfluralin	55283-68-6
Fenarimol	60168-88-9
Fenbutatin oxide	13356-08-6
Fenitrothion	122-14-5
Fenthion	55-38-9
PCB 153	35065-27-1
Permethrin	52645-53-1
Perylene	198-55-0
Polychlorinated biphenyls (PCBs)	1336-36-3
Prothiofos	34643-46-4
Quinalphos	13593-03-8
Triclosan	3380-34-5
Zinc	7440-66-6

In this approach, in order to obtain weighting factors, the two methods were compared and graded under three main headings which are

- Scope/Extent of the assessments (in terms of exposure, hazard and risk)
- Protectiveness of the methods
- Applicability of the methods

The details of the comparison and evaluation of the methods are explained in Table 74.

Table 74. Evaluation of the COMMPS and NORMAN Methods

Criteria	**Subcriteria**	**Indicators**	**COMMPS**	**NORMAN**
Scope/Extent of the assessments				
	Exposure			
		Modelling techniques	++++	++
		Monitoring techniques	+	+++
		Persistency	+	+++
		Bioaccumulation	++	+
		Long-range transport potential		+
	Hazard			
		Usage of the ecotoxicological data	+	+
		Inclusion of CMR effect	+	+
		Inclusion of ED property		+
		Consideration of other health effects		+

Table 74. Evaluation of the COMMPS and NORMAN Methods (cont'd)

Criteria	Subcriteria	Indicators	COMMPS	NORMAN
		Consideration of secondary poisoning and EQS in PNEC calculations		+
	Risk			
		Calculation of frequency of exceedance of the lowest PNEC		+
		Calculation of extent of exceedance of the lowest PNEC		+
Protectiveness of the methods				
	Consideration of the worst-case scenario			
		During environmental concentration calculation	+	++
		During environmental effect(PNEC) calculation	+	++
	Scoring in case of uncertainty or no data		++	+
Applicability of the methods				
	Feasibility			
		Simplicity	++	+

*Positive signs (+) were assigned in accordance with number of parameters that are considered for the evaluation of the criteria in each method as described in the following section.

Highlights in Table 74

Scope/Extent of the assessments

For exposure:

- Modelling techniques: COMMPS method includes distribution-degradation analysis of chemicals along with production/usage amounts and usage patterns data whereas NORMAN includes only production/usage amounts and use patterns of chemicals.
- Monitoring techniques: Surface water analysis is done in the COMMPS method. In the NORMAN method, appearance of a chemical both in surface water and groundwater are considered. Also, spatial and temporal distribution analyses of chemicals are done.
- Persistency: Biodegradability is considered for only modelling-based approach of the COMMPS method whereas half-lives of a chemical in water, sediment and air are regarded in the NORMAN Method.
- Bioaccumulation: In the COMMPS method, both $\log K_{ow}$ and BCF of chemicals are evaluated while only BCF of chemicals is evaluated for the scoring process in the NORMAN method.
- Long-range transport potential: Vapor pressure and/or half-life of chemicals in the air are evaluated only in the NORMAN method.

For hazard:

- Usage of ecotoxicological data: Both methods use these data.
- Inclusion of CMR effect: Both methods regard CMR effect via risk phrases (COMMPS method) or via research of CMR category (NORMAN method)
- Inclusion of ED property: Only NORMAN method considers ED effect.
- Consideration of other health effects: In the NORMAN method, non-standards toxicity indicators are also included for hazard assessment.
- Consideration of secondary poisoning and EQS in PNEC calculations: Only NORMAN method applies them.

For risk:

- Calculation of frequency of exceedance of the lowest PNEC: It is considered only in the NORMAN method.
- Calculation of extent of exceedance of the lowest PNEC: It is considered only in the NORMAN method.

Protectiveness of the methods

For consideration of the worst-case scenario:

- During environmental concentration calculation: 90^{th} percentile of average environmental concentrations of a substance at each monitoring point is calculated in the COMMPS method whereas 95^{th} percentile of maximum environmental concentrations of a substance at each monitoring point is calculated in the NORMAN method.
- During environmental effect (PNEC) calculation: The lowest chronic toxicity value (PNEC) is preferred in the COMMPS method while the lowest toxicity value (PNEC) among acute and chronic data is used in the NORMAN method along with consideration of sediment and biota compartments.

For scoring in case of uncertainty or no data: Higher score is assigned to be on the safe side in the COMMPS method.

Applicability of the methods

For feasibility:

- Simplicity: The NORMAN method is more complex in terms of applicability and data requirement.

As a result of the comparison and evaluation of the methods, the weighting factors of 0.4 and 0.6 were calculated for the COMMPS and NORMAN methods, respectively. Necessary calculations and determined weighting factors are shown in Table 75, and number of positive signs (+) used for the evaluation/grading of the methods (as indicated in Table 74) were considered.

Table 75. Weighting Factor Approach

Criteria	Subcriteria	Weight of importance*	COMMPS**	NORMAN**
Extent / Scope of the assessments		**0.5**		
	Exposure	0.33	8/18 (0.44)	10/18(0.56)
	Hazard	0.33	2/7 (0.29)	5/7 (0.71)
	Risk	0.34	0/2 (0)	2/2 (1)
Protectiveness of the methods		**0.34**		
	Consideration of worst case scenario	0.5	2/6 (0.33)	4/6 (0.67)
	Scoring in case of uncertainty or no data	0.5	2/3 (0.67)	1/3 (0.33)
Applicability of the methods		**0.16**		
	Feasibility	1	2/3 (0.67)	1/3 (0.33)
Weighting Factor* **			**0.4**	**0.6**

*Weight of importance values for each criterion were assigned and arranged in proportion to number of subcriteria. Equal weights are given to each subcriterion.
Scope/Extent of the assessments – 3 subcriteria
Protectiveness of the methods – 2 subcriteria
Applicability of the methods – 1 subcriterion
**Number of positive signs (+) in Table 74 were used and number of signs assigned in particular method for each subcriterion were divided by total number of signs for that subcriterion. (e.g. for exposure subcriterion NORMAN method received 10 signs out of 18).
****For COMMPS method*: 0.5 x (0.33x0.44 + 0.33x0.29 + 0.34x0) + 0.34 x (0.5x0.33 + 0.5x0.67) + 0.16 x (0.67) = 0.4, *For NORMAN method*: 0.5 x (0.33x0.56 + 0.33x0.71 + 0.34x1) + 0.34 x (0.5x0.67+ 0.5x0.33) + 0.16 x (0.33) = 0.6

If equal weights were given to each score and subscore, the weight of importance factors would be 0.48 and 0.52 for the COMMPS and NORMAN methods, respectively. In both cases, NORMAN method is more dominant over the total score.

For the calculation of the integrated score for each substance, firstly NORMAN scores were multiplied by 33.333 since the range of the scores are 0-3 for the NORMAN method and 0-100 for the COMMPS method. After the ranges had been equalized, the COMMPS and NORMAN scores were added up by multiplying determined weighting factors (0.4 and 0.6, respectively). Then, the integrated score was calculated for each substance, and substances were ranked depending on the values in order to determine river basin specific pollutants for Yesilirmak among 250 national specific pollutants.

As an example, calculations of the scores for arsenic and permethrin are given below.

For arsenic

- Calculation of the integrated score for arsenic (0-100):

Integrated score is obtained by using weighting factor approach (Equation (63)) after range of NORMAN and COMMPS scores have been equalized.

$$\textbf{Integrated Score} = \textbf{0.4} \times (\textbf{COMMPS Score}) + \textbf{0.6} \times (\textbf{33.333} \times \textbf{NORMAN Score}) \quad (63)$$

Integrated Score (for arsenic) $= 0.4 \times 45.885 + 0.6 \times (33.333 \times 2.073)$

Integrated Score (for arsenic) ≈ 59.82

For permethrin

- Calculation of the integrated score for permethrin (0-100):

Integrated score is obtained by using weighting factor approach (Equation (63)) after the range of NORMAN and COMMPS scores have been equalized.

$$\textbf{Integrated Score} = \textbf{0.4} \times (\textbf{COMMPS Score}) + \textbf{0.6} \times (\textbf{33.333} \times \textbf{NORMAN Score}) \quad (63)$$

Integrated Score (for permethrin) = $0.4 \times 41.477 + 0.6 \times (33.333 \times 1.469)$

Integrated Score (for permethrin) ≈ 46

Final ranking results of top 70 candidate substances for the identification of specific pollutants of the Yesilirmak River Basin are shown in Table 76. The complete list of the results by using weighting factor approach is given in APPENDIX E-Table 82.

Table 76. Final Ranking Results of the Weighting Factor Approach

RANK	***CHEMICAL NAME***	***COMMPS SCORE***	***NORMAN SCORE***	***INTEGRATED SCORE****
1	Arsenic	45.885	2.073	59.820
2	Chromium	37.892	1.893	53.023
3	Zinc	29.945	2.048	52.944
4	Antimony	45.589	1.610	50.433
5	Cobalt	27.504	1.877	48.534
6	DDT (Total)	36.765	1.681	48.330
7	Perylene	46.337	1.452	47.576
8	Fenarimol	61.076	1.096	46.356
9	Permethrin	41.477	1.469	45.965
10	Fenthion	40.833	1.404	44.416
11	Diflubenzuron	33.169	1.538	44.037
12	Endrin	28.337	1.626	43.855
13	Copper	20.333	1.768	43.500
14	Aluminium	17.846	1.772	42.571
15	Cyfluthrin	30.310	1.483	41.789
16	**Fenitrothion**	33.480	1.417	41.725
17	Vanadium	24.204	1.602	41.715
18	Chlorobenzilate	34.226	1.385	41.398
19	Silver	18.151	1.699	41.231
20	Prothiofos	39.530	1.245	40.719
21	**Dieldrin**	33.377	1.367	40.684
22	Iron	16.367	1.627	39.080
23	Ethalfluralin	43.557	1.078	38.986

Table 76. Final Ranking Results of the Weighting Factor Approach (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE**
24	Barium	18.340	1.577	38.869
25	Polychlorinated biphenyls (PCBs)	36.958	1.201	38.807
26	**Malathion**	26.122	1.392	38.282
27	Acetochlor	25.021	1.402	38.048
28	PCB 28	25.259	1.359	37.275
29	Atrazine-desethyl (Deethylatrazine)	33.281	1.197	37.249
30	**Triclosan**	30.577	1.233	36.897
31	**Quinalphos**	33.979	1.155	36.692
32	**Tris(nonylphenyl) phosphite; TNPP**	42.000	0.975	36.300
33	PCB 153	29.956	1.204	36.068
34	Diflufenican	27.617	1.246	35.963
35	PCB 180	27.649	1.243	35.916
36	**Fenbutatin oxide**	31.687	1.150	35.675
37	Pendimethalin	26.485	1.251	35.614
38	PCB 138	23.990	1.291	35.419
39	Diazinon	20.047	1.351	35.039
40	Carbendazim	31.980	1.094	34.662
41	**Oxadiazon**	33.544	1.058	34.584
42	4.4'-DDD	35.135	1.001	34.083
43	2-Chloronaphthalene	45.874	0.785	34.042
44	Carbofuran	23.370	1.234	34.035
45	Chlorothalonil	32.760	1.034	33.785
46	**Tolfenpyrad**	35.702	0.955	33.381
47	Fenpropathrin	26.411	1.134	33.252
48	Benzo[*e*]pyrene	31.963	1.013	33.040
49	PCB 52	24.402	1.145	32.662
50	4.4'-DDE	24.904	1.126	32.479
51	**Propetamphos**	29.125	1.025	32.150
52	Boron	13.264	1.341	32.124
53	**Phenthoate**	28.326	1.030	31.930

Table 76. Final Ranking Results of the Weighting Factor Approach (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE**
54	Trifloxystrobin	28.091	1.034	31.924
55	**Pyridaben**	33.979	0.908	31.758
56	Phenanthrene	27.672	1.032	31.712
57	**Chlordane**	25.364	1.067	31.479
58	**4.5-dichloro-2-octyl-2H-isothiazol-3-on; DCOIT**	33.979	0.875	31.092
59	Silicon	13.333	1.285	31.033
60	4-Chloroaniline	25.858	1.028	30.902
61	**Methomyl**	19.052	1.155	30.721
62	Azinphos-methyl	22.939	1.076	30.696
63	**Clofibric acid**	35.035	0.825	30.514
64	**Pirimicarb**	19.919	1.117	30.301
65	Methidathion	22.123	1.064	30.119
66	Fenpropimorph	40.351	0.699	30.119
67	Lindane	28.341	0.939	30.107
68	**Prometryn**	15.682	1.192	30.106
69	1.4-Dichlorobenzene	26.678	0.968	30.025
70	Cadusafos	22.086	1.059	30.022

*Integrated score= 0.4 x (COMMPS score) + 0.6 x (33.333 x NORMAN score)

Since NORMAN scores are more dominant over the total integrated scores, metals and pesticides were observed to be at the top places.

As a result of analysis of the distribution of the scores (as indicated in Figure 7), it was seen that curve of the graph decreases exponentially until the score of 30. Then, there is a relatively rapid and nearly linear decline after the score of 30 out of 100. Therefore, 70 substances which exceeded the score of 30 were determined as high priority pollutants for the Yesilirmak River Basin. Substances which were detected but not quantified in any monitoring period indicated in bold font. They should be reconsidered by performing modelling-based prioritization approach

based on amount of usage/production and usage pattern data of chemicals. In order to obtain more reasonable and feasible number by considering studies of other EU member states related to identification of river basin specific pollutants, non-quantified chemicals among 70 high priority pollutants were excluded. As a result, 52 water phase relevant specific pollutants were proposed for the Yesilirmak River Basin to be monitored periodically instead of monitoring all 250 national specific pollutants of Turkey.

