EVALUATION OF MICROPOLLUTANT TOXICITY IN ERGENE RIVER DURING A DRY MONTH

by

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ABSTRACT

EVALUATION OF MICROPOLLUTANT TOXICITY IN ERGENE RIVER DURING A DRY MONTH

In this study, micropollutant analyses were carried out on water samples taken from Ergene River in August 2017. Additionally, acute toxicity values of each sample were determined by using Microtox test and relationship between micropollutants and toxicity was investigated. About 222 micropollutants analyzed in samples, 131 of which were detected at least once. Among them were priority pollutants, antibiotics, brominated flame retardants, nonylphenols, disinfectants, pesticides, plasticizers, fragrances and cyanotoxins. Benzyldimethyldodecylammonium (BAC-12), benzyldimethyltetradecylammonium (BAC-14), N,N-diethyl-m-toluamide (DEET), ofloxacin and 3,3',4,4',5,5'-hexachlorobiphenyl (PCB-169) were detected in all samples. Most substances were found in sample taken from Çorlu Creek while, least substances were detected in sample taken from the source of Ergene River. The highest toxicity was reported in sample taken from near to Ergene-1 Organized Industrial Zone and at this sample 15 heavy metals and 33 micropollutants were detected. Especially, hexa(methoxymethyl)melamine, damascone, PCB-169, aluminum, nickel, boron and zinc were found in high concentrations. Although relation of each pollutant with toxicity showed that BAC-14, benzylamine, nonylphenol diethoxylate, PCB-169, BAC-12, dicyclohexylamine, celestolide were probably contributed to toxicity, the regression was relatively low. Moreover, relation between actual toxicity and predicted mixture toxicity derived by using Concentration Addition and Independent Action toxicity prediction models. When water quality and toxicity were examined, the highest pollution were observed in Çorlu and Ergene Creek which are under pressure of textile and leather organized industrial areas and domestic discharges. Outcomes of this study may contribute in understanding the risk of micropollutants in Ergene River and developing discharge limits for these pollutants.

ÖZET

ERGENE NEHRİ’NDE KURAK DÖNEMDE TESPİT EDİLEN MİKROKİRLETİCİLERİN TOKSİSİTE DEĞERLENDİRMESİ

Bu tez çalışmasında, Ağustos 2017 ayında Ergene Nehri’nden alınan numunelerde mikrokirletici analizleri yapılmıştır. Ayrıca, her bir su numunesi için Microtox toksisite testi kullanılarak akut toksisite değerleri hesaplanmış ve saptanan mikrokirleticiler ile toksisite arasındaki ilişki araştırılmıştır. Numunelerde analiz edilen 222 mikrokirleticiden 131 tanesi en az bir numunede saptanmıştır. Bu mikrokirleticiler arasında öncelikli kirleticiler, antibiyotikler, bromlu alev geciktiriciler, nonilfenoller, dezenfektanlar, böcek ilaçları, plastikleştiriciler, koku maddeleri ve siyanotoksinler bulunmaktadır. Ergene Nehri’nden alınan bütün numunelerde, benzildimetildodesilamonyum (BAC 12), benzildimetiltetradesilamonyum (BAC 14), N,N-dietil-m-toluamid (DEET), ofloksasin ve 3,3',4,4',5,5'-hekzaklorlubifenil (PCB-169) tespit edilmiştir. En fazla kimyasal madde Ergene Nehri’nin yan kolu olan Çorlu Deresi’nden alınan numunede bulunurken, en az kimyasal madde Ergene Nehri'ni besleyen kaynaklardan alınan numunede saptanmıştır. En yüksek toksisite değeri, Ergene-1 Organize Sanayi Bölgesi’ne yakın bir yerden alınan numunede tespit edilmiş olup bu numunede 15 ağır metal ve 33 mikrokirletici madde saptanmıştır. Numunelerde, özellikle hekza(metoksimetil)melamin, damascone, PCB-169, alüminyum, nikel, bor ve çinko maddelerine yüksek konsantrasyonlarda rastlanmıştır. BAC 14, benzilamin, nonilfenol dietoksilat, PCB-169, BAC 12, disikloheksilamin ve celestolide maddelerinin toksisiteye en çok katkıda bulunan maddeler olduğu belirlenmiştir. Ayrıca, Konsantrasyon Ekleme ve Bağımsız Eylem toksisite tahmin modelleri kullanılarak her bir numune noktası için karışım toksisitesi hesaplanmış ve ölçülen toksisite değerleriyle arasındaki ilişki incelenmiştir. Su kalitesi ve toksisite incelendiğinde en yüksek kirlilik değerleri, tekstil ve deri organize sanayi bölgeleri ile evsel ve kentsel atık su deşarjlarının baskısı altında olan Çorlu ve Ergene Derelerinden alınan su numunelerinde gözlenmiştir. Çalışma kapsamında elde edilen sonuçlar Ergene Nehri’nde mikrokirleticilerden kaynaklanan riski anlamakta ve kirletici kaynakları için deşarj standartları belirlemekte kullanılabilir.