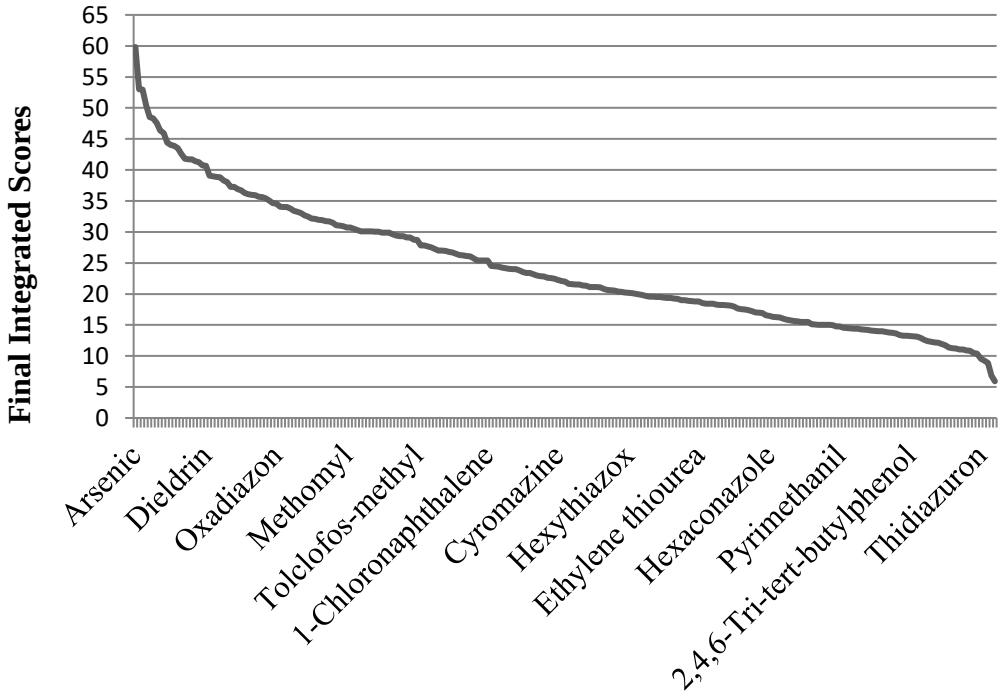

Figure 7. Distribution of the Integrated Scores

Moreover, a sensitivity analysis was done by giving equal weighting factors for each method (0.5 for COMMPS and 0.5 for NORMAN prioritization methods) since the weighting factor approach includes some subjectivity. Candidate substances were again scored and ranked for comparison. It was seen that a similar pattern was observed with small changes (as shown in APPENDIX F-

Table 83). Unlike the previous approach; silicon, methomyl, pirimicarb, methidathion, prometryn, cadusafos were not included among 70 high priority pollutants. Instead of them, musk xylene, pyriproxyfen, triflumuron, bis (2-ethylhexyl) terephthalate, PCB 101 and parathion-methyl took part. The rest was same.

4.4. Uncertainties and Recommendations

Uncertainties about monitoring results due to the inadequacy of the analytical methods can cause mistakes during exposure assessment. Therefore, there is a need to improve existing analytical methods. Within the scope of the WFD, since monitoring is a legal necessity, more accurate and sensitive analytical techniques are required for water quality management. The analytical methods advanced have to fulfill technical specifications related to monitoring of environmental compartments and chemical analysis as declared in Commission Directive 2009/90/EC. It must be ensured that 30% of the relevant EQS value is equal or exceeded by the LOQ value of the analytical techniques and uncertainty of the results is 50% or below the predicted EQS with 95% confidence level (coverage factor of 2) in order to make comparison results more accurate (EC, 2009).

Uncertainties about effect (toxicity) data can cause mistakes during hazard assessment since higher assessment factors are used. This results in relatively low threshold values such as PNEC and EQS (Casado-Martinez et al., 2018). Therefore, deficiencies should be eliminated. In addition, the presence of different toxicity values (belonging to same chemical substances) reported in different databases affects ranking results depending on the selection of different data.

The existence of any degradation by-products or products of the parent chemicals should be researched since these products can be more dangerous than parent chemicals and they should be included in the monitoring studies.

Sediment monitoring studies (especially for hydrophobic substances) should also be carried out since it offers to see and interpret long-term anthropogenic effects.

Performing prioritization procedure with long-term monitoring data enables to see the big picture of fluctuations of concentration data. As a result of the stabilization of concentration data for related chemicals, more accurate and realistic results can be obtained.

Using weighting factor approach can lead to different results depending on the magnitude of coefficients determined as a result of the evaluations and judgments. However, instead of application of one method, combination/integration of different methods can be more realistic and reliable since different methods put emphasis on different aspects. In order to increase reliability and decrease uncertainty, sensitivity analysis can be done as another option. The results can be compared and interpreted in the stage of final decision about selection of river basin specific pollutants.

CHAPTER 5

CONCLUSION

As a requirement of the EU WFD (2000/60/EC) and as a part of river basin management plans, substances posing a relatively higher risk to the environment and human health in each river basin, so called river basin specific pollutants, must be identified and controlled to achieve good (ecological) water status. In Turkey, 250 substances and group of substances were identified as national river basin specific pollutants by the Ministry of Agriculture and Forestry (The General Directorate of Water Management) in 2016. However, depending on industrial and agricultural profile, there is a need to identify specific pollutants for each river basin by choosing environmentally relevant chemicals. By this means, waste of resources (time, workforce and budget) will be prevented in terms of monitoring/auditing and risk assessment works. Within this scope, specific pollutants of the Yesilirmak River Basin were identified by using the COMMPS and NORMAN prioritization methods in this study.

The studies carried out and the data used in this thesis are summarized as noted below:

- A set of 1.5-year surface water quality monitoring data which was obtained from 42 monitoring points from the basin between years of August 2016 and January 2018 were used.

- National 250 specific pollutants of Turkey were selected as candidate substances. The EU suggested COMMPS and NORMAN prioritization methods were separately applied to score and rank the chemicals and to identify most relevant chemicals for the Yesilirmak River Basin.

- As there were differences in the ranking patterns of the candidate substances by the COMMPS and NORMAN methods, COMMPS and NORMAN scores were combined for each substance by using weighting factor approach in order to obtain a single ranking list. In selecting weighting factors to use, the two methods were compared and graded in terms of the extent of the exposure-hazard-risk assessments, protectiveness and applicability of the methods. Candidate substances were scored and ranked again according to these integrated scores created.

The following conclusions were drawn based on the outputs of the study:

- By analyzing the distribution of the integrated scores, 70 dangerous substances with scores exceeding the arbitrarily selected integrated score of 30 were determined as high priority pollutants for the Yesilirmak River Basin (as shown in Table 76). Pollutants indicated in bold font represent pollutants that were detected but not quantified in any of the monitoring periods. They were included in the ranking/prioritization procedure by taking their concentrations as LOD/ 2. They require a review via modelling-based approaches by using amount of usage and use pattern data. In order to obtain more reasonable and feasible number by considering studies of other EU member states related to identification of river basin specific pollutants, non-quantified chemicals (in any of the monitoring periods) among 70 high priority pollutants were excluded. As a result, 52 water phase relevant specific pollutants were proposed for the Yesilirmak River Basin (as shown in Table 77).

- Since the weighting factor approach includes some subjectivity, a sensitivity analysis was also done by giving equal weights for each method. It was observed that 64 substances were same out of 70 determined high priority substances. Besides, (as a difference) silicon, methomyl, pirimicarb, methidathion, prometryn, cadusafos were found in the top 70 instead of musk xylene, pyriproxyfen, triflumuron, bis (2-ethylhexyl) terephthalate, PCB 101 and parathion-methyl. These additional substances can also be regarded.

❖ As a requirement of the EU WFD, instead of monitoring all 250 national specific pollutants of Turkey, monitoring 52 proposed specific pollutants in the Yesilirmak River Basin will make auditing works easy. Moreover, thanks to prioritization and ranking processes, much higher efforts will be made for hazardous substances posing relatively higher risk and ranking at the top places in terms of their control at the sources or wastewater treatment plants.

Table 77. Proposed Specific Pollutants for the Yesilirmak River Basin

Proposed specific pollutants	**CAS No**	**EC No**
Arsenic	7440-38-2	231-148-6
Chromium	7440-47-3	231-157-5
Zinc	7440-66-6	231-175-3
Antimony	7440-36-0	231-146-5
Cobalt	7440-48-4	231-158-0
DDT (Total)	50-29-3	200-024-3
Perylene	198-55-0	205-900-9
Fenarimol	60168-88-9	262-095-7
Permethrin	52645-53-1	258-067-9
Fenthion	55-38-9	200-231-9
Diflubenzuron	35367-38-5	252-529-3
Endrin	72-20-8	200-775-7
Copper	7440-50-8	231-159-6
Aluminium	7429-90-5	231-072-3
Cyfluthrin	68359-37-5	269-855-7
Vanadium	7440-62-2	231-171-1
Chlorobenzilate	510-15-6	208-110-2
Silver	7440-22-4	231-131-3
Prothiofos	34643-46-4	252-125-7
Barium	7440-39-3	231-149-1
Iron	7439-89-6	231-096-4

Table 77. Proposed Specific Pollutants for the Yesilirmak River Basin (cont'd)

Proposed specific pollutants	CAS No	EC No
Ethalfluralin	55283-68-6	259-564-3
Polychlorinated biphenyls (PCBs)	1336-36-3	215-648-1
Acetochlor	34256-82-1	251-899-3
PCB 28	7012-37-5	n.a.
Atrazine-desethyl (Deethylatrazine)	6190-65-4	n.a.
PCB 153	35065-27-1	n.a.
Diflufenican	83164-33-4	617-446-2
PCB 180	35065-29-3	n.a.
Pendimethalin	40487-42-1	254-938-2
PCB 138	35065-28-2	n.a.
Diazinon	333-41-5	206-373-8
Carbendazim	10605-21-7	234-323-0
4,4'-DDD	72-54-8	200-783-0
2-Chloronaphthalene	91-58-7	202-079-9
Carbofuran	1563-66-2	216-353-0
Chlorothalonil	1897-45-6	217-588-1
Fenpropathrin	39515-41-8	254-485-0
Benzo[*e*]pyrene	192-97-2	205-892-7
PCB 52	35693-99-3	n.a.
4,4'-DDE	72-55-9	200-784-6
Boron	7440-42-8	231-151-2
Trifloxystrobin	141517-21-7	604-237-6
Phenanthrene	85-01-8	201-581-5
Silicon	7440-21-3	231-130-8
4-Chloroaniline	106-47-8	203-401-0
Azinphos-methyl	86-50-0	201-676-1
Methidathion	950-37-8	213-449-4
Fenpropimorph	67564-91-4	266-719-9

Table 77. Proposed Specific Pollutants for the Yesilirmak River Basin (cont'd)

Proposed specific pollutants	CAS No	EC No
Lindane	58-89-9	210-168-9
1,4-Dichlorobenzene	106-46-7	203-400-5
Cadusafos	95465-99-9	619-129-4

CHAPTER 6

RECOMMENDATIONS FOR FUTURE STUDIES

It is expected that following recommendations will help to make significant improvements in the identification of river basin specific pollutants:

- The Ministry of Forestry and Agriculture should have a comprehensive database including physicochemical and toxicological properties of chemical substances in order to be used in the identification of specific pollutants for all river basins of Turkey.

- To obtain more reliable and realistic results from the identification of river basin specific pollutants, water quality monitoring programs should be continued as required by WFD.

- Amount of usage and use pattern of chemicals should be reported regularly to be used for modelling-based prioritization approaches and for interpretation of chemicals which are detected but not quantified as exact values because of insufficiency of analytical methods.

- Apart from a ranking of water phase relevant specific pollutants, sediment phase relevant substances should be also prioritized by performing complementary approach because of the affinity of particular substances to partition into sediment phase due to hydrophobic characteristics. For this purpose, monitoring of sediment phase should be carried out

- Analytical methods must be improved since some of the emerging pollutants exist at very low concentrations, and they are hazardous and pose risk to the environment and human health.

- Deficiencies in effect (toxicity) data should be eliminated. Otherwise, the usage of high assessment factor will lead to relatively low PNEC and EQS values.

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APPENDICES

APPENDIX A

CONCENTRATIONS OF THE NATIONAL 250 SPECIFIC POLLUTANTS OF TURKEY IN THE YESILIRMAK RIVER BASIN

Table 78. Concentrations of the Candidate Substances in the Basin

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
1,1-dichloroethane	75-34-3	0.188	1.237
1,2,4,5-tetrachlorobenzene	95-94-3	0.003	0.003
1,2,4-Trimethylbenzene	95-63-6	0.050	0.050
1,3,5-trimethylbenzene (Mesitylene)	108-67-8	0.050	0.050
1,3-Dichlorobenzene	541-73-1	0.058	0.110
1,4-Dichlorobenzene	106-46-7	0.060	0.130
17 alpha Ethinyl Estradiol	57-63-6	0.050	0.050
17 beta Estradiol	50-28-2	0.013	0.013
1-chloro-2,4-dinitrobenzene	97-00-7	0.011	0.050
1-Chloronaphthalene	90-13-1	0.818	6.530
1-Methylnaphthalene	90-12-0	0.038	0.784
2,3,4,5,6-Pentachlorotoluene	877-11-2	0.050	0.050
2,4,6-Tri-tert-butylphenol	732-26-3	0.001	0.001
2,6-Di-*tert*-butylphenol	128-39-2	0.008	0.070
2,6-Xylenol	576-26-1	1.044	8.605
2-Amino-4-chlorophenol	95-85-2	0.050	0.050
2-Chloronaphthalene	91-58-7	0.866	6.910
3,6-dimethylphenanthrene	1576-67-6	0.008	0.077

Table 78. Concentrations of the Candidate Substances in the Basin (cont'd)

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
4,4'-DDD	72-54-8	0.005	0.036
4,4'-Dibromodiphenyl Ether	2050-47-7	0.002	0.002
4,5-dichloro-2-octyl-2H-isothiazol-3-on; DCOIT	64359-81-5	0.025	0.025
4-Aminoazobenzene	60-09-3	0.050	0.050
4-Chloro-3-methylphenol	59-50-7	0.015	0.195
4-Chloroaniline	106-47-8	0.006	0.026
Aldrin	309-00-2	0.003	0.003
Aluminium	7429-90-5	674.802	5681.882
Antimony	7440-36-0	20.888	65.937
Arsenic	7440-38-2	23.314	51.289
Acenaphthene	83-32-9	0.004	0.031
Acetochlor	34256-82-1	0.050	0.072
Azinphos-methyl	86-50-0	0.030	0.064
Copper	7440-50-8	27.525	154.548
Barium	7440-39-3	91.086	222.720
Benzyl benzoate	120-51-4	0.068	0.592
Benzyl butyl phthalate	85-68-7	0.005	0.029
Benzo(a)fluorene	238-84-6	0.001	0.001
Benzo[*e*]pyrene	192-97-2	0.003	0.123
Beryllium	7440-41-7	0.055	0.293
Biphenyl	92-52-4	0.010	0.286
Bis(2-ethylhexyl) terephthalate	6422-86-2	0.075	6.052
Bisphenol A	80-05-7	0.010	0.088
Boron	7440-42-8	358.984	905.559
Bromide	7726-95-6	Excluded	Excluded
Zinc	7440-66-6	97.315	458.608
DDT (Total)	50-29-3	0.004	0.017
Decamethylcyclopentasiloxane	541-02-6	0.001	0.813
Demeton	8065-48-3	0.005	0.005
Iron	7439-89-6	1067.180	6576.703
Diazinon	333-41-5	0.005	0.027

Table 78. Concentrations of the Candidate Substances in the Basin (cont'd)

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
Dibutyl phthalate (DBP)	84-74-2	0.030	0.275
Dibutyltin oxide	818-08-6	0.005	0.005
Dieldrin	60-57-1	0.003	0.003
Diethyl phthalate	84-66-2	0.083	1.255
Diphenyl ether (Diphenyl oxide)	101-84-8	0.873	25.848
Diphenylamine	122-39-4	0.001	0.013
Diisobutyl adipate	141-04-8	0.026	0.213
Diclofenac	15307-79-6	0.097	0.429
Dioctyl Phthalate	117-84-0	0.098	0.747
EDTA**	60-00-4	-	-
Endrin	72-20-8	0.007	0.040
Ethylene thiourea	96-45-7	0.113	0.202
Phenanthrene	85-01-8	0.029	0.296
Fenitrothion	122-14-5	0.250	0.250
Fenthion	55-38-9	0.073	0.408
Fluorene	86-73-7	0.009	0.097
Silver	7440-22-4	0.217	1.968
Isopropylbenzene, cumene	98-82-8	0.050	0.050
Isodrin	465-73-6	0.002	0.013
Tin	7440-31-5	13.280	46.952
Carbon tetrachloride	56-23-5	0.050	0.050
Clofibric acid	882-09-7	0.750	0.750
Chloroacetic acid	79-11-8	0.025	0.025
Chlorothalonil	1897-45-6	0.063	0.621
Cobalt	7440-48-4	2.311	31.165
Chrysene	218-01-9	0.002	0.010
Chromium	7440-47-3	5.996	16.880
Meta-xylene	108-38-3	0.070	0.253
Ortho-xylene	95-47-6	0.050	0.050
Musk xylene	81-15-2	0.050	0.050
Linuron	330-55-2	0.010	0.010
2-Mercaptobenzothiazole	149-30-4	0.034	0.272

Table 78. Concentrations of the Candidate Substances in the Basin (cont'd)

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
N,N,N',N'-tetramethyl-4,4'-methylenedianiline (Michler's base)	101-61-1	0.003	0.003
Butyltin Trichloride	1118-46-3	0.006	0.026
Nitrobenzene	98-95-3	0.555	14.280
p-(1,1-dimethylpropyl)phenol	80-46-6	0.035	8.498
Polychlorinated biphenyls (PCBs)	1336-36-3	0.010	0.058
PCB 101	37680-73-2	0.003	0.003
PCB 138	35065-28-2	0.001	0.021
PCB 153	35065-27-1	0.002	0.016
PCB 180	35065-29-3	0.003	0.021
PCB 28	7012-37-5	0.001	0.010
PCB 31	16606-02-3	0.001	0.001
PCB 52	35693-99-3	0.001	0.004
Perylene	198-55-0	0.021	0.132
Permethrin	52645-53-1	0.072	0.540
Total petroleum hydrocarbons (TPH)	n.a.	Excluded	Excluded
Pyrene	129-00-0	0.005	0.044
Pyriproxyfen	95737-68-1	0.010	0.010
Prochloraz	67747-09-5	0.025	0.025
Propetamphos	31218-83-4	0.025	0.025
Propylbenzene	103-65-1	0.050	0.050
Free Cyanide	57-12-5	Excluded	Excluded
Silicon	7440-21-3	9915.740	19682.500
Styrene; Vinylbenzene	100-42-5	0.050	0.050
Sulfamethoxazole	723-46-6	0.073	0.545
Tert-butyl-4-methoxyphenol**	25013-16-5	-	-
Tetrabromobisphenol A (TBBP-A)	79-94-7	0.050	0.050
Titanium	7440-32-6	11.104	80.468
Triadimenol	55219-65-3	0.050	0.050

Table 78. Concentrations of the Candidate Substances in the Basin (cont'd)

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
Tribromobiphenyl ether	49690-94-0	0.002	0.002
Tributyl phosphate	126-73-8	0.001	0.001
Tridecane	629-50-5	0.056	4.343
Triphenyltin; Fentin	668-34-8	0.000	0.000
Trichloroethylene (TRI)	79-01-6	0.050	0.050
Triclosan	3380-34-5	0.050	0.050
Tris(nonylphenyl) phosphite; TNPP	26523-78-4	0.750	0.750
Vanadium	7440-62-2	7.909	24.213
2,4,5-Trichlorophenoxyacetic acid	93-76-5	0.250	0.250
2,4-D, isooctyl ester	25168-26-7	0.100	0.100
2,4-Dichlorophenoxyacetic acid	94-75-7	0.013	0.013
2-Methyl-4,6-dinitrophenol	534-52-1	0.025	0.025
Acetamiprid	135410-20-7	0.025	0.025
Atrazine-desethyl (Deethylatrazine)	6190-65-4	0.217	0.940
Azoxystrobin	131860-33-8	0.032	0.077
Bentazon	25057-89-0	0.025	0.025
Lindane	58-89-9	0.004	0.027
Boscalid	188425-85-6	0.020	0.020
Bromophos-ethyl	4824-78-6	0.001	0.001
Bromophos-methyl	2104-96-3	0.001	0.001
Bromopropylate	18181-80-1	0.005	0.005
Bromoxynil	1689-84-5	0.025	0.025
Buprofezin	69327-76-0	0.054	0.322
Butralin	33629-47-9	0.025	0.025
Cadusafos	95465-99-9	0.006	0.015
Captan	133-06-2	0.051	0.402
Carbaryl	63-25-2	0.007	0.018
Carbendazim	10605-21-7	0.058	0.718
Carbofuran	1563-66-2	0.060	0.133

Table 78. Concentrations of the Candidate Substances in the Basin (cont'd)

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
Carboxin (Vitavax)	5234-68-4	0.025	0.025
Chlorantraniliprole	500008-45-7	0.025	0.025
Chlorobenzilate	510-15-6	0.341	0.977
Chlordane	57-74-9	0.003	0.003
Chlorfenapyr	122453-73-0	0.008	0.044
Chloridazon, pyrazon	1698-60-8	0.047	0.315
Chlorsulfuron	64902-72-3	0.015	0.073
Clofentezine	74115-24-5	0.005	0.005
Clopyralid	1702-17-6	0.008	0.056
Clothianidin	210880-92-5	0.032	0.079
Cyclanilide	113136-77-9	0.250	0.250
Cyfluthrin	68359-37-5	0.034	0.390
Cyprodinil	121552-61-2	0.007	0.015
Cyromazine	66215-27-8	0.062	0.212
4,4'-DDE	72-55-9	0.001	0.001
Dichlobenil	1194-65-6	0.003	0.003
Diethofencarb	87130-20-9	0.025	0.025
Difenoconazole	119446-68-3	0.025	0.025
Diflubenzuron	35367-38-5	0.074	1.628
Diflufenican	83164-33-4	0.012	0.060
Dimethenamid	87674-68-8	0.005	0.005
Dimethoate	60-51-5	0.029	0.394
Dimethomorph	110488-70-5	0.005	0.005
Dimethylaminosulfanilide	4710-17-2	0.020	0.020
Dinobuton	973-21-7	0.005	0.005
Epoxiconazole	133855-98-8	0.016	0.324
Ethalfluralin	55283-68-6	0.196	3.107
Ethofumesate	26225-79-6	0.025	0.025
Ethoprophos	13194-48-4	0.025	0.025
Fenamiphos	22224-92-6	0.005	0.005
Fenarimol	60168-88-9	39.409	315.093
Fenbutatin oxide	13356-08-6	0.050	0.050

Table 78. Concentrations of the Candidate Substances in the Basin (cont'd)

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
Fenhexamid	126833-17-8	0.020	0.020
Fenpropathrin	39515-41-8	0.012	0.061
Fenpropimorph	67564-91-4	0.271	1.819
Fluazifop-P-butyl	79241-46-6	0.025	0.025
Fludioxonil	131341-86-1	0.025	0.025
Fluopyram	658066-35-4	0.005	0.005
Fluquinconazole	136426-54-5	0.013	0.013
Fluroxypyr	69377-81-7	0.108	0.868
Flutolanil	66332-96-5	0.025	0.025
Flutriafol	76674-21-0	0.069	1.976
Fosetyl-al	39148-24-8	0.085	0.296
Fosthiazate	98886-44-3	0.003	0.003
Hexaconazole	79983-71-4	0.023	0.044
Hexythiazox	78587-05-0	0.025	0.025
Imazalil	35554-44-0	0.013	0.031
Imazapyr	81334-34-1	0.020	0.020
Imidacloprid	138261-41-3	0.027	0.671
Lenacil	2164-08-1	0.025	0.130
Malathion	121-75-5	0.050	0.050
Mandipropamid	374726-62-2	0.025	0.025
Mepiquat Chloride	24307-26-4	3.450	27.428
Mesotrione	104206-82-8	0.034	0.138
Metalaxyl	57837-19-1	0.020	0.142
Metam Potassium	137-41-7	0.064	0.162
Metamitron	41394-05-2	0.035	0.077
Metazachlor	67129-08-2	0.025	0.025
Methamidophos	10265-92-6	0.005	0.005
Methidathion	950-37-8	0.032	0.078
Methomyl	16752-77-5	0.025	0.025
Methoxyfenozide	161050-58-4	0.050	0.050
Metolachlor	51218-45-2	0.038	0.129
Metrafenone	220899-03-6	0.223	1.749

Table 78. Concentrations of the Candidate Substances in the Basin (cont'd)

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
Molinate	2212-67-1	0.032	0.073
Monocrotophos	6923-22-4	0.028	0.051
Myclobutanil	88671-89-0	0.063	0.363
Nicosulfuron	111991-09-4	0.019	0.081
Nitrofen	1836-75-5	0.005	0.005
Omethoate	1113-02-6	0.010	0.010
Oxadiazon	19666-30-9	0.025	0.025
Oxadixyl	77732-09-3	0.025	0.025
Parathion-methyl	298-00-0	0.018	0.110
Penconazole	66246-88-6	0.013	0.034
Pendimethalin	40487-42-1	0.035	0.105
Phenthoate	2597-03-7	0.025	0.025
Picloram	1918-02-1	0.086	0.509
Piperonyl butoxide	51-03-6	0.035	0.355
Pirimicarb	23103-98-2	0.025	0.025
Procymidone	32809-16-8	0.015	0.082
Prometryn	7287-19-6	0.025	0.025
Propamocarb Hydrochloride	25606-41-1	0.005	0.023
Propazine	139-40-2	0.005	0.005
Propham	122-42-9	0.039	0.138
Propiconazole	60207-90-1	0.020	0.020
Propyzamide	23950-58-5	0.025	0.025
Prothiofos	34643-46-4	0.071	4.161
Pyraclostrobin	175013-18-0	0.025	0.025
Pyridaben	96489-71-3	0.025	0.025
Pyrimethanil	53112-28-0	0.013	0.033
Quinalphos	13593-03-8	0.025	0.025
Quizalofop-p-ethyl	100646-51-3	0.025	0.025
Spiroxamine	118134-30-8	0.025	0.025
Tebuconazole	107534-96-3	0.035	0.214
Tebuthiuron	34014-18-1	0.025	0.025
Tecnazene	117-18-0	0.005	0.005

Table 78. Concentrations of the Candidate Substances in the Basin (cont'd)

CHEMICAL NAME	CAS NO	Avg EC_{90}*	MEC_{95}*
Tefluthrin	79538-32-2	0.005	0.005
Terbuthylazine	5915-41-3	0.025	0.025
Thiabendazole	148-79-8	0.005	0.005
Thiacloprid	111988-49-9	0.050	0.228
Thiamethoxam	153719-23-4	0.006	0.042
Thidiazuron	51707-55-2	0.050	0.050
Thiometon	640-15-3	0.005	0.005
Thiophanate-methyl	23564-05-8	0.005	0.005
Tolclofos-methyl	57018-04-9	0.250	0.250
Tolfenpyrad	129558-76-5	0.025	0.025
Triasulfuron	82097-50-5	0.005	0.005
Tribenuron-methyl	101200-48-0	0.020	0.020
Trifloxystrobin	141517-21-7	0.057	0.285
Triflumuron	64628-44-0	0.025	0.025
Trinexapac-ethyl	95266-40-3	0.010	0.073
Vinclozolin	50471-44-8	0.005	0.005

*90^{th} percentile of average environmental concentrations of each monitoring point was used for exposure calculations in the COMMPS method. And, 95^{th} percentile of maximum environmental concentrations at each monitoring point was used for exposure/risk calculations in the NORMAN method.

**Not measured

***Chemicals which were detected but not quantified in any of the monitoring periods are indicated in bold font. They were included in the ranking/prioritization procedure by taking their concentrations as LOD/ 2.