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LIST OF SYMBOLS/ABBREVIATIONS

Symbol	**Explanation**	**Unit**
Al	Aluminum	µg/L
B	Boron	µg/L
Ba	Barium	µg/L
Cd	Cadmium	µg/L
Co	Cobalt	µg/L
Cr	Chromium	µg/L
Cu	Copper	µg/L
Ni	Nickel	µg/L
R^2	Regression Coefficient	
Sn	Tin	µg/L
V	Vanadium	µg/L
Zn	Zinc	µg/L
µg/L	Micrograms per Liter	
(m/z)	mass-to-charge ratio	

Abbreviation	**Explanation**
AF	Assessment Factor
APAP	Acetaminophen
APCI	Atmospheric Pressure Chemical Ionization
APs	Alkyl Phenols
BAC 12	Benzyldimethyldodecylammonium
BAC 14	Benzyldimethyltetradecylammonium
BDE	Brominated Diphenyl Ethers
BPA	Bisphenol-A
CA	Concentration Addition
CAD	Nitrogen Gas
CAS	Chemical Abstract System
CE	Collision Energy
CECs	Contaminants of Emerging Concern
CUR	Curtain gas flow

DEET	N,N-Diethyl-m-toluamide
DEHP	Di(2-ethylhexyl)phthalate
DNPs	Dinitropyrenes
DP	Declustering Potential
EC_{50}	50% Effective Concentration
ECOSAR	Ecological Structure Activity Relations
EDA	Effect Directed Analysis
EDCs	Endocrine Disrupting Compounds
EI	Electron Impact
EMS	Enhanced Mass Scanning
EP	Entrance Potential
EPA	Environmental Protection Agency
EPI	Enhanced Product Ion
EQSs	Environmental Quality Standards
ESI	Electrospray Ionization
EU	European Union
FAB	Fast Atom Bombardment
FT-ICR	Fourier Transform Ion Cyclotron Resonance
GC	Gas Chromatography
GC-MS	Gas Chromatography-Mass Spectrometry
GC-MS/MS	Gas Chromatography - Tandem Mass Spectrometry
HBCDs	Hexabromocyclododecanes
HMMM	Hexa(methoxymethyl)melamine
HPLC	High-Performance Liquid Chromatography
HRMS	High-Resolution Mass Spectrometry
HTS	High-Throughput Screening
IA	Independent Action
IS	Ion Spray Voltage
LC	Liquid Chromatography
LC50	50% Lethal Concentration
LC-HRMS	Liquid Chromatography- High Resolution Mass Spectrometry
LC-MS	Liquid Chromatography-Mass Spectrometry
LC-MS/MS	Liquid Chromatography - Tandem Mass Spectrometry
LC-TOF-MS	Liquid Chromatography–Time of Flight Mass Spectrometry

LLE	Liquid-Liquid Extraction
LLME	Liquid-Liquid Microextraction
LOD	Limit of Detection
LogP	Octanol/Water Partition Coefficient
LOQ	Limit of Quantitation
MALDI	Matrix Assisted Laser Desorption Ionization
MCs	Microcystins
MRM	Multiple Reaction Monitoring
MS	Mass Spectrometry
MSD	Mass Detector
NOEC	No Observed Effective Concentration
NJ	Neighbor Joining
NVOCs	Non-Volatile Organic Compounds
OECD	Organization for Economic Co-operation and Development
PAHs	Polycyclic Aromatic Hydrocarbons
PBDEs	Polybrominated Diphenyl Ethers
PCPs	Personal Care Products
PFCs	Perfluorinated Compounds
PNEC	Predicted No Effect Concentration
PNEdf	Predicted No Effect Dilution Factor
POPs	Persistent Organic Pollutants
Q1	Parent ion
Q3	Fragment ion
QACs	Quaternary Ammonium Compounds
QqQ	Triple-Quadrupole
QSAR	Quantitative Structure-Activity Relationship
RC	Regenerated Cellulose
REACH	Registration, Evaluation, Authorization and Restriction of Chemicals
RT	Retention Time
SAR	Structure Activity Relations
SIM	Selected Ion Monitoring
SP	Sample Point
SPE	Solid-Phase Extraction

SPME	Solid-Phase Microextraction
SVOCs	Semi-Volatile Organic Compounds
TBEP	Tris(2-butoxyethyl) phosphate
TEM	Temperature
TIM	Total Ion Monitoring
TOF	Time-of-Flight
TUBITAK	Scientific and Technological Research Council of Turkey
UPLC	Ultra-Performance Liquid Chromatography
UPLC-MS/MS	Ultra-Performance Liquid Chromatography - Tandem Mass Spectrometry
UV	Ultraviolet
WFD	Water Framework Directive
WWTP	Waste Water Treatment Plant

1. INTRODUCTION

Nearly 142 million organic and inorganic chemical substances are registered to the Chemical Abstract System (CAS) and some of these chemicals are released into water bodies by various ways. Contamination of water resources with these chemical substances is one of the challenging environmental problems as polluted water resources are threatening both ecosystem and human health. The European Water Framework Directive (WFD) 2000/60/EC was introduced by the European Commission to combat water pollution through an audit policy. WFD aims to protect groundwater and surface waters and their dependent ecosystems, considering their natural, geographical and hydrological characteristics (EC, 2000). In this context, a list of "priority substances" that pose a risk to nature due to their high toxicity, high environmental resistance and high hydrophobicity was established and a Directive 2008/105/EC to set Environmental Quality Standards (EQSs) of priority substances in the field of water policy was published (EC, 2008). EQSs are needed to determine the concentrations of specific substances or substance groups that should not exceed in water, sediment or biota to protect human and environmental health. In order to set EQSs, acute and chronic toxicity data of the substances available in the literature are used (European Commission, 2003). Turkey also have several regulations to improve quality of the water bodies such as; "Water Pollution Control Regulation", "Surface Water Quality Regulation", "Monitoring of Surface Water and Groundwater Regulation", "Protection of Water Watersheds and Preparation of Management Plans Regulation", and "Pollution Caused by Dangerous Substances in and around Water Control Regulation" (Ministry of Environment and Urbanization, 2016).

However, the list of "priority substances" comprises only a part of many substances discharged into water bodies. In addition to priority substances, "contaminants of emerging concern (CECs)", whose existence and importance in the environment have been currently noticed, created an increasing concern as well, because despite of their high transformation and removal rates, they are released into the environment continuously (Barceló and Petrovic, 2008). More than one thousand chemicals, including pharmaceuticals, personal care products (PCPs), endocrine disrupting compounds (EDCs), pesticides, biocides, flame retardants, algal toxins, metals, surfactants, artificial sweeteners, gasoline additives and industrial chemicals, have been listed as CECs by the EU NORMAN Network (Gomez et al., 2011; Gasperi et al., 2008; Boxall, 2012; Bletsou et al., 2015).