APPENDIX B

LOCATIONS OF THE MONITORING STATIONS IN THE YESILIRMAK RIVER BASIN

Table 79. Locations of the Monitoring Stations

ID	Locations	N	E
YESIL-1	Ozbeyli-Kose-Gumushane	40° 11' 27" N	39° 42' 41" E
YESIL -2	Baspinar-Kelkit-Gumushane	40° 06' 29" N	39° 17' 57" E
YESIL -3	Bayir-Camoluk-Giresun	40° 08' 15" N	38° 33' 18" E
YESIL -4	Erentepe-Sebinkarahisar-Giresun	40° 13' 22" N	38° 23' 57" E
YESIL -5	Kilicpinari-Koyuluhisar-Sivas	40° 13' 35" N	38° 01' 20" E
YESIL -6	Derekoy-Zara-Sivas	40° 07' 44" N	37° 45' 12" E
YESIL -7	Karsikent-Resadiye-Tokat	40° 22' 56" N	37° 21' 25" E
YESIL -8	Resadiye-Tokat	40° 23' 22" N	37° 19' 56" E
YESIL -9	Cayirpinar- Resadiye-Tokat	40° 24' 04" N	37° 17' 37" E
YESIL-10	Muhtarduzu-Niksar-Tokat	40° 26' 58" N	37° 04' 36" E
YESIL-11	Bakisli-Merkez-Tokat	40° 21' 01" N	36° 37' 42" E
YESIL-12	Kinik-Almus-Tokat	40° 20' 16" N	36° 53' 30" E
YESIL-13	Gumeleonu-Almus-Tokat	40° 18' 42" N	37° 07' 34" E
YESIL-14	Pazar-Tokat	40° 17' 32" N	36° 16' 57" E
YESIL-15	Kesikkopru-Saraykent-Yozgat	39° 55' 02" N	35° 38' 47" E
YESIL-16	Sulusaray-Yozgat	39° 59' 45" N	36° 04' 16" E
YESIL-17	Turhal-Tokat	40° 22' 44" N	36° 05' 20" E
YESIL-18	Sutluce- Turhal-Tokat	40° 24' 57" N	36° 05' 56" E
YESIL-19	Helvaci-Merkez-Amasya	40° 37' 09" N	35° 48' 41" E
YESIL-20	Gollubaglari-Merkez-Amasya	40° 40' 34" N	35° 50' 03" E
YESIL-21	Kuyubasi- Merkez-Amasya	40° 33' 48" N	35° 45' 41" E
YESIL-22	Kutu- Merkez-Amasya	40° 31' 49" N	35° 38' 21" E

Table 79. Locations of the Monitoring Stations (cont'd)

ID	Locations	N	E
YESIL-23	Bekdemir-Goynucek-Amasya	40° 28' 05" N	35° 34' 41" E
YESIL-24	Seyhoglu- Goynucek-Amasya	40° 27' 05" N	35° 25' 01" E
YESIL-25	Baliyakup-Merkez-Corum	40° 22' 43" N	35° 03' 27" E
YESIL-26	Corakbucagi- Merkez-Corum	40° 20' 23" N	35° 03' 50" E
YESIL-27	Kazankaya-Aydincik-Yozgat	40° 13' 37" N	35° 19' 37" E
YESIL-28	Kochisar-Alaca-Corum	40° 06' 20" N	34° 56' 30" E
YESIL-29	Evcikuzkusla-Merkez-Corum	40° 23' 12" N	34° 38' 21" E
YESIL-30	Uctutlar- Merkez-Corum	40° 34' 25" N	34° 58' 29" E
YESIL-31	Cayirozu-Merzifon-Amasya	40° 46' 49" N	35° 29' 33" E
YESIL-32	Kulu-Suluova-Amasya	40° 45' 55" N	35° 37' 26" E
YESIL-33	Kuzgece-Merkez-Amasya	40° 44' 56" N	36° 01' 27" E
YESIL-34	Dutluk-Tasova-Amasya	40° 44' 29" N	36° 16' 03" E
YESIL-35	Cilkidir-Tasova-Amasya	40° 44' 45" N	36° 21' 44" E
YESIL-36	Kalekoy-Erbaa-Tokat	40° 46' 06" N	36° 30' 44" E
YESIL-37	Catili- Erbaa-Tokat	40° 42' 11" N	36° 34' 31" E
YESIL-38	**CANCELLED**		
YESIL-39	Kumbetli-Niksar-Tokat	40° 42' 09" N	36° 41' 59" E
YESIL-40	Mazlumoglu-Ladik-Samsun	40° 55' 13" N	36° 01' 16" E
YESIL-41	Ilkadim-Samsun	41° 16' 14" N	36° 20' 42" E
YESIL-42	Irmaksirti-Carsamba-Samsun	41° 13' 43" N	36° 35' 11" E
YESIL-43	Carsamba-Samsun	41° 12' 23" N	36° 43' 35" E

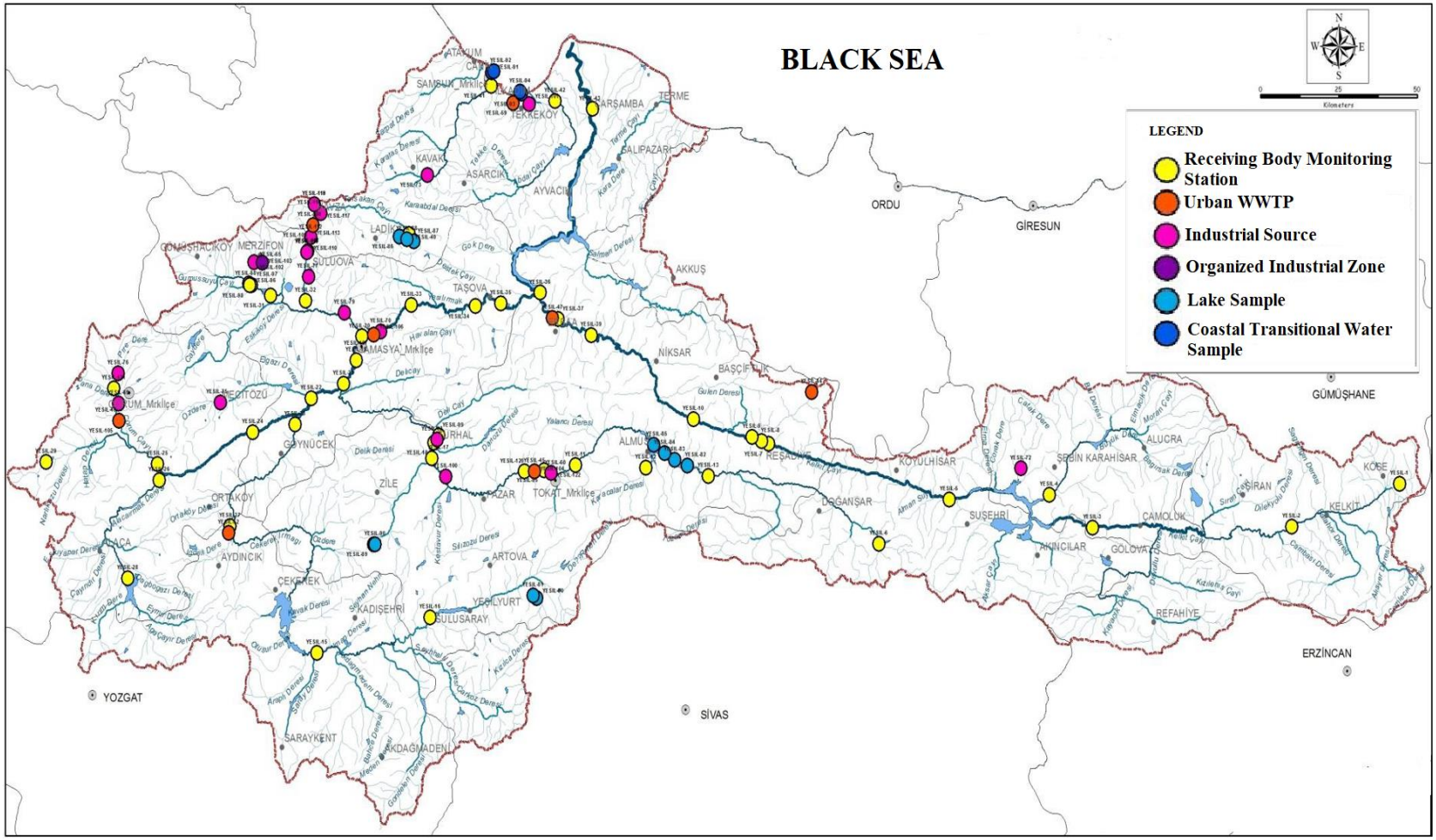

Figure 8. Locations of the Monitoring Stations on the Map of the Yesilirmak River Basin

APPENDIX C

RANKING RESULTS OF THE COMMPS METHOD

Table 80. Complete List of the COMMPS Ranking Results

RANK	***CHEMICAL NAME***	***EXPOSURE SCORE***	***EFFECT SCORE***	***COMMPS SCORE****
1	Fenarimol	9.422	6.482	61.076
2	Perylene	4.743	9.770	46.337
3	Arsenic	7.666	5.985	45.885
4	2-Chloronaphthalene	7.054	6.504	45.874
5	Antimony	7.547	6.041	45.589
6	Ethalfluralin	6.132	7.104	43.557
7	**Tris(nonylphenyl) phosphite; TNPP**	6.964	6.031	42.000
8	Permethrin	5.509	7.528	41.477
9	Fenthion	5.518	7.400	40.833
10	Fenpropimorph	6.333	6.371	40.351
11	**2-Amino-4-chlorophenol**	5.284	7.628	40.306
12	Prothiofos	5.505	7.181	39.530
13	Chromium	6.192	6.119	37.892
14	Polychlorinated biphenyls (PCBs)	4.312	8.571	36.958
15	DDT (Total)	3.761	9.776	36.765
16	**Butralin**	4.854	7.571	36.753
17	Tridecane	5.357	6.786	36.355
18	**2.4-D. isooctyl ester**	5.714	6.356	36.322
19	Metam Potassium	5.437	6.671	36.274
20	**Tolfenpyrad**	4.854	7.355	35.702
21	4.4'-DDD	3.853	9.118	35.135

Table 80. Complete List of the COMMPS Ranking Results (cont'd)

RANK	***CHEMICAL NAME***	***EXPOSURE SCORE***	***EFFECT SCORE***	***COMMPS SCORE****
22	**Clofibric acid**	6.964	5.031	35.035
23	Chlorobenzilate	6.475	5.286	34.226
24	**4.5-dichloro-2-octyl-2H-isothiazol-3-on; DCOIT**	4.854	7.000	33.979
25	**Pyridaben**	4.854	7.000	33.979
26	**Quinalphos**	4.854	7.000	33.979
27	**Oxadiazon**	4.854	6.910	33.544
28	**Fenitrothion**	6.283	5.329	33.480
29	**Dieldrin**	3.426	9.743	33.377
30	Atrazine-desethyl (Deethylatrazine)	6.196	5.371	33.281
31	Diflubenzuron	5.528	6.000	33.169
32	Chlorothalonil	5.432	6.031	32.760
33	**Musk xylene**	5.284	6.123	32.354
34	**17 alpha Ethinyl Estradiol**	5.284	6.072	32.087
35	Carbendazim	5.379	5.945	31.980
36	Benzo[*e*]pyrene	3.551	9.000	31.963
37	**Fenbutatin oxide**	5.284	5.997	31.687
38	**Pyriproxyfen**	4.286	7.136	30.583
39	**Triclosan**	5.284	5.786	30.577
40	**2.3.4.5.6-Pentachlorotoluene**	5.284	5.776	30.520
41	Cyfluthrin	5.052	6.000	30.310
42	**Dibutyltin oxide**	3.856	7.857	30.295
43	PCB 153	3.410	8.785	29.956
44	Zinc	9.218	3.249	29.945
45	**Prochloraz**	4.854	6.156	29.884
46	Dioctyl Phthalate	5.700	5.214	29.718
47	Captan	5.298	5.511	29.201
48	**Propetamphos**	4.854	6.000	29.125
49	**Triflumuron**	4.854	6.000	29.125
50	**4-Aminoazobenzene**	5.284	5.463	28.866

Table 80. Complete List of the COMMPS Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*EXPOSURE SCORE*	*EFFECT SCORE*	*COMMPS SCORE**
51	Tebuconazole	5.072	5.657	28.691
52	Bis(2-ethylhexyl) terephthalate	5.538	5.156	28.553
53	**Aldrin**	3.426	8.301	28.435
54	**Nitrofen**	3.856	7.356	28.364
55	Lindane	3.759	7.540	28.341
56	Endrin	4.081	6.943	28.337
57	**Phenthoate**	4.854	5.835	28.326
58	1-Methylnaphthalene	5.120	5.531	28.319
59	Fluorene	4.190	6.751	28.286
60	Trifloxystrobin	5.370	5.231	28.091
61	1-Chloronaphthalene	7.019	3.968	27.848
62	Phenanthrene	4.954	5.585	27.672
63	PCB 180	3.552	7.785	27.649
64	Diflufenican	4.394	6.286	27.617
65	Cobalt	5.157	5.333	27.504
66	**17 beta Estradiol**	4.424	6.211	27.477
67	Parathion-methyl	4.657	5.783	26.930
68	**Hexythiazox**	4.854	5.510	26.745
69	1.4-Dichlorobenzene	5.397	4.943	26.678
70	Pendimethalin	5.063	5.231	26.485
71	Fenpropathrin	4.402	6.000	26.411
72	Dibutyl phthalate (DBP)	4.976	5.301	26.378
73	**Malathion**	5.284	4.943	26.122
74	Benzyl benzoate	5.472	4.766	26.083
75	4-Chloroaniline	3.978	6.501	25.858
76	**Fluazifop-P-butyl**	4.854	5.316	25.807
77	Pyrene	3.873	6.571	25.453
78	**Chlordane**	3.426	7.404	25.364
79	**Boscalid**	4.716	5.373	25.337
80	PCB 28	2.875	8.785	25.259

Table 80. Complete List of the COMMPS Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*EXPOSURE SCORE*	*EFFECT SCORE*	*COMMPS SCORE**
81	Diphenyl ether (Diphenyl oxide)	7.058	3.573	25.219
82	**PCB 101**	3.426	7.341	25.148
83	Acetochlor	5.284	4.735	25.021
84	4.4'-DDE	2.541	9.800	24.904
85	Penconazole	4.446	5.601	24.899
86	PCB 52	2.778	8.785	24.402
87	Diethyl phthalate	5.599	4.326	24.224
88	Vanadium	6.493	3.728	24.204
89	PCB 138	2.731	8.785	23.990
90	Nitrobenzene	6.777	3.529	23.915
91	**Tolclofos-methyl**	6.283	3.801	23.878
92	Carbofuran	5.401	4.327	23.370
93	Piperonyl butoxide	5.059	4.601	23.273
94	3.6-dimethylphenanthrene	4.175	5.571	23.261
95	**Tefluthrin**	3.856	6.000	23.134
96	**Propylbenzene**	5.284	4.356	23.020
97	Azinphos-methyl	4.965	4.620	22.939
98	Myclobutanil	5.427	4.227	22.939
99	**Styrene; Vinylbenzene**	5.284	4.338	22.922
100	**N.N.N'.N'-tetramethyl-4.4'-methylenedianiline (Michler's base)**	3.426	6.604	22.623
101	**Vinclozolin**	3.856	5.851	22.560
102	**Pyraclostrobin**	4.854	4.641	22.527
103	Chlorfenapyr	4.123	5.439	22.423
104	Metrafenone	6.212	3.606	22.398
105	**Fludioxonil**	4.854	4.571	22.191
106	**Trichloroethylene (TRI)**	5.284	4.198	22.185
107	Methidathion	5.000	4.424	22.123
108	Cadusafos	3.996	5.527	22.086

Table 80. Complete List of the COMMPS Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*EXPOSURE SCORE*	*EFFECT SCORE*	*COMMPS SCORE**
109	**Difenoconazole**	4.854	4.536	22.020
110	Epoxiconazole	4.573	4.734	21.648
111	Chrysene	3.236	6.658	21.549
112	**Carbon tetrachloride**	5.284	4.076	21.541
113	Benzyl butyl phthalate	3.893	5.516	21.477
114	Flutriafol	5.483	3.913	21.455
115	Biphenyl	4.306	4.968	21.390
116	**PCB 31**	2.427	8.785	21.322
117	**Bromopropylate**	3.856	5.515	21.264
118	Ethylene thiourea	5.788	3.644	21.091
119	**Triadimenol**	5.284	3.943	20.835
120	**Linuron**	4.286	4.857	20.816
121	Isodrin	3.305	6.229	20.585
122	Buprofezin	5.334	3.845	20.509
123	Copper	7.847	2.591	20.333
124	**Benzo(a)fluorene**	2.427	8.313	20.177
125	Molinate	5.005	4.028	20.158
126	Diazinon	3.818	5.251	20.047
127	**Propazine**	3.856	5.189	20.007
128	**Dinobuton**	3.856	5.181	19.978
129	**Pirimicarb**	4.854	4.103	19.919
130	**Quizalofop-p-ethyl**	4.854	4.098	19.893
131	Monocrotophos	4.930	4.027	19.855
132	**Carboxin (Vitavax)**	4.854	4.081	19.811
133	**Spiroxamine**	4.854	4.071	19.760
134	1-chloro-2.4-dinitrobenzene	4.354	4.515	19.656
135	**Tecnazene**	3.856	5.091	19.631
136	**Bromophos-methyl**	2.427	8.000	19.417
137	**Diethofencarb**	4.854	3.996	19.395
138	**Tetrabromobisphenol A (TBBP-A)**	5.284	3.642	19.246

Table 80. Complete List of the COMMPS Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*EXPOSURE SCORE*	*EFFECT SCORE*	*COMMPS SCORE**
139	**Methomyl**	4.854	3.925	19.052
140	**1.2.4-Trimethylbenzene**	5.284	3.591	18.975
141	p-(1.1-dimethylpropyl)phenol	5.066	3.731	18.901
142	**Propyzamide**	4.854	3.886	18.865
143	**4.4'-Dibromodiphenyl Ether**	3.287	5.731	18.840
144	Procymidone	4.522	4.156	18.789
145	**Propiconazole**	4.716	3.977	18.754
146	**Chlorantraniliprole**	4.854	3.821	18.549
147	Thiacloprid	5.289	3.490	18.458
148	Chlorsulfuron	4.532	4.071	18.450
149	Diclofenac	5.698	3.229	18.396
150	**Tebuthiuron**	4.854	3.786	18.380
151	Barium	9.146	2.005	18.340
152	Imazalil	4.433	4.119	18.259
153	Cyromazine	5.422	3.356	18.198
154	**Tribenuron-methyl**	4.716	3.856	18.182
155	Silver	2.589	7.012	18.151
156	**1.3.5-trimethylbenzene (Mesitylene)**	5.284	3.427	18.110
157	Tin	7.055	2.545	17.957
158	Cyprodinil	4.066	4.396	17.874
159	**1.2.4.5-tetrachlorobenzene**	3.426	5.211	17.850
160	Aluminium	10.000	1.785	17.846
161	**Bromophos-ethyl**	2.427	7.333	17.797
162	Nicosulfuron	4.679	3.786	17.717
163	Carbaryl	4.035	4.373	17.645
164	Bisphenol A	4.278	4.081	17.458
165	**2.4.5-Trichlorophenoxyacetic acid**	6.283	2.776	17.439
166	**Clofentezine**	3.856	4.515	17.408
167	**Fluquinconazole**	4.424	3.916	17.327

Table 80. Complete List of the COMMPS Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*EXPOSURE SCORE*	*EFFECT SCORE*	*COMMPS SCORE**
168	**Omethoate**	4.286	4.041	17.319
169	**Bromoxynil**	4.854	3.545	17.211
170	Imidacloprid	4.910	3.467	17.022
171	**Methoxyfenozide**	5.284	3.220	17.015
172	Azoxystrobin	4.999	3.356	16.778
173	Hexaconazole	4.802	3.478	16.701
174	**Fenamiphos**	3.856	4.286	16.524
175	**Thiometon**	3.856	4.286	16.524
176	**Demeton**	3.856	4.274	16.477
177	**Terbuthylazine**	4.854	3.372	16.370
178	Iron	10.000	1.637	16.367
179	**2.4.6-Tri-tert-butylphenol**	2.427	6.730	16.334
180	**Triasulfuron**	3.856	4.229	16.306
181	**Ethoprophos**	4.854	3.341	16.219
182	**Cyclanilide**	6.283	2.573	16.165
183	Decamethylcyclopentasiloxane	2.959	5.426	16.056
184	**Prometryn**	4.854	3.231	15.682
185	**Chloroacetic acid**	4.854	3.198	15.525
186	Diisobutyl adipate	4.867	3.186	15.507
187	**Tribromobiphenyl ether**	3.287	4.711	15.487
188	Mepiquat Chloride	7.911	1.928	15.252
189	2.6-Xylenol	7.170	2.119	15.193
190	**Thidiazuron**	5.284	2.857	15.098
191	Metalaxyl	4.715	3.126	14.739
192	Propham	5.132	2.857	14.663
193	Titanium	6.861	2.113	14.500
194	**Flutolanil**	4.854	2.961	14.371
195	Clothianidin	5.001	2.801	14.007
196	2-Mercaptobenzothiazole	5.054	2.771	14.004
197	Acenaphthene	3.757	3.696	13.885
198	Lenacil	4.854	2.857	13.869

Table 80. Complete List of the COMMPS Ranking Results (cont'd)

RANK	***CHEMICAL NAME***	***EXPOSURE SCORE***	***EFFECT SCORE***	***COMMPS SCORE****
199	Diphenylamine	3.023	4.549	13.753
200	1.3-Dichlorobenzene	5.371	2.539	13.638
201	2.6-Di-*tert*-butylphenol	4.150	3.281	13.618
202	Metamitron	5.068	2.642	13.391
203	Silicon	10.000	1.333	13.333
204	Boron	10.000	1.326	13.264
205	Butyltin Trichloride	3.926	3.356	13.177
206	**Fenhexamid**	4.716	2.766	13.045
207	1.1-dichloroethane	6.107	2.125	12.976
208	**Methamidophos**	3.856	3.356	12.941
209	Sulfamethoxazole	5.519	2.338	12.904
210	**Metazachlor**	4.854	2.642	12.825
211	**Thiabendazole**	3.856	3.300	12.723
212	Metolachlor	5.115	2.487	12.719
213	**2-Methyl-4.6-dinitrophenol**	4.854	2.506	12.165
214	**Dimethenamid**	3.856	3.141	12.112
215	Meta-xylene	5.493	2.204	12.109
216	Chloridazon. pyrazon	5.247	2.301	12.075
217	Dimethoate	4.943	2.427	11.998
218	Picloram	5.617	2.113	11.871
219	**Dimethomorph**	3.856	3.072	11.845
220	**Bentazon**	4.854	2.391	11.604
221	**Triphenyltin; Fentin**	1.997	5.571	11.126
222	**Ethofumesate**	4.854	2.281	11.074
223	**Ortho-xylene**	5.284	2.071	10.945
224	**Fluopyram**	3.856	2.764	10.657
225	Fosetyl-al	5.616	1.859	10.439
226	**Mandipropamid**	4.854	2.143	10.402
227	**2.4-Dichlorophenoxyacetic acid**	4.424	2.340	10.352
228	**Dichlobenil**	3.426	3.016	10.330

Table 80. Complete List of the COMMPS Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*EXPOSURE SCORE*	*EFFECT SCORE*	*COMMPS SCORE**
229	**Isopropylbenzene. cumene**	5.284	1.898	10.031
230	4-Chloro-3-methylphenol	4.544	2.143	9.737
231	Pyrimethanil	4.459	2.162	9.640
232	**Fosthiazate**	3.426	2.801	9.594
233	**Thiophanate-methyl**	3.856	2.460	9.484
234	Trinexapac-ethyl	4.263	2.204	9.397
235	**Tributyl phosphate**	2.427	3.728	9.048
236	Mesotrione	5.037	1.683	8.479
237	**Acetamiprid**	4.854	1.698	8.241
238	**Oxadixyl**	4.854	1.669	8.104
239	Thiamethoxam	3.988	1.928	7.687
240	**Imazapyr**	4.716	1.535	7.238
241	Dimethylaminosulfanilide	4.716	1.443	6.803
242	Beryllium	1.089	5.317	5.791
243	Clopyralid	4.138	1.214	5.022
244	Propamocarb Hydrochloride	3.863	1.149	4.440
245	Fluroxypyr	5.762	0.679	3.913
246	**EDTA**	Not measured		
247	**Tert-butyl-4-methoxyphenol**	Not measured		
248	Bromide	Excluded		
249	Total petroleum hydrocarbons	Excluded		
250	Free Cyanide	Excluded		

*COMMPS score= Exposure score x Effect score

**Chemicals which were detected but not quantified in any of the monitoring periods are indicated in bold font. They were included in the ranking/prioritization procedure by taking their concentrations as LOD/ 2.

***Mixtures and inorganics other than metals-metalloids were not included in the ranking/ prioritization process.

APPENDIX D

RANKING RESULTS OF THE NORMAN METHOD

Table 81. Complete List of the NORMAN Ranking Results

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
1	Arsenic	0.833	0.615	0.625	2.073
2	Zinc	0.833	0.465	0.750	2.048
3	Chromium	0.833	0.435	0.625	1.893
4	Cobalt	0.667	0.460	0.750	1.877
5	Aluminium	0.667	0.355	0.750	1.772
6	Copper	0.833	0.310	0.625	1.768
7	Silver	0.664	0.410	0.625	1.699
8	DDT (Total)	0.106	0.950	0.625	1.681
9	Iron	0.667	0.210	0.750	1.627
10	Endrin	0.101	0.900	0.625	1.626
11	Antimony	0.659	0.385	0.565	1.610
12	Vanadium	0.667	0.310	0.625	1.602
13	Barium	0.667	0.360	0.550	1.577
14	Diflubenzuron	0.088	0.450	1.000	1.538
15	Cyfluthrin	0.083	0.400	1.000	1.483
16	Permethrin	0.069	0.650	0.750	1.469
17	Perylene	0.102	0.600	0.750	1.452
18	**Fenitrothion**	0.167	0.500	0.750	1.417
19	Fenthion	0.204	0.575	0.625	1.404
20	Acetochlor	0.127	0.650	0.625	1.402
21	**Malathion**	0.167	0.600	0.625	1.392
22	Chlorobenzilate	0.035	0.725	0.625	1.385

Table 81. Complete List of the NORMAN Ranking Results (cont'd)

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
23	**Dieldrin**	0.067	0.750	0.550	1.367
24	PCB 28	0.156	0.950	0.252	1.359
25	Diazinon	0.101	0.625	0.625	1.351
26	Boron	0.667	0.160	0.514	1.341
27	PCB 138	0.145	0.950	0.196	1.291
28	Silicon	0.500	0.160	0.625	1.285
29	Pendimethalin	0.101	0.525	0.625	1.251
30	Diflufenican	0.071	0.425	0.750	1.246
31	Prothiofos	0.085	0.410	0.750	1.245
32	PCB 180	0.108	0.950	0.185	1.243
33	Carbofuran	0.034	0.575	0.625	1.234
34	**Triclosan**	0.033	0.575	0.625	1.233
35	PCB 153	0.145	0.950	0.110	1.204
36	Polychlorinated biphenyls (PCBs)	0.201	1.000	0.000	1.201
37	Atrazine-desethyl (Deethylatrazine)	0.147	0.500	0.550	1.197
38	**Prometryn**	0.067	0.500	0.625	1.192
39	**Terbuthylazine**	0.167	0.450	0.550	1.167
40	**Methomyl**	0.000	0.605	0.550	1.155
41	**Quinalphos**	0.000	0.530	0.625	1.155
42	**Fenbutatin oxide**	0.000	0.525	0.625	1.150
43	PCB 52	0.109	0.950	0.086	1.145
44	Fenpropathrin	0.034	0.350	0.750	1.134
45	4.4'-DDE	0.102	0.950	0.074	1.126
46	**Pirimicarb**	0.067	0.500	0.550	1.117
47	Fenarimol	0.034	0.550	0.512	1.096
48	Carbendazim	0.128	0.650	0.315	1.094
49	Ethalfluralin	0.094	0.425	0.560	1.078
50	Azinphos-methyl	0.201	0.250	0.625	1.076
51	**Metazachlor**	0.067	0.450	0.550	1.067

Table 81. Complete List of the NORMAN Ranking Results (cont'd)

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
52	**Chlordane**	0.167	0.900	0.000	1.067
53	Methidathion	0.039	0.400	0.625	1.064
54	Cadusafos	0.034	0.400	0.625	1.059
55	Monocrotophos	0.034	0.475	0.550	1.059
56	**Oxadiazon**	0.033	0.475	0.550	1.058
57	**Fludioxonil**	0.000	0.500	0.550	1.050
58	Trifloxystrobin	0.034	0.375	0.625	1.034
59	Chlorothalonil	0.078	0.700	0.256	1.034
60	Phenanthrene	0.282	0.750	0.000	1.032
61	**Phenthoate**	0.000	0.405	0.625	1.030
62	4-Chloroaniline	0.246	0.625	0.157	1.028
63	**Propetamphos**	0.000	0.400	0.625	1.025
64	Benzo[*e*]pyrene	0.144	0.500	0.369	1.013
65	4.4'-DDD	0.040	0.900	0.062	1.001
66	**PCB 101**	0.067	0.925	0.000	0.992
67	**Fenamiphos**	0.033	0.400	0.550	0.983
68	**Tris(nonylphenyl) phosphite; TNPP**	0.000	0.425	0.550	0.975
69	**Tefluthrin**	0.000	0.350	0.625	0.975
70	1.4-Dichlorobenzene	0.368	0.600	0.000	0.968
71	**Tolclofos-methyl**	0.033	0.375	0.550	0.958
72	**Tolfenpyrad**	0.000	0.405	0.550	0.955
73	**Quizalofop-p-ethyl**	0.000	0.400	0.550	0.950
74	**PCB 31**	0.000	0.950	0.000	0.950
75	Decamethylcyclopentasiloxane	0.112	0.775	0.062	0.949
76	Lindane	0.039	0.900	0.000	0.939
77	Parathion-methyl	0.204	0.550	0.173	0.927
78	**Pyridaben**	0.033	0.250	0.625	0.908
79	Nitrobenzene	0.144	0.700	0.062	0.906
80	**Chlorantraniliprole**	0.000	0.350	0.550	0.900
81	**Pyraclostrobin**	0.000	0.350	0.550	0.900