It is crucial to identify the sources of those contaminants in order to minimize their effect on receiving water environment. Such contaminants are released into water bodies through point or non-point sources. In general, non-point sources are diffused sources such as agricultural areas from where contaminants such as pesticides are released into the aquatic environment through irrigation run-off (Chen et al., 2014). On the other hand, point sources such as; wastewater discharges of urban and industrial areas contain contaminants such as alkyl phenols (APs), phthalates, phenols, anilines, polycyclic aromatic hydrocarbons (PAHs), flame retardants, personal care products, pharmaceuticals and biocides (Sanchez-Avila et al., 2009). Untreated municipal wastewater and wastewater treatment plant (WWTP) effluents are the primary point sources of CECs in the surface water (Petrovic et al., 2003). Since such contaminants cannot be treated with conventional wastewater treatment systems and regulations have not been developed to limit their release into the environment in many countries, they reach threatening levels and pose risk to human health and environment (Sanchez-Avila et al., 2009). Presence of those chemical substances in receiving environments leads to toxicity and endocrine disruption in marine organisms (Porte et al., 2006), neurotoxicity (Tiffany-Castiglioni et al., 2006), and ecosystem transformation.

Conventionally, chemical analysis methods are used to monitor environmental risks associated with priority substances and CECs. That is, if the measured concentration of a contaminant is higher than its environmental quality standard or any standard set by a regulatory agency, the water body and associated ecosystem as well as population that use the water are under risk. However, priority substances and CECs are commonly present in water bodies at a very low concentration together and they produce unidentified by-products by biotransformation. Thus, it is complicated and difficult to evaluate the overall risk that is posed by the complex mixtures of those toxic chemicals in water bodies. For this reason, in addition to sensitive instrumental methods like liquid chromatography (LC) or gas chromatography (GC) coupled with tandem mass spectrometry (MS), high throughout toxicity screening tools must be used for the rapid evaluation of overall quality of a water body and the associated risk (Galassi et al., 2004; Marugan et al., 2012; Latif and Licek, 2004).

As suggested by WFD, the combination of chemical analysis and toxicity tests is necessary to assess water quality comprehensively and evaluate the impact of chemical pollution in a surface water more realistically (Müller et al., 2018), since chemicals may contribute to mixture effects, even though they are present at low concentrations (Tang et al., 2013). Combined application of chemical and biological analysis is a completing strategy for water quality monitoring since, chemical analysis cannot estimate the bioavailability of substances and cannot predict mixture effects of contaminants in complex water matrices. On the other hand, bioassays play significant role to analyze possible adverse effects of chemicals such pesticides, hormones, pharmaceuticals etc. in water bodies (Hernando et al., 2006).

The study area, Ergene Watershed, is in the Thrace Region of Turkey and it is one the most important watersheds in Turkey. However, the watershed is facing a major environmental deterioration due to rapid and uncontrolled urbanization, industrialization and agricultural activities. Since 1970s, many organized industrial zones were established around the Thrace Region. Increased industrialization and population density led to significant environmental pollution on the Ergene Basin and the Ergene River. This pollution is caused by discharging of domestic and industrial wastewater to the river without or inadequate treatment. Moreover, agricultural wastewater contaminated with pesticides and fertilizers also reach the river with the surface run-off (Ministry of Agriculture and Forestry, 2018).

Ergene River is the most important surface water source of the region and water quality of the Ergene River has seriously decreased due to agricultural and industrial activities and lack of properly working WWTPs. In order to improve Ergene River water quality, Ministry of Environment and Urbanization has published two circulars as “Circular on Ergene Watershed Protection Action Plan” and “Circular on Restriction of Discharge Standards in Ergene River”. Poor water quality of Ergene River affects adversely the public health and the agricultural production in the region. Ergene River is mostly used for irrigation in agriculture while the groundwater resources are used for drinking and utility water, but the drastic decline in the groundwater levels leads to the possibility of using Ergene River as a source of drinking water. (Ministry of Environment and Urbanization, 2016). Therefore, improving the water quality of the Ergene River is of great importance. In order to improve the water quality of the Ergene River, proper treatment of the domestic and industrial wastewater before their discharge to the receiving environment and reduction of the chemicals used for agricultural activities is necessary (Ministry of Environment and Urbanization, 2016).

The objective of this study is to evaluate the contribution of micropollutants present in the Ergene River to the toxicity. Specific objectives are (1) to identify contaminants and their potential sources in Ergene River; (2) to evaluate toxicity along the Ergene River; (3) to determine toxicity-pollutant relationship; (4) to predict mixture toxicity and to identify the potential toxicity risk zones in the Ergene Watershed.

2. LITERATURE REVIEW

2.1. Study Area

Ergene Watershed, which is the subject of this study, is a part of Thrace Region located in northwest of Turkey. Ergene Watershed has a total catchment area of 12 438 km^2 with an east-west length of 160 km and a north-south length of 140 km. The most important surface water resources in the watershed are the Ergene River and its streams (Ministry of Agriculture and Forestry, 2018). The topographical map showing the Ergene River and its streams is given in Figure 2.1.

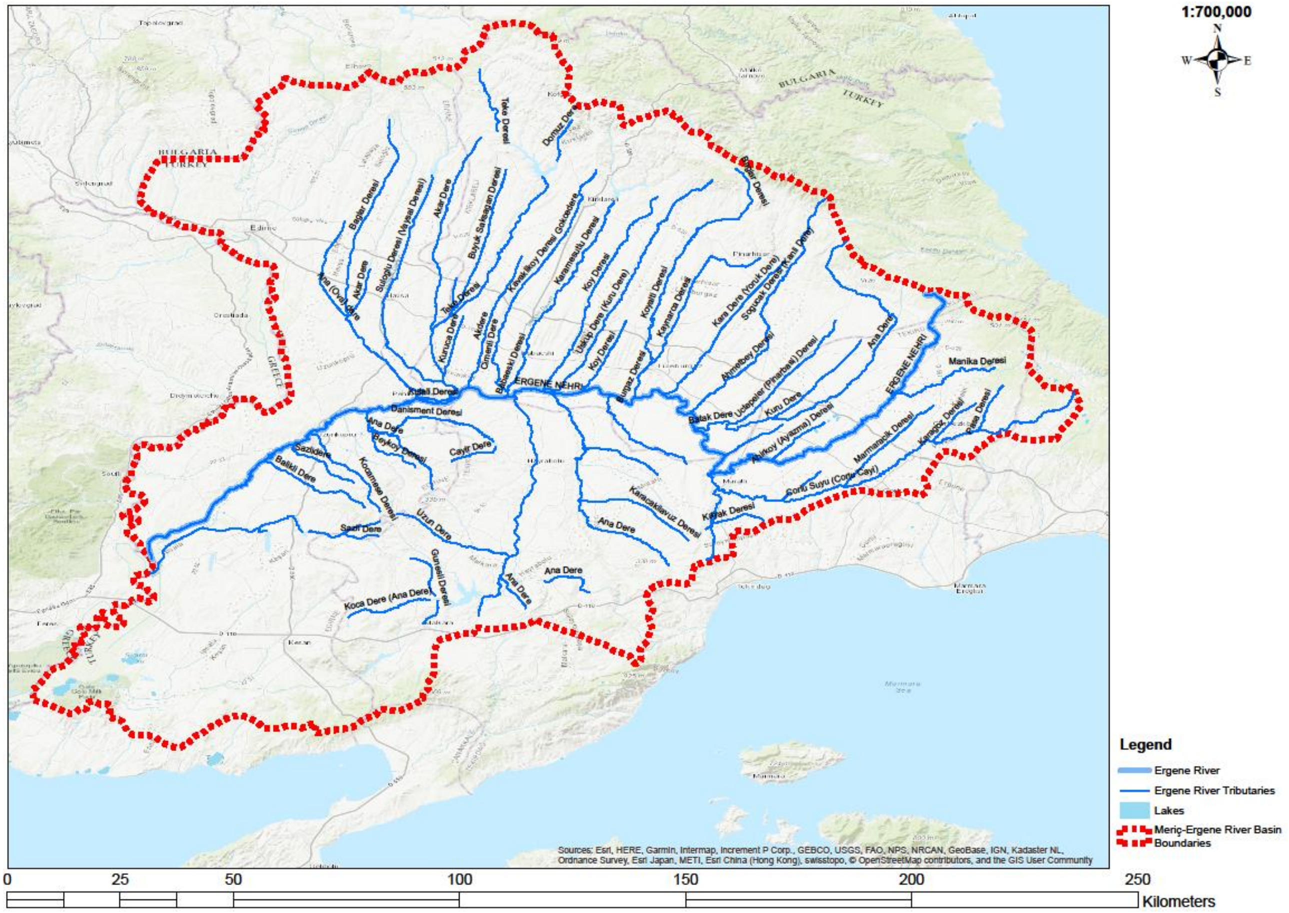

Figure 2.1. Topographic map of the Ergene River Basin.

Tekirdağ, Kırklareli and Edirne are three cities in Ergene Watershed where total of 1 768 000 people lives (TurkStat, 2017). When the population distribution of the provinces in Ergene Basin is examined, it is observed that the population density of Tekirdağ province is higher than other provinces. Population density in Tekirdağ has increased as a result of the decentralization of industrial facilities from Istanbul to Tekirdağ. The population showed a similar trend of increase in the other provinces of Ergene Basin from 2012 to 2017 (Table 2.2.).

Table 2.2. Population for districts within provinces of Edirne, Kırklareli, and Tekirdağ (TurkStat, 2017).

	2012	2013	2014	2015	2016	2017
EDİRNE						
Merkez	162 161	164 048	165 979	171 386	173 037	178 910
Enez	10 516	10 497	11 203	10 580	10 494	10 434
Havsa	20 457	20 248	19 976	19 380	19 292	18 881
İpsala	29 770	29 021	28 915	28 249	27 822	27 402
Keşan	79 716	79 889	80 486	81 054	80 894	81 747
Lalapaşa	7 279	7 194	7 077	6 979	6 834	6 601
Meriç	15 365	14 782	14 509	14 259	14 028	13 801
Süloğlu	8 383	7 870	7 823	7 457	7 000	7 159
Uzunköprü	66 061	65 033	64 312	63 193	62 300	61 920
Total	**399 708**	**398 582**	**400 280**	**402 537**	**401 701**	**406 855**
KIRKLARELİ						
Merkez	88 956	89 509	92 514	95 274	97 626	100 116
Babaeski	50 559	49 992	49 121	47 851	47 950	48 229
Demirköy	8 782	8 455	8 566	8 448	8 464	8 482
Kofçaz	2 924	2 702	2 707	2 644	2 564	2 434
Lüleburgaz	137 872	138 827	140 236	142 840	145 263	147 325
Pehlivanköy	4 211	4 140	3 965	3 790	3 681	3 593
Pınarhisar	19 686	19 035	18 914	18 704	18 580	18 513
Vize	28 228	27 899	27 700	27 422	27 556	27 358
Total	**341 218**	**340 559**	**343 723**	**346 973**	**351 684**	**356 050**
TEKİRDAĞ						
Merkez	176 848	179 239	182 522	187 727	191 864	196 031
Çerkezköy	188 712	113 134	123 119	133 626	146 319	157 931
Çorlu	273 362	225 540	235 630	245 588	253 551	260 437
Hayrabolu	34 478	33 839	33 488	32 602	32 158	32 035
Malkara	54 121	53 293	53 014	52 663	52 331	52 456
Marmara E.	21 469	22 816	23 476	23 452	24 043	24 598
Muratlı	23 341	26 764	26 821	26 987	27 561	28 127
Saray	46 999	47 171	47 522	48 272	48 834	49 180
Kapaklı	-	85 898	92 003	97 700	105 243	112 269
Ergene	-	56 787	57 613	58 311	59 641	60 881
Şarköy	29 991	29 994	31 524	30 982	31 330	31 518
Total	**852 321**	**874 475**	**906 732**	**937 910**	**972 875**	**1 005 463**
TOTAL	**1 593 247**	**1 613 616**	**1 650 735**	**1 687 420**	**1 726 260**	**1 768 368**