Table 81. Complete List of the NORMAN Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*ES**	*HS**	*RS**	*NORMAN SCORE**
82	**Triflumuron**	0.000	0.275	0.625	0.900
83	Bis(2-ethylhexyl) terephthalate	0.077	0.200	0.619	0.896
84	**4.5-dichloro-2-octyl-2H-isothiazol-3-on; DCOIT**	0.000	0.325	0.550	0.875
85	**Spiroxamine**	0.000	0.250	0.625	0.875
86	Diethyl phthalate	0.114	0.750	0.000	0.864
87	Dibutyl phthalate (DBP)	0.258	0.605	0.000	0.863
88	**Pyriproxyfen**	0.033	0.275	0.550	0.858
89	Epoxiconazole	0.158	0.600	0.098	0.856
90	1-chloro-2.4-dinitrobenzene	0.106	0.725	0.000	0.831
91	1.3-Dichlorobenzene	0.201	0.630	0.000	0.831
92	**Clofibric acid**	0.000	0.275	0.550	0.825
93	**Nitrofen**	0.000	0.825	0.000	0.825
94	Meta-xylene	0.420	0.405	0.000	0.825
95	1.1-dichloroethane	0.266	0.555	0.000	0.821
96	**Triphenyltin; Fentin**	0.067	0.750	0.000	0.817
97	**Musk xylene**	0.033	0.775	0.000	0.808
98	**Tetrabromobisphenol A (TBBP-A)**	0.000	0.805	0.000	0.805
99	Diphenyl ether (Diphenyl oxide)	0.086	0.400	0.315	0.802
100	Biphenyl	0.249	0.475	0.074	0.798
101	**1.2.4.5-tetrachlorobenzene**	0.167	0.625	0.000	0.792
102	**Linuron**	0.167	0.625	0.000	0.792
103	2-Chloronaphthalene	0.068	0.655	0.062	0.785
104	Beryllium	0.318	0.465	0.000	0.783
105	Fluorene	0.273	0.500	0.000	0.773
106	**Aldrin**	0.067	0.700	0.000	0.767
107	**Ortho-xylene**	0.333	0.425	0.000	0.758
108	Cyromazine	0.039	0.625	0.086	0.749
109	Benzyl butyl phthalate	0.117	0.630	0.000	0.747

Table 81. Complete List of the NORMAN Ranking Results (cont'd)

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
110	**Chloroacetic acid**	0.167	0.575	0.000	0.742
111	Myclobutanil	0.035	0.705	0.000	0.740
112	Tebuconazole	0.039	0.600	0.098	0.736
113	Bisphenol A	0.173	0.555	0.000	0.728
114	Imidacloprid	0.128	0.525	0.074	0.727
115	4-Chloro-3-methylphenol	0.251	0.475	0.000	0.726
116	Dimethoate	0.249	0.475	0.000	0.724
117	1-Chloronaphthalene	0.101	0.475	0.137	0.713
118	2-Mercaptobenzothiazole	0.075	0.575	0.062	0.712
119	Chlorsulfuron	0.084	0.375	0.252	0.712
120	Chrysene	0.206	0.505	0.000	0.711
121	**Propylbenzene**	0.033	0.675	0.000	0.708
122	Piperonyl butoxide	0.104	0.525	0.074	0.703
123	Fenpropimorph	0.041	0.450	0.208	0.699
124	**Methamidophos**	0.167	0.525	0.000	0.692
125	**Trichloroethylene (TRI)**	0.033	0.650	0.000	0.683
126	**2-Methyl-4.6-dinitrophenol**	0.033	0.650	0.000	0.683
127	**Bromopropylate**	0.000	0.675	0.000	0.675
128	**2.4.5-Trichlorophenoxyacetic acid**	0.167	0.505	0.000	0.672
129	**2.4-Dichlorophenoxyacetic acid**	0.167	0.505	0.000	0.672
130	**Omethoate**	0.167	0.500	0.000	0.667
131	**Bromoxynil**	0.033	0.625	0.000	0.658
132	Tridecane	0.083	0.250	0.304	0.637
133	p-(1.1-dimethylpropyl)phenol	0.087	0.480	0.062	0.629
134	**Carbon tetrachloride**	0.000	0.625	0.000	0.625
135	Procymidone	0.041	0.580	0.000	0.621
136	Dioctyl Phthalate	0.070	0.550	0.000	0.620
137	Clopyralid	0.069	0.550	0.000	0.619
138	Titanium	0.198	0.310	0.110	0.617

Table 81. Complete List of the NORMAN Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*ES**	*HS**	*RS**	*NORMAN SCORE**
139	Imazalil	0.034	0.575	0.000	0.609
140	**Propiconazole**	0.033	0.575	0.000	0.608
141	**Triadimenol**	0.000	0.600	0.000	0.600
142	**Tebuthiuron**	0.000	0.600	0.000	0.600
143	Lenacil	0.036	0.500	0.062	0.598
144	**Dibutyltin oxide**	0.067	0.530	0.000	0.597
145	**Isopropylbenzene. cumene**	0.167	0.425	0.000	0.592
146	Acenaphthene	0.160	0.425	0.000	0.585
147	**17 alpha Ethinyl Estradiol**	0.000	0.580	0.000	0.580
148	**17 beta Estradiol**	0.000	0.580	0.000	0.580
149	**Vinclozolin**	0.000	0.580	0.000	0.580
150	Thiacloprid	0.043	0.475	0.062	0.580
151	**Dichlobenil**	0.000	0.575	0.000	0.575
152	**Tecnazene**	0.000	0.575	0.000	0.575
153	**Styrene; Vinylbenzene**	0.067	0.505	0.000	0.572
154	Cyprodinil	0.040	0.525	0.000	0.565
155	**Tribromobiphenyl ether**	0.000	0.560	0.000	0.560
156	Carbaryl	0.034	0.525	0.000	0.559
157	Captan	0.071	0.425	0.062	0.558
158	Metolachlor	0.101	0.455	0.000	0.556
159	Flutriafol	0.092	0.455	0.000	0.547
160	Pyrimethanil	0.041	0.505	0.000	0.546
161	Picloram	0.037	0.505	0.000	0.542
162	Isodrin	0.068	0.400	0.062	0.530
163	**N.N.N'.N'-tetramethyl-4.4'-methylenedianiline (Michler's base)**	0.000	0.525	0.000	0.525
164	Chlorfenapyr	0.036	0.400	0.086	0.522
165	**Tributyl phosphate**	0.067	0.455	0.000	0.522
166	**Bentazon**	0.167	0.355	0.000	0.522
167	Pyrene	0.244	0.275	0.000	0.519

Table 81. Complete List of the NORMAN Ranking Results (cont'd)

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
168	Ethylene thiourea	0.068	0.450	0.000	0.518
169	Sulfamethoxazole	0.117	0.400	0.000	0.517
170	Molinate	0.035	0.475	0.000	0.510
171	**Propazine**	0.033	0.475	0.000	0.508
172	**Propyzamide**	0.000	0.505	0.000	0.505
173	**4-Aminoazobenzene**	0.000	0.500	0.000	0.500
174	**Difenoconazole**	0.000	0.500	0.000	0.500
175	Metrafenone	0.035	0.400	0.062	0.497
176	**2-Amino-4-chlorophenol**	0.067	0.430	0.000	0.497
177	Nicosulfuron	0.034	0.400	0.062	0.496
178	Tin	0.106	0.310	0.074	0.490
179	Hexaconazole	0.034	0.455	0.000	0.489
180	1-Methylnaphthalene	0.133	0.355	0.000	0.488
181	**Tribenuron-methyl**	0.033	0.450	0.000	0.483
182	Chloridazon. pyrazon	0.149	0.330	0.000	0.479
183	**2.4-D. isooctyl ester**	0.000	0.475	0.000	0.475
184	**Hexythiazox**	0.000	0.475	0.000	0.475
185	Penconazole	0.036	0.425	0.000	0.461
186	**Prochloraz**	0.033	0.425	0.000	0.458
187	**Fenhexamid**	0.000	0.455	0.000	0.455
188	**Dimethomorph**	0.000	0.450	0.000	0.450
189	Mepiquat Chloride	0.034	0.350	0.062	0.446
190	Fluroxypyr	0.090	0.350	0.000	0.440
191	Propamocarb Hydrochloride	0.035	0.400	0.000	0.435
192	Diphenylamine	0.110	0.325	0.000	0.435
193	**Dinobuton**	0.000	0.430	0.000	0.430
194	**Butralin**	0.000	0.425	0.000	0.425
195	**Clofentezine**	0.000	0.425	0.000	0.425
196	**Diethofencarb**	0.000	0.425	0.000	0.425
197	**Dimethenamid**	0.000	0.425	0.000	0.425
198	**Ethoprophos**	0.000	0.425	0.000	0.425

Table 81. Complete List of the NORMAN Ranking Results (cont'd)

RANK	*CHEMICAL NAME*	*ES**	*HS**	*RS**	*NORMAN SCORE**
199	**Flutolanil**	0.000	0.425	0.000	0.425
200	**Demeton**	0.067	0.355	0.000	0.422
201	**4.4'-Dibromodiphenyl Ether**	0.000	0.410	0.000	0.410
202	Trinexapac-ethyl	0.078	0.330	0.000	0.408
203	**Boscalid**	0.000	0.405	0.000	0.405
204	**Cyclanilide**	0.000	0.405	0.000	0.405
205	**Fluazifop-P-butyl**	0.000	0.405	0.000	0.405
206	**Fluopyram**	0.000	0.400	0.000	0.400
207	**Oxadixyl**	0.000	0.400	0.000	0.400
208	**Triasulfuron**	0.000	0.400	0.000	0.400
209	Fosetyl-al	0.043	0.355	0.000	0.398
210	Metam Potassium	0.036	0.360	0.000	0.396
211	Metamitron	0.071	0.325	0.000	0.396
212	Butyltin Trichloride	0.039	0.355	0.000	0.394
213	Thiamethoxam	0.039	0.350	0.000	0.389
214	Diclofenac	0.037	0.350	0.000	0.387
215	Mesotrione	0.077	0.305	0.000	0.382
216	**Fluquinconazole**	0.000	0.375	0.000	0.375
217	**Fosthiazate**	0.000	0.375	0.000	0.375
218	**Thiabendazole**	0.000	0.375	0.000	0.375
219	**Thiometon**	0.000	0.375	0.000	0.375
220	**1.2.4-Trimethylbenzene**	0.067	0.305	0.000	0.372
221	Metalaxyl	0.043	0.325	0.000	0.368
222	Azoxystrobin	0.034	0.325	0.000	0.359
223	**Carboxin (Vitavax)**	0.000	0.355	0.000	0.355
224	**Thiophanate-methyl**	0.000	0.355	0.000	0.355
225	2.6-Xylenol	0.100	0.155	0.098	0.353
226	3.6-dimethylphenanthrene	0.146	0.205	0.000	0.351
227	Clothianidin	0.035	0.305	0.000	0.340
228	**1.3.5-trimethylbenzene (Mesitylene)**	0.033	0.305	0.000	0.338

Table 81. Complete List of the NORMAN Ranking Results (cont'd)

RANK	***CHEMICAL NAME***	***ES****	***HS****	***RS****	***NORMAN SCORE****
229	**Ethofumesate**	0.033	0.305	0.000	0.338
230	**2.4.6-Tri-tert-butylphenol**	0.033	0.300	0.000	0.333
231	Buprofezin	0.129	0.200	0.000	0.329
232	**Bromophos-ethyl**	0.000	0.325	0.000	0.325
233	**Methoxyfenozide**	0.000	0.305	0.000	0.305
234	**Bromophos-methyl**	0.000	0.300	0.000	0.300
235	**Imazapyr**	0.000	0.300	0.000	0.300
236	Diisobutyl adipate	0.090	0.210	0.000	0.300
237	**Benzo(a)fluorene**	0.067	0.230	0.000	0.297
238	Propham	0.043	0.250	0.000	0.293
239	2.6-Di-*tert*-butylphenol	0.081	0.200	0.000	0.281
240	Benzyl benzoate	0.106	0.160	0.012	0.278
241	**Mandipropamid**	0.000	0.255	0.000	0.255
242	**Acetamiprid**	0.000	0.175	0.000	0.175
243	**Thidiazuron**	0.000	0.175	0.000	0.175
244	**2.3.4.5.6-Pentachlorotoluene**	0.000	0.165	0.000	0.165
245	**Dimethylaminosulfanilide**	0.000	0.160	0.000	0.160
246	**EDTA**	Not measured			
247	**Tert-butyl-4-methoxyphenol**	Not measured			
248	Bromide	Excluded			
249	Total petroleum hydrocarbons	Excluded			
250	Free Cyanide	Excluded			

**NORMAN Score= ES +HS+ RS where ES: Exposure Score. HS: Hazard Score. RS: Risk Score

**Chemicals which were detected but not quantified in any of the monitoring periods are indicated in bold font. They were included in the ranking/prioritization procedure by taking their concentrations as LOD/ 2

***Mixtures and inorganics other than metals-metalloids were not included in the ranking/ prioritization process.

APPENDIX E

FINAL RANKING RESULTS BY USING WEIGHTING FACTOR APPROACH

Table 82. Complete Final Ranking List of Weighting Factor Approach

RANK	***CHEMICAL NAME***	***COMMPS SCORE***	***NORMAN SCORE***	***INTEGRATED SCORE***
1	Arsenic	45.885	2.073	59.820
2	Chromium	37.892	1.893	53.023
3	Zinc	29.945	2.048	52.944
4	Antimony	45.589	1.610	50.433
5	Cobalt	27.504	1.877	48.534
6	DDT (Total)	36.765	1.681	48.330
7	Perylene	46.337	1.452	47.576
8	Fenarimol	61.076	1.096	46.356
9	Permethrin	41.477	1.469	45.965
10	Fenthion	40.833	1.404	44.416
11	Diflubenzuron	33.169	1.538	44.037
12	Endrin	28.337	1.626	43.855
13	Copper	20.333	1.768	43.500
14	Aluminium	17.846	1.772	42.571
15	Cyfluthrin	30.310	1.483	41.789
16	**Fenitrothion**	33.480	1.417	41.725
17	Vanadium	24.204	1.602	41.715
18	Chlorobenzilate	34.226	1.385	41.398
19	Silver	18.151	1.699	41.231
20	Prothiofos	39.530	1.245	40.719
21	**Dieldrin**	33.377	1.367	40.684

Table 82. Complete Final Ranking List of Weighting Factor Approach (cont'd)

RANK	***CHEMICAL NAME***	***COMMPS SCORE***	***NORMAN SCORE***	***INTEGRATED SCORE***
22	Iron	16.367	1.627	39.080
23	Ethalfluralin	43.557	1.078	38.986
24	Barium	18.340	1.577	38.869
25	Polychlorinated biphenyls (PCBs)	36.958	1.201	38.807
26	**Malathion**	26.122	1.392	38.282
27	Acetochlor	25.021	1.402	38.048
28	PCB 28	25.259	1.359	37.275
29	Atrazine-desethyl (Deethylatrazine)	33.281	1.197	37.249
30	**Triclosan**	30.577	1.233	36.897
31	**Quinalphos**	33.979	1.155	36.692
32	**Tris(nonylphenyl) phosphite; TNPP**	42.000	0.975	36.300
33	PCB 153	29.956	1.204	36.068
34	Diflufenican	27.617	1.246	35.963
35	PCB 180	27.649	1.243	35.916
36	**Fenbutatin oxide**	31.687	1.150	35.675
37	Pendimethalin	26.485	1.251	35.614
38	PCB 138	23.990	1.291	35.419
39	Diazinon	20.047	1.351	35.039
40	Carbendazim	31.980	1.094	34.662
41	**Oxadiazon**	33.544	1.058	34.584
42	4.4'-DDD	35.135	1.001	34.083
43	2-Chloronaphthalene	45.874	0.785	34.042
44	Carbofuran	23.370	1.234	34.035
45	Chlorothalonil	32.760	1.034	33.785
46	**Tolfenpyrad**	35.702	0.955	33.381
47	Fenpropathrin	26.411	1.134	33.252
48	Benzo[*e*]pyrene	31.963	1.013	33.040
49	PCB 52	24.402	1.145	32.662