Ergene River, which is a 289 km long river, is the only running surface water in the area. It is born in Strandzha Mountain and joins to Maritsa River, then flows into the Aegean Sea from Gulf of Saros. Ergene River is one of the most polluted rivers in Turkey. Agricultural and industrial activities have increased significantly in the region over the last 20 years. About 18 organized industrial zones (Table 2.2.) and more than 1300 industrial facilities that operating in textile, leather, metal and chemical industries are located at the watershed and a significant portion of industrial plants are mainly located at the Çorlu – Çerkezköy sub-basin, for that reason pollution starts from this region (Ergene Basin Action Plan, 2008). Due to agricultural and industrial activities, pollution of the river has become easily visible, in fact a major part of Ergene River has “4th Class” (very dirty water) of water quality, currently (Ministry of Environment and Urbanization, 2016).

Table 2.3. Organized Industrial Zones located in Ergene Basin.

No	Name	Province	District	Latitude	Longitude
1	Çerkezköy OIZ	Tekirdağ	Çerkezköy	41.313944	27.978931
2	Çorlu Leather OIZ	Tekirdağ	Çorlu	41.184269	27.773839
3	Hayrabolu OIZ	Tekirdağ	Hayrabolu	41.223700	27.047100
4	Malkara OIZ	Tekirdağ	Malkara	40.872764	27.024051
5	Veliköy OIZ	Tekirdağ	Çerkezköy	41.263171	27.942033
6	Ergene-1 OIZ	Tekirdağ	Çorlu	41.267096	27.645467
7	Ergene-2 OIZ	Tekirdağ	Çorlu	41.236373	27.708831
8	Çorlu-1 OIZ	Tekirdağ	Çorlu	41.133080	27.858531
9	Velimeşe OIZ	Tekirdağ	Çorlu	41.208639	27.844655
10	Muratlı OIZ	Tekirdağ	Muratlı	41.186670	27.510065
11	Kapaklı OIZ	Tekirdağ	Çerkezköy	41.317251	27.969479
12	Yalıboyu OIZ	Tekirdağ	Çerkezköy	41.241804	27.932651
13	Tekirdağ OIZ	Tekirdağ	Merkez	40.965278	27.415833
14	Edirne OIZ	Edirne	Merkez	41.825073	26.832100
15	Uzunköprü OIZ	Edirne	Uzunköprü	41.181104	26.669983
16	Kırklareli OIZ	Kırklareli	Merkez	41.691950	27.335536
17	Büyükkarıştıran OIZ	Kırklareli	Lüleburgaz	41.281977	27.573291
18	Evrensekiz OIZ	Kırklareli	Lüleburgaz	41.353343	27.469081

Agricultural areas cover nearly 70% of the watershed and Ergene River is predominantly used for irrigation purposes while the drinking water demand of the region is mostly supplied from groundwater sources. However, because of the population growth and industrial activities, substantial reductions are observed in the groundwater levels, therefore the use of Ergene River water as drinking water in the future is possible. In addition to water pollution, soil contamination, desertification and deterioration of crop quality is taking place because of the usage of polluted river as a source of irrigation water (Ministry of Agriculture and Forestry, 2016).

Ergene Watershed is an important agricultural area, since the substantial portion of Turkey's wheat, sunflower and rice need is met by this region. About 55% of the rice produced in Turkey is produced in Ergene Watershed. Moreover, due to its fertile soil, many agricultural products are grown in this region such as sugar beet, barley, watermelon, onion, oats, corn, clover, vetch, tomatoes and other vegetables (Ministry of Environment and Urbanization, 2016).

2.2. Micropollutants: Analysis, Sources and Occurrence in the Surface Water

Micropollutants are bioactive and persistent contaminants which are mostly entered in aquatic environments due to anthropogenic activities. Micropollutants such as priority pollutants and CECs are commonly present in water bodies at trace concentrations ranging from ng/L to µg/L but they cannot be effectively removed with conventional treatment techniques. Although they are found at low concentrations, there is an emerging concern about their impact on both human health and ecosystem, since they continuously enter water bodies and they cause toxicity at very low concentrations. Continuous release of these contaminants into the environment has long-term detrimental effects on living organisms, because they are bioaccumulative and their impacts on environment as mixture are not known. In addition, biotransformation of these chemical substances forms unknown by-products, therefore precise and accurate analytical methods are required to detect micropollutants in water bodies such as; gas chromatography (GS) or liquid chromatography (LC) coupled with mass spectrometry (MS) (Pochodylo and Helbling, 2017).

However, it is difficult to detect and quantify micropollutants in the aquatic environment due to very low concentrations and complexity of water matrices. For instance, wastewater samples contain lots of interfering substances that cause complex matrix effects and hence comprehensive extraction methods are required to obtain the analytes. Therefore, it is critical to extract, concentrate and clean-up the samples before the detection and so sample preparation is an essential step because of the trace levels of substances in complex matrices (Bohdziewicz et al., 2015). Various sample preparation techniques are available for effective analysis of substances at trace levels such as; liquid-liquid extraction (LLE), solid-phase extraction (SPE), liquid-liquid microextraction (LLME) and solid-phase microextraction (SPME) (Çeçen and Tezel, 2017).