Table 82. Complete Final Ranking List of Weighting Factor Approach (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
50	4.4'-DDE	24.904	1.126	32.479
51	**Propetamphos**	29.125	1.025	32.150
52	Boron	13.264	1.341	32.124
53	**Phenthoate**	28.326	1.030	31.930
54	Trifloxystrobin	28.091	1.034	31.924
55	**Pyridaben**	33.979	0.908	31.758
56	Phenanthrene	27.672	1.032	31.712
57	**Chlordane**	25.364	1.067	31.479
58	**4.5-dichloro-2-octyl-2H-isothiazol-3-on; DCOIT**	33.979	0.875	31.092
59	Silicon	13.333	1.285	31.033
60	4-Chloroaniline	25.858	1.028	30.902
61	**Methomyl**	19.052	1.155	30.721
62	Azinphos-methyl	22.939	1.076	30.696
63	**Clofibric acid**	35.035	0.825	30.514
64	**Pirimicarb**	19.919	1.117	30.301
65	Methidathion	22.123	1.064	30.119
66	Fenpropimorph	40.351	0.699	30.119
67	Lindane	28.341	0.939	30.107
68	**Prometryn**	15.682	1.192	30.106
69	1.4-Dichlorobenzene	26.678	0.968	30.025
70	Cadusafos	22.086	1.059	30.022
71	**PCB 101**	25.148	0.992	29.893
72	**Terbuthylazine**	16.370	1.167	29.881
73	**Fludioxonil**	22.191	1.050	29.876
74	**Triflumuron**	29.125	0.900	29.650
75	**Pyriproxyfen**	30.583	0.858	29.400
76	Bis(2-ethylhexyl) terephthalate	28.553	0.896	29.343
77	Parathion-methyl	26.930	0.927	29.307
78	Monocrotophos	19.855	1.059	29.129

Table 82. Complete Final Ranking List of Weighting Factor Approach (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
79	**Musk xylene**	32.354	0.808	29.108
80	**Tefluthrin**	23.134	0.975	28.753
81	**Tolclofos-methyl**	23.878	0.958	28.718
82	**Nitrofen**	28.364	0.825	27.845
83	Dibutyl phthalate (DBP)	26.378	0.863	27.816
84	Nitrobenzene	23.915	0.906	27.678
85	**PCB 31**	21.322	0.950	27.529
86	Tridecane	36.355	0.637	27.279
87	**Pyraclostrobin**	22.527	0.900	27.010
88	Diethyl phthalate	24.224	0.864	26.978
89	**Quizalofop-p-ethyl**	19.893	0.950	26.957
90	Fluorene	28.286	0.773	26.770
91	**Aldrin**	28.435	0.767	26.707
92	**Metazachlor**	12.825	1.067	26.463
93	**Fenamiphos**	16.524	0.983	26.276
94	Tebuconazole	28.691	0.736	26.199
95	Diphenyl ether (Diphenyl oxide)	25.219	0.802	26.125
96	**2-Amino-4-chlorophenol**	40.306	0.497	26.056
97	Epoxiconazole	21.648	0.856	25.777
98	**Chlorantraniliprole**	18.549	0.900	25.419
99	Decamethylcyclopentasiloxane	16.056	0.949	25.409
100	**Spiroxamine**	19.760	0.875	25.404
101	1-Chloronaphthalene	27.848	0.713	25.398
102	Biphenyl	21.390	0.798	24.510
103	1-chloro-2.4-dinitrobenzene	19.656	0.831	24.487
104	**17 alpha Ethinyl Estradiol**	32.087	0.580	24.435
105	Dioctyl Phthalate	29.718	0.620	24.283
106	**Linuron**	20.816	0.792	24.160
107	**Dibutyltin oxide**	30.295	0.597	24.051
108	**2.4-D. isooctyl ester**	36.322	0.475	24.029

Table 82. Complete Final Ranking List of Weighting Factor Approach (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
109	Myclobutanil	22.939	0.740	23.984
110	**Tetrabromobisphenol A (TBBP-A)**	19.246	0.805	23.798
111	Benzyl butyl phthalate	21.477	0.747	23.523
112	**Propylbenzene**	23.020	0.708	23.375
113	Piperonyl butoxide	23.273	0.703	23.366
114	**Butralin**	36.753	0.425	23.201
115	**1.2.4.5-tetrachlorobenzene**	17.850	0.792	22.973
116	Chrysene	21.549	0.711	22.844
117	Captan	29.201	0.558	22.835
118	**17 beta Estradiol**	27.477	0.580	22.591
119	**Trichloroethylene (TRI)**	22.185	0.683	22.541
120	Metam Potassium	36.274	0.396	22.439
121	Cyromazine	18.198	0.749	22.264
122	1.3-Dichlorobenzene	13.638	0.831	22.076
123	**Bromopropylate**	21.264	0.675	22.005
124	Chlorsulfuron	18.450	0.712	21.614
125	1.1-dichloroethane	12.976	0.821	21.601
126	**4-Aminoazobenzene**	28.866	0.500	21.546
127	Bisphenol A	17.458	0.728	21.539
128	Imidacloprid	17.022	0.727	21.346
129	Meta-xylene	12.109	0.825	21.338
130	**Prochloraz**	29.884	0.458	21.120
131	**Carbon tetrachloride**	21.541	0.625	21.116
132	1-Methylnaphthalene	28.319	0.488	21.092
133	**Chloroacetic acid**	15.525	0.742	21.043
134	**Triphenyltin; Fentin**	11.126	0.817	20.784
135	**Vinclozolin**	22.560	0.580	20.624
136	**Styrene; Vinylbenzene**	22.922	0.572	20.602
137	Pyrene	25.453	0.519	20.555
138	**2.4.5-Trichlorophenoxyacetic acid**	17.439	0.672	20.409

Table 82. Complete Final Ranking List of Weighting Factor Approach (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
139	**Triadimenol**	20.835	0.600	20.334
140	**Omethoate**	17.319	0.667	20.261
141	**Hexythiazox**	26.745	0.475	20.198
142	p-(1.1-dimethylpropyl)phenol	18.901	0.629	20.147
143	**Bromoxynil**	17.211	0.658	20.051
144	Procymidone	18.789	0.621	19.928
145	2-Mercaptobenzothiazole	14.004	0.712	19.839
146	**Propiconazole**	18.754	0.608	19.668
147	**N.N.N'.N'-tetramethyl-4.4'-methylenedianiline (Michler's base)**	22.623	0.525	19.549
148	**Ortho-xylene**	10.945	0.758	19.544
149	Flutriafol	21.455	0.547	19.514
150	Imazalil	18.259	0.609	19.491
151	Chlorfenapyr	22.423	0.522	19.412
152	**Tecnazene**	19.631	0.575	19.352
153	**Tebuthiuron**	18.380	0.600	19.352
154	Dimethoate	11.998	0.724	19.277
155	Penconazole	24.899	0.461	19.189
156	**Methamidophos**	12.941	0.692	19.010
157	Thiacloprid	18.458	0.580	18.975
158	Metrafenone	22.398	0.497	18.905
159	Isodrin	20.585	0.530	18.826
160	**Difenoconazole**	22.020	0.500	18.808
161	Ethylene thiourea	21.091	0.518	18.790
162	**2-Methyl-4.6-dinitrophenol**	12.165	0.683	18.533
163	Cyprodinil	17.874	0.565	18.441
164	**Fluazifop-P-butyl**	25.807	0.405	18.423
165	4-Chloro-3-methylphenol	9.737	0.726	18.414
166	Molinate	20.158	0.510	18.271
167	Carbaryl	17.645	0.559	18.245

Table 82. Complete Final Ranking List of Weighting Factor Approach (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
168	**Boscalid**	25.337	0.405	18.235
169	**Propazine**	20.007	0.508	18.170
170	Titanium	14.500	0.617	18.142
171	Beryllium	5.791	0.783	17.986
172	**Propyzamide**	18.865	0.505	17.646
173	**2.4-Dichlorophenoxyacetic acid**	10.352	0.672	17.574
174	Lenacil	13.869	0.598	17.515
175	**Tribromobiphenyl ether**	15.487	0.560	17.395
176	Acenaphthene	13.885	0.585	17.261
177	Nicosulfuron	17.717	0.496	17.012
178	Tin	17.957	0.490	16.983
179	**Tribenuron-methyl**	18.182	0.483	16.940
180	**Dinobuton**	19.978	0.430	16.591
181	Hexaconazole	16.701	0.489	16.468
182	3.6-dimethylphenanthrene	23.261	0.351	16.320
183	**Diethofencarb**	19.395	0.425	16.258
184	Metolachlor	12.719	0.556	16.208
185	Benzyl benzoate	26.083	0.278	15.994
186	**Isopropylbenzene. cumene**	10.031	0.592	15.846
187	**4.4'-Dibromodiphenyl Ether**	18.840	0.410	15.736
188	**Dichlobenil**	10.330	0.575	15.632
189	Picloram	11.871	0.542	15.598
190	**2.3.4.5.6-Pentachlorotoluene**	30.520	0.165	15.508
191	Sulfamethoxazole	12.904	0.517	15.494
192	**Clofentezine**	17.408	0.425	15.463
193	Diclofenac	18.396	0.387	15.108
194	**Bentazon**	11.604	0.522	15.075
195	Mepiquat Chloride	15.252	0.446	15.026

Table 82. Complete Final Ranking List of Weighting Factor Approach (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
196	**Carboxin (Vitavax)**	19.811	0.355	15.025
197	**Demeton**	16.477	0.422	15.024
198	**1.2.4-Trimethylbenzene**	18.975	0.372	15.023
199	**Ethoprophos**	16.219	0.425	14.988
200	Buprofezin	20.509	0.329	14.783
201	Pyrimethanil	9.640	0.546	14.768
202	**Cyclanilide**	16.165	0.405	14.566
203	**Triasulfuron**	16.306	0.400	14.522
204	**Fluquinconazole**	17.327	0.375	14.431
205	Chloridazon. pyrazon	12.075	0.479	14.408
206	Clopyralid	5.022	0.619	14.383
207	**Fenhexamid**	13.045	0.455	14.318
208	**Flutolanil**	14.371	0.425	14.248
209	Diphenylamine	13.753	0.435	14.209
210	**Thiometon**	16.524	0.375	14.110
211	**Tributyl phosphate**	9.048	0.522	14.052
212	**1.3.5-trimethylbenzene (Mesitylene)**	18.110	0.338	14.010
213	**Benzo(a)fluorene**	20.177	0.297	14.004
214	Azoxystrobin	16.778	0.359	13.899
215	**Bromophos-methyl**	19.417	0.300	13.767
216	**Dimethomorph**	11.845	0.450	13.738
217	**Bromophos-ethyl**	17.797	0.325	13.619
218	**Dimethenamid**	12.112	0.425	13.345
219	Metamitron	13.391	0.396	13.273
220	Metalaxyl	14.739	0.368	13.249
221	**2.4.6-Tri-tert-butylphenol**	16.334	0.333	13.200
222	Butyltin Trichloride	13.177	0.394	13.149
223	2.6-Xylenol	15.193	0.353	13.127
224	**Methoxyfenozide**	17.015	0.305	12.906
225	**Thiabendazole**	12.723	0.375	12.589

Table 82. Complete Final Ranking List of Weighting Factor Approach (cont'd)

RANK	***CHEMICAL NAME***	***COMMPS SCORE***	***NORMAN SCORE***	***INTEGRATED SCORE***
226	Clothianidin	14.007	0.340	12.411
227	**Fluopyram**	10.657	0.400	12.263
228	Diisobutyl adipate	15.507	0.300	12.193
229	Fosetyl-al	10.439	0.398	12.129
230	Trinexapac-ethyl	9.397	0.408	11.921
231	Propham	14.663	0.293	11.719
232	**Fosthiazate**	9.594	0.375	11.337
233	**Oxadixyl**	8.104	0.400	11.241
234	**Ethofumesate**	11.074	0.338	11.196
235	2.6-Di-*tert*-butylphenol	13.618	0.281	11.071
236	Mesotrione	8.479	0.382	11.032
237	**Thiophanate-methyl**	9.484	0.355	10.894
238	Thiamethoxam	7.687	0.389	10.845
239	Propamocarb Hydrochloride	4.440	0.435	10.484
240	Fluroxypyr	3.913	0.440	10.356
241	**Thidiazuron**	15.098	0.175	9.539
242	**Mandipropamid**	10.402	0.255	9.261
243	**Imazapyr**	7.238	0.300	8.895
244	**Acetamiprid**	8.241	0.175	6.796
245	Dimethylaminosulfanilide	6.803	0.160	5.921
246	**EDTA**	Not measured		
247	**Tert-butyl-4-methoxyphenol**	Not measured		
248	Bromide	Excluded		
249	Total petroleum hydrocarbons (TPH)	Excluded		
250	Free Cyanide	Excluded		

APPENDIX F

SENSITIVITY ANALYSIS RESULTS OF THE WEIGHTING FACTOR APPROACH

Table 83. Ranking Results of the Sensitivity Analysis

RANK	***CHEMICAL NAME***	***COMMPS SCORE***	***NORMAN SCORE***	***INTEGRATED SCORE***
1	Arsenic	45.885	2.073	57.498
2	Chromium	37.892	1.893	50.501
3	Antimony	45.589	1.610	49.626
4	Zinc	29.945	2.048	49.111
5	Fenarimol	61.076	1.096	48.809
6	Perylene	46.337	1.452	47.369
7	DDT (Total)	36.765	1.681	46.403
8	Permethrin	41.477	1.469	45.217
9	Cobalt	27.504	1.877	45.029
10	Fenthion	40.833	1.404	43.819
11	Diflubenzuron	33.169	1.538	42.226
12	Endrin	28.337	1.626	41.269
13	Prothiofos	39.530	1.245	40.521
14	**Fenitrothion**	33.480	1.417	40.351
15	Chlorobenzilate	34.226	1.385	40.203
16	Cyfluthrin	30.310	1.483	39.876
17	Ethalfluralin	43.557	1.078	39.748
18	Copper	20.333	1.768	39.639
19	**Dieldrin**	33.377	1.367	39.466
20	Vanadium	24.204	1.602	38.796
21	Polychlorinated biphenyls (PCBs)	36.958	1.201	38.498

Table 83. Ranking Results of the Sensitivity Analysis (cont'd)

RANK	***CHEMICAL NAME***	***COMMPS SCORE***	***NORMAN SCORE***	***INTEGRATED SCORE***
22	Aluminium	17.846	1.772	38.451
23	Silver	18.151	1.699	37.385
24	**Tris(nonylphenyl) phosphite; TNPP**	42.000	0.975	37.250
25	Atrazine-desethyl (Deethylatrazine)	33.281	1.197	36.587
26	**Malathion**	26.122	1.392	36.255
27	**Quinalphos**	33.979	1.155	36.240
28	2-Chloronaphthalene	45.874	0.785	36.014
29	Acetochlor	25.021	1.402	35.877
30	**Triclosan**	30.577	1.233	35.844
31	Barium	18.340	1.577	35.448
32	Iron	16.367	1.627	35.294
33	PCB 28	25.259	1.359	35.272
34	PCB 153	29.956	1.204	35.049
35	**Fenbutatin oxide**	31.687	1.150	35.010
36	Diflufenican	27.617	1.246	34.572
37	PCB 180	27.649	1.243	34.538
38	**Oxadiazon**	33.544	1.058	34.411
39	4.4'-DDD	35.135	1.001	34.258
40	Carbendazim	31.980	1.094	34.215
41	Pendimethalin	26.485	1.251	34.093
42	**Tolfenpyrad**	35.702	0.955	33.768
43	Chlorothalonil	32.760	1.034	33.614
44	PCB 138	23.990	1.291	33.514
45	Benzo[*e*]pyrene	31.963	1.013	32.861
46	Diazinon	20.047	1.351	32.540
47	Carbofuran	23.370	1.234	32.258
48	**Pyridaben**	33.979	0.908	32.128
49	Fenpropathrin	26.411	1.134	32.112
50	Fenpropimorph	40.351	0.699	31.824

Table 83. Ranking Results of the Sensitivity Analysis (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
51	**Propetamphos**	29.125	1.025	31.646
52	**4.5-dichloro-2-octyl-2H-isothiazol-3-on; DCOIT**	33.979	0.875	31.573
53	**Phenthoate**	28.326	1.030	31.330
54	PCB 52	24.402	1.145	31.285
55	Trifloxystrobin	28.091	1.034	31.285
56	**Clofibric acid**	35.035	0.825	31.267
57	4.4'-DDE	24.904	1.126	31.217
58	Phenanthrene	27.672	1.032	31.038
59	**Chlordane**	25.364	1.067	30.459
60	4-Chloroaniline	25.858	1.028	30.061
61	Lindane	28.341	0.939	29.812
62	**Musk xylene**	32.354	0.808	29.649
63	**Pyriproxyfen**	30.583	0.858	29.597
64	**Triflumuron**	29.125	0.900	29.562
65	1.4-Dichlorobenzene	26.678	0.968	29.467
66	Azinphos-methyl	22.939	1.076	29.403
67	Bis(2-ethylhexyl) terephthalate	28.553	0.896	29.211
68	**PCB 101**	25.148	0.992	29.102
69	Boron	13.264	1.341	28.981
70	Parathion-methyl	26.930	0.927	28.911
71	Tridecane	36.355	0.637	28.792
72	Methidathion	22.123	1.064	28.787
73	**Methomyl**	19.052	1.155	28.776
74	Cadusafos	22.086	1.059	28.699
75	**Fludioxonil**	22.191	1.050	28.595
76	**Pirimicarb**	19.919	1.117	28.570
77	**2-Amino-4-chlorophenol**	40.306	0.497	28.431
78	Silicon	13.333	1.285	28.083
79	**Nitrofen**	28.364	0.825	27.932
80	**Tolclofos-methyl**	23.878	0.958	27.911

Table 83. Ranking Results of the Sensitivity Analysis (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
81	**Tefluthrin**	23.134	0.975	27.817
82	**Prometryn**	15.682	1.192	27.702
83	**Terbuthylazine**	16.370	1.167	27.629
84	Monocrotophos	19.855	1.059	27.583
85	Dibutyl phthalate (DBP)	26.378	0.863	27.576
86	Nitrobenzene	23.915	0.906	27.051
87	Fluorene	28.286	0.773	27.023
88	**Aldrin**	28.435	0.767	26.995
89	Tebuconazole	28.691	0.736	26.614
90	Diethyl phthalate	24.224	0.864	26.519
91	**PCB 31**	21.322	0.950	26.494
92	**Pyraclostrobin**	22.527	0.900	26.263
93	**2.4-D. isooctyl ester**	36.322	0.475	26.078
94	Diphenyl ether (Diphenyl oxide)	25.219	0.802	25.974
95	1-Chloronaphthalene	27.848	0.713	25.806
96	**Quizalofop-p-ethyl**	19.893	0.950	25.780
97	**17 alpha Ethinyl Estradiol**	32.087	0.580	25.710
98	**Butralin**	36.753	0.425	25.460
99	Dioctyl Phthalate	29.718	0.620	25.189
100	**Dibutyltin oxide**	30.295	0.597	25.092
101	Epoxiconazole	21.648	0.856	25.089
102	Metam Potassium	36.274	0.396	24.744
103	**Fenamiphos**	16.524	0.983	24.651
104	**Spiroxamine**	19.760	0.875	24.463
105	**Chlorantraniliprole**	18.549	0.900	24.274
106	**Metazachlor**	12.825	1.067	24.190
107	Biphenyl	21.390	0.798	23.990
108	Captan	29.201	0.558	23.896
109	Decamethylcyclopentasiloxane	16.056	0.949	23.850
110	Myclobutanil	22.939	0.740	23.809

Table 83. Ranking Results of the Sensitivity Analysis (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
111	1-chloro-2.4-dinitrobenzene	19.656	0.831	23.682
112	**Linuron**	20.816	0.792	23.602
113	**17 beta Estradiol**	27.477	0.580	23.405
114	Piperonyl butoxide	23.273	0.703	23.351
115	**Propylbenzene**	23.020	0.708	23.316
116	Benzyl butyl phthalate	21.477	0.747	23.182
117	**Tetrabromobisphenol A (TBBP-A)**	19.246	0.805	23.039
118	**4-Aminoazobenzene**	28.866	0.500	22.766
119	Chrysene	21.549	0.711	22.628
120	**Prochloraz**	29.884	0.458	22.581
121	**Trichloroethylene (TRI)**	22.185	0.683	22.481
122	1-Methylnaphthalene	28.319	0.488	22.296
123	**1.2.4.5-tetrachlorobenzene**	17.850	0.792	22.119
124	**Bromopropylate**	21.264	0.675	21.882
125	Cyromazine	18.198	0.749	21.586
126	Pyrene	25.453	0.519	21.372
127	**Hexythiazox**	26.745	0.475	21.289
128	**Carbon tetrachloride**	21.541	0.625	21.187
129	Chlorsulfuron	18.450	0.712	21.086
130	**Styrene; Vinylbenzene**	22.922	0.572	20.989
131	**Vinclozolin**	22.560	0.580	20.946
132	Bisphenol A	17.458	0.728	20.859
133	1.3-Dichlorobenzene	13.638	0.831	20.670
134	Imidacloprid	17.022	0.727	20.625
135	**Triadimenol**	20.835	0.600	20.417
136	1.1-dichloroethane	12.976	0.821	20.163
137	Penconazole	24.899	0.461	20.140
138	**Chloroacetic acid**	15.525	0.742	20.123
139	**N.N.N'.N'-tetramethyl-4.4'-methylenedianiline (Michler's base)**	22.623	0.525	20.062

Table 83. Ranking Results of the Sensitivity Analysis (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
140	p-(1.1-dimethylpropyl)phenol	18.901	0.629	19.940
141	**2.4.5-Trichlorophenoxyacetic acid**	17.439	0.672	19.914
142	Chlorfenapyr	22.423	0.522	19.914
143	Flutriafol	21.455	0.547	19.837
144	Meta-xylene	12.109	0.825	19.800
145	**Omethoate**	17.319	0.667	19.771
146	Procymidone	18.789	0.621	19.738
147	**Fluazifop-P-butyl**	25.807	0.405	19.653
148	**Bromoxynil**	17.211	0.658	19.577
149	**Propiconazole**	18.754	0.608	19.516
150	Metrafenone	22.398	0.497	19.487
151	**Boscalid**	25.337	0.405	19.419
152	**Tecnazene**	19.631	0.575	19.399
153	**Difenoconazole**	22.020	0.500	19.343
154	Imazalil	18.259	0.609	19.286
155	**Tebuthiuron**	18.380	0.600	19.190
156	**Triphenyltin; Fentin**	11.126	0.817	19.174
157	Ethylene thiourea	21.091	0.518	19.174
158	Isodrin	20.585	0.530	19.119
159	Thiacloprid	18.458	0.580	18.889
160	2-Mercaptobenzothiazole	14.004	0.712	18.866
161	Molinate	20.158	0.510	18.586
162	**Propazine**	20.007	0.508	18.476
163	Cyprodinil	17.874	0.565	18.346
164	Carbaryl	17.645	0.559	18.145
165	**Ortho-xylene**	10.945	0.758	18.111
166	Dimethoate	11.998	0.724	18.064
167	**2.3.4.5.6-Pentachlorotoluene**	30.520	0.165	18.010
168	**Methamidophos**	12.941	0.692	17.998
169	**Propyzamide**	18.865	0.505	17.849

Table 83. Ranking Results of the Sensitivity Analysis (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
170	Benzyl benzoate	26.083	0.278	17.675
171	Titanium	14.500	0.617	17.535
172	3.6-dimethylphenanthrene	23.261	0.351	17.477
173	**2-Methyl-4.6-dinitrophenol**	12.165	0.683	17.472
174	**Dinobuton**	19.978	0.430	17.155
175	**Tribenuron-methyl**	18.182	0.483	17.147
176	Tin	17.957	0.490	17.146
177	Nicosulfuron	17.717	0.496	17.130
178	**Tribromobiphenyl ether**	15.487	0.560	17.077
179	4-Chloro-3-methylphenol	9.737	0.726	16.968
180	Lenacil	13.869	0.598	16.907
181	**Diethofencarb**	19.395	0.425	16.781
182	Acenaphthene	13.885	0.585	16.698
183	Hexaconazole	16.701	0.489	16.506
184	**2.4-Dichlorophenoxyacetic acid**	10.352	0.672	16.370
185	**4.4'-Dibromodiphenyl Ether**	18.840	0.410	16.253
186	Beryllium	5.791	0.783	15.953
187	**Carboxin (Vitavax)**	19.811	0.355	15.822
188	**Clofentezine**	17.408	0.425	15.787
189	Buprofezin	20.509	0.329	15.737
190	**1.2.4-Trimethylbenzene**	18.975	0.372	15.682
191	Diclofenac	18.396	0.387	15.656
192	Metolachlor	12.719	0.556	15.627
193	**Demeton**	16.477	0.422	15.266
194	**Ethoprophos**	16.219	0.425	15.193
195	Mepiquat Chloride	15.252	0.446	15.064
196	Sulfamethoxazole	12.904	0.517	15.062
197	**Benzo(a)fluorene**	20.177	0.297	15.033
198	Picloram	11.871	0.542	14.977
199	**Fluquinconazole**	17.327	0.375	14.913

Table 83. Ranking Results of the Sensitivity Analysis (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
200	**Isopropylbenzene. cumene**	10.031	0.592	14.876
201	**Cyclanilide**	16.165	0.405	14.832
202	**Triasulfuron**	16.306	0.400	14.820
203	**Dichlobenil**	10.330	0.575	14.748
204	**Bromophos-methyl**	19.417	0.300	14.708
205	**1.3.5-trimethylbenzene (Mesitylene)**	18.110	0.338	14.694
206	**Thiometon**	16.524	0.375	14.512
207	**Bentazon**	11.604	0.522	14.496
208	Azoxystrobin	16.778	0.359	14.378
209	**Bromophos-ethyl**	17.797	0.325	14.315
210	**Flutolanil**	14.371	0.425	14.269
211	Diphenylamine	13.753	0.435	14.133
212	**Fenhexamid**	13.045	0.455	14.106
213	Chloridazon. pyrazon	12.075	0.479	14.019
214	Pyrimethanil	9.640	0.546	13.913
215	**2.4.6-Tri-tert-butylphenol**	16.334	0.333	13.723
216	**Methoxyfenozide**	17.015	0.305	13.591
217	Metalaxyl	14.739	0.368	13.498
218	2.6-Xylenol	15.193	0.353	13.471
219	**Dimethomorph**	11.845	0.450	13.423
220	Metamitron	13.391	0.396	13.293
221	**Tributyl phosphate**	9.048	0.522	13.218
222	Butyltin Trichloride	13.177	0.394	13.153
223	**Dimethenamid**	12.112	0.425	13.139
224	Clopyralid	5.022	0.619	12.823
225	Diisobutyl adipate	15.507	0.300	12.745
226	Clothianidin	14.007	0.340	12.677
227	**Thiabendazole**	12.723	0.375	12.612
228	Propham	14.663	0.293	12.209
229	**Fluopyram**	10.657	0.400	11.995

Table 83. Ranking Results of the Sensitivity Analysis (cont'd)

RANK	*CHEMICAL NAME*	*COMMPS SCORE*	*NORMAN SCORE*	*INTEGRATED SCORE*
230	Fosetyl-al	10.439	0.398	11.847
231	Trinexapac-ethyl	9.397	0.408	11.500
232	2.6-Di-*tert*-butylphenol	13.618	0.281	11.496
233	**Ethofumesate**	11.074	0.338	11.176
234	**Fosthiazate**	9.594	0.375	11.047
235	**Oxadixyl**	8.104	0.400	10.719
236	**Thiophanate-methyl**	9.484	0.355	10.659
237	Mesotrione	8.479	0.382	10.607
238	**Thidiazuron**	15.098	0.175	10.466
239	Thiamethoxam	7.687	0.389	10.319
240	Propamocarb Hydrochloride	4.440	0.435	9.477
241	**Mandipropamid**	10.402	0.255	9.451
242	Fluroxypyr	3.913	0.440	9.282
243	**Imazapyr**	7.238	0.300	8.619
244	**Acetamiprid**	8.241	0.175	7.037
245	Dimethylaminosulfanilide	6.803	0.160	6.068
246	**EDTA**	Not measured		
247	**Tert-butyl-4-methoxyphenol**	Not measured		
248	Bromide	Excluded		
249	Total petroleum hydrocarbons (TPH)	Excluded		
250	Free Cyanide	Excluded		