LLE is used to transfer the analytes from an aqueous phase to another (generally an organic solvent) based on the partition coefficients in two different immiscible liquids. Although it is one of the first extraction methods, a significant amount of toxic solvent usage does not make it appealing. However, it is still widely used for some aqueous pollutants. After LLE, analytes are preconcentrated by evaporation of the solvent (Çeçen and Tezel, 2017).

SPE is used to immobilize the analytes in a liquid sample (mobile phase) on an adsorbent bed (stationary phase) and then to separate. The beds are usually made from polymeric or silica-based cartridges, small disks or 96-well plates. SPE is preferred to LLE, because most of the hydrophilic contaminants are not well separated in an organic solvent and due to their low extraction efficiencies. SPE is a simple, time-saving method that uses a smaller amount of toxic solvent and can be better adapted to automation (Çeçen and Tezel, 2017).

Mass spectrometry is a detection method that is used to identify molecules by means of the separation of gaseous ions with respect to their mass to charge ratio by using electric and magnetic fields. It also provides information about structures of the molecules by fragmentation of the ions. Mass spectrometry, which has been used since the early 1900s, was first used to determine the atomic weights of the elements (De Hoffmann, 2000).

Several methods of ionization are used in mass spectrometry techniques. Electron Impact (EI) and Fast Atom Bombardment (FAB) are the classical and most common methods. However, in current MS techniques these methods are slightly applied except from EI is used with GC-MS for environmental studies. Instead of EI and FAB methods, Atmospheric Pressure Chemical Ionization (APCI), Electrospray Ionization (ESI) and Matrix Assisted Laser Desorption Ionization (MALDI) methods are presently used in mass spectrometry. APCI is preferred over EI because APCI generates a protonated or deprotonated ion and complies with LC, whereas EI does not complies with LC and leads to uncertain detection of the molecular weight since it has higher possibility of ion fragmentation. FAB was the earlier method that made protonation of non-volatile compounds possible. MALDI and ESI abolished the use of FAB because they allow ionization and analysis of heavier molecules than FAB. ESI is conveniently compatible with LC, while MALDI is mainly applied in imaging mass spectrometry (De Hoffmann, 2000).

Various mass spectrometry systems are available with different mass-to-charge ratio (m/z) separation techniques, such as magnetic sector MS, triple-quadrupole (QqQ) MS, time-of-flight

(TOF) MS, Fourier transform ion cyclotron resonance (FT-ICR) MS or Orbitrap MS. TOF, FTICR and Orbitrap emerged as new analytical techniques in trace environmental analyses due to their high-resolution mass spectrometry (HRMS) capabilities (Günthardt, 2016). Modern HRMS instruments provide accurate mass data while combining enough selectivity and sensitivity, which allows the determination of trace substances in complex environmental matrices (Bader et al.,2016).

The advantage of using HRMS, such as TOF MS or Orbitrap MS for analysis is the use of a full-scan operating mode, which can provide high precision without limiting the number of simultaneously monitored substances. HRMS can be used to identify both target and non-target compounds in complex matrices since it has high resolution, accurate mass measurement and high full-scan accuracy (Gómez-Ramos et al., 2013).

Methods such as gas chromatography-mass spectrometry (GC-MS) and liquid chromatography-mass spectrometry (LC-MS) are widely used for identification and quantification of chemical substances at low concentrations. Whereas GC-MS is generally used for measurement of volatile and semi-volatile nonpolar chemical substances, LC-MS is used for analysis of a broader contaminants range including both nonpolar and polar compounds. Also, LC-MS is more applicable and accurate instrumental method for measurement of chemical substances in water bodies since sample extraction, which is an essential pretreatment for aqueous samples in GC-MS analysis, is not required most of the times in LC-MS analysis (Eken et al., 2017).

LC analysis is steady, rapid and comparatively simple to attach to a mass spectrometer or other detection devices and has satisfying repeatability. There are various compounds of interest that have different chemical properties. In this manner, numerous chromatographic separation methods are developed (Tohmola, 2015).

LC attached with mass spectrometry is a method that used extensively for the detection of micropollutants in water samples. There are two types of LC; such high-performance liquid chromatography (HPLC) and ultra-performance liquid chromatography (UPLC), is used to determine chemicals in water samples. HPLC is a highly effective analytical tool used for separation, identification, and quantitation of chemicals in a water sample. UPLC is derived from HPLC. UPLC is recent and improved method that has increased resolution, speed, and sensitivity (McPeters, 2012). In UPLC, tinier particle and column sizes are used, and analytes are separated under very high pressure. The main benefits of UPLC is narrower peaks, higher peak capacities and reduced analyze times that leads to sensitivity and efficiency increase (Swartz, 2005).

A lot of chemicals can be detected at once by liquid chromatography coupled with high-resolution mass spectrometry (LC-HRMS). However, targeted analysis methods are only capable of detecting specific analytes and they cannot track the possible transformation by-products and other unknown analytes despite of their high concentrations (Bletsou et al., 2015).

Anthropogenically polluted surface waters are mainly dominated by surfactants, PCPs, pharmaceuticals, antibiotics, hormones, pesticides, flame retardants, chlorinated benzenes, ultraviolet (UV) filters, industrial compounds and their transformation by-products. These compounds are called as emerging contaminants and they entered to the water bodies due to point sources such as municipal, hospital and industrial WWTP discharges, sewer leakage, landfill leachate or non-point sources such as urban runoff from agricultural regions (Müller et al., 2018; Stasinakis et al., 2012; Yan et al., 2018; Torres et al., 2017; Kasprzyk-Hordern et al., 2009, Tran et al., 2018).

In the recent studies, existence of pharmaceuticals and hormones in the water bodies are recognized as an important environmental problem and substantial data on their formation became important to develop new effective treatment techniques to prevent or reduce their discharge to the environment. Discharges of pharmaceuticals into the environment may adversely affect the aquatic organisms living in receiving environments, because pharmaceuticals are designed to have a biological effect. Antibiotics and hormones that are extensively used in human and veterinary medication are also draw attention because of their possible role in the evolution of resistance mechanisms and their endocrine disruptive effects (Sousa et al., 2018).

Industrial discharges are also one of the major pollutant sources in the contamination of aquatic environments. The chemical properties and combination of the industrial wastewater vary according to the type of production process. Certain chemical substances are often discharged only by industries that apply specific manufacturing processes. For instance, halogenated anilines, benzenes, anthraquinones, volatile organic solvents and much more chemical substances were detected in the effluents from textile industries, while benzothiazoles, aniline derivatives, toluene and further compounds were found in the effluents from rubber and tire production (Dsikowitzky and Schwarzbauer, 2013).

Various industrial chemical substances such as phthalates, alkylphenols and perfluorinated compounds are known as priority pollutants and they pose a serious environmental risk due to their high detection frequency toxicity, persistence and bioaccumulation. Shores and estuaries are considered as the most sensitive environmental bodies to discharges of these contaminants directly or indirectly (Sousa et al., 2018).

Polycyclic aromatic hydrocarbons (PAHs) and polybrominated diphenyl ethers (PBDEs) are known as persistent organic pollutants (POPs) and they have been regularly monitored in surface waters. POPs are bioaccumulative, non-degradable and toxic compounds. Seven of the known PAHs are defined as possible human carcinogens. PAHs consist of two or more fused aromatic rings resulting from incomplete combustion of both anthropogenic sources like fossil fuels and natural sources like biomass. PAHs are generally released into the environment by engine exhausts, industrial activities, heating systems and forest fires and they cause atmospheric deposition in water bodies. Similarly, PBDEs are brominated flame retardants and they are continuously emitted to the atmosphere from urban areas, since they are widely used in consumer goods and industrial products. PBDEs are accumulated in the aquatic environment by wet and dry deposition. PBDEs and PAHs can also be emitted from low temperature burns, such as waste fires (Ruge et al., 2015; Sousa et al., 2018).

Organic UV filters are another group of compounds that are found in sunscreens, cosmetics, adhesives, plastics, paint and rubber. UV filters show resistance to degradation during traditional water treatment processes and increase bioaccumulation in the aquatic organisms and humans since they are lipophilic (Sousa et al., 2018).

Several studies have been performed in point of the occurrence of micropollutants in the water bodies such as surface water (Pal et al., 2010), groundwater (Lapworth et al., 2012), wastewater (Deblonde et al., 2011) and stormwater (Gasperi et al., 2013).

The occurrence of 30 micropollutants in the surface water bodies of 9 different countries was reviewed and the results were summarized in Table 2.3. According to the collected data and chemical analyses carried out through this study, chemical concentrations in surface waters of Turkey were higher for most of the reviewed chemicals as compared to other countries.

The occurrence of endocrine disrupting compounds (EDCs), personal care products (PCPs), pharmaceuticals, hormones, antibiotics, and flame retardants in Korean surface waters were studied by Kim et al. and Yoon et al. in 2007 and 2010, respectively. In both studies, solid phase extraction (SPE) was used to extract analytes and liquid chromatography with tandem mass spectrometry (LC-MS/MS) was used for analyzing.

Stasinakis and coworkers (2012) were investigated the presence of phenolic EDCs in Greek surface waters in 2012. In the study, first, samples were filtered, adjusted to pH 2.5 and extracted using C18 SPE cartridges, then analytes were analyzed using gas chromatography coupled with mass spectrometry (GC-MS). Likewise, Terzopoulou and colleagues (2014) were analyzed 70 organic micropollutants from different chemical classes, such as phenols, polycyclic aromatic hydrocarbons (PAHs), polychlorinated biphenyls (PCBs), pharmaceuticals and triazines, in Greek surface waters by using gas chromatography coupled to tandem mass spectrometry (GC-MS/MS).

Monitoring of 1300 organic micropollutants in Chinese surface waters was carried out by Kong and coworkers (2015). In the study, GC-MS, operating in both selected ion monitoring (SIM) and total ion monitoring (TIM) mode, was used for monitoring semi-volatile organic compounds (SVOCs), while liquid chromatography–time of flight mass spectrometry (LC-TOF-MS) was used for monitoring non-volatile organic chemicals (NVOCs) (Kong et al., 2015). Similarly, Yan and colleagues (2018) investigated the concentrations of various classes of organic micropollutants, such as pharmaceuticals, UV filters, perfluorinated compounds (PFCs), organochlorine pesticides, PCBs, PAHs and hexabromocyclododecanes (HBCDs) in the Chinese surface waters. In the study, samples were extracted using SPE and analyzed using an ultra-performance liquid chromatography with tandem mass spectrometry (UPLC-MS/MS) with an electrospray ionization (ESI) source or a gas chromatography coupled to a triple quadrupole mass spectrometer (GC-MS/MS).

Table 2.3. Occurrence of some micropollutants in surface waters in different countries.

Compound	Concentration (ng/L)								
	Korea[a,b]	Greece[c,d]	China[e,f,g]	Portugal[h]	USA[i]	Germany[j,k,l]	Canada[m]	Bulgaria[n]	Turkey*
3-Chloroaniline	-	-	3.3×104	-	-	-	-	-	1.6×10^{3}
Acetaminophen (Paracetamol)	73	-	395	-	342	53	298	-	1.1×10^{5}
Acetamiprid	-	-	82	-	14	-	-	-	1.9×10^{3}
Atrazine	0.61	-	183	41	204	-	-	18.11	50
Atrazine-desethyl	-	-	-	-	81	56	-	-	9.6×10^{3}
Azithromycin	-	-	-	50	-	-	-	-	79×10^{3}
Benzo(a)pyrene	-	-	16	-	-	-	-	-	980
Benzo(b)fluoranthene	-	40	87	-	-	-	-	-	4.4×10^{3}
Benzyldimethyldodecylammonium	-	-	-	-	-	-	-	-	2.4×10^{4}
Benzyldimethyltetradecylammonium	-	-	-	-	-	-	-	-	7.6×10^{3}
Bisphenol-A	59	162	25	-	-	215	87	4.8	4.9×10^{4}
Carbamazepine	61	-	5.3	177	262	-	749	78.6	-
Carbendazim	-	-	28	-	207	-	-	14.9	6.3×10^{3}
Chlorfenvinphos	-	880	-	-	-	-	-	-	440
Ciprofloxacin	-	-	25.5	-	207	-	-	-	5.2×10^{4}
Clarithromycin	-	-	25	44	266	-	-	2.51	2.7×10^{3}
Diuron	-	420	7	-	90	8	-	6.1	2.6×10^{3}
Erythromycin	4.8	-	25.1	-	-	-	145	5.18	1.1×10^{3}
Hexa(methoxymethyl)melamine	-	-	-	-	-	-	-	156	3.3×10^{7}
Isoproturon	-	860	-	92	4	72	-	-	-
N,N-Diethyl-m-toluamide (DEET)	69	-	-	-	3.9×10^{3}	-	-	15.8	3.6×10^{4}
Nonylphenol diethoxylate	-	-	-	-	-	-	-	-	1.2×10^{4}
Norfloxacin	-	-	39.17	-	24	-	-	-	4.2×10^{4}
Ofloxacin	-	-	23.47	-	195	-	-	-	5.3×10^{5}
Oxybenzone	2.7	-	-	-	404	-	-	-	650

Table 2.3. Occurrence of some micropollutants in surface waters in different countries (continued).

Compound	Concentration (ng/L)								
	Korea[a,b]	Greece[c,d]	China[e,f,g]	Portugal[h]	USA[i]	Germany[j,k,l]	Canada[m]	Bulgaria[n]	Turkey*
Polychlorinated biphenyls	-	-	18.18	-	-	-	-	-	4.7×10^5
Simazine	-	-	26	-	53	-	-	-	-
Sulfamethoxazole	36	-	40	-	678	322	284	37.2	3.3×10^3
Terbutryn	-	-	-	-	-	-	-	-	30
Triclosan	29	39	3	-	428	220	-	6.32	-
Trimethoprim	5.3	-	45	-	531	66	25	15	200
Tris(2-butoxyethyl) phosphate	-	-	-	-	-	652	-	-	2.7×10^5

[a] Kim et al., 2007; [b] Yoon et al., 2010; [c] Terzopoulou et al., 2014; [d] Stasinakis et al., 2012; [e] Kong et al., 2015; [f] Bu et al, 2015; [g] Yan et al., 2018; [h] Barbosa et al., 2018; [i] Carpenter and Helbling, 2018; [j] Müller et al., 2018; [k] Regnery and Püttmann, 2010; [l] Reinstorf et al., 2008; [m] Kleywegt et al., 2011; [n] Neale et al., 2015

* The highest concentrations determined in Ergene River within this study were used.

2.3. Evaluation of Micropollutant Toxicity

Environmental toxicology is a multidisciplinary scientific field that examines the harmful effects of chemical substances on living organisms. Based on the nature and scope of the antagonistic effects, fate and behavior of the substances, potential damage to the environment can be predicted. Environmental toxicology outcomes are used to forecast environmental hazard and risk caused by specific substances. The threat of these substances originates from their ability to adversely affect organisms, their chemical structures, physicochemical properties and environmental fate. Chemical substances are always in interaction with the environment and the main effect depends on this interaction (Gruiz et al., 2016).

2.3.1. Toxicity Prediction

There are thousands of chemical substances present in the environment and the possible effects of only a part of these substances on humans have been evaluated. The significance of toxicity has been increased since the scientists realized that many chemical substances are toxic to living organisms at levels below the limit of detection. Therefore, toxicity prediction methods are required to understand better the effects of these substances on humans and other living beings.

The Ecological Structure Activity Relationships (ECOSAR) program is used to predict aquatic toxicity by a computerized estimation system. The program forecasts the acute and chronic toxicity of chemicals by applying computerized Structure Activity Relationships (SARs) for marine organisms (ECOSAR, 2012).

The quantitative structure-activity relationship (QSAR) concept has been originally developed by Corwin Hansch and colleagues in the early 1960s and since then, it has been used for various purposes (Hansch et al., 1962). QSAR tries to obtain a quantitative relationship between the geometric and chemical properties of a molecule and its biological activity. QSAR models have been generated from correlation between chemical structures and toxicity. Due to elimination of experimental part, QSAR models save money and time, moreover most of times they take the place of animal testing and they promote greener chemistry by preventing experiments (Cronin, 2010).

U.S. EPA ToxCast Program (Kavlock et al., 2012) and the Tox21 program, which is a joint program of the National Institutes of Health, U.S. Environmental Protection Agency (EPA), and U.S.

Food and Drug Administration, are used to enhance molecular toxicology, systems biology and computational toxicology to reduce defects of *in vivo* testing. These programs rely on high-throughput screening (HTS) that is being used to identify chemical probes of gene, pathway, and cell functions, with the goal of comprehensively delineating relationships between chemical structures and biological activities (Escher et al., 2014).

2.3.2. Toxicity Assays

Toxicity assays analyze possible adverse effects of chemical substances on living organisms when released into the environment and aim to protect public health and improve water quality by screening negative impacts of test substances on both living beings and receiving environments.

Conventionally, *in vivo* toxicity tests on laboratory animals are conducted to predict adverse health effects of test substances on human beings. But, only a small number of substances can be analyzed since, these tests are expensive, time-consuming and they require high doses to obtain data (Krewski et al., 2010). On the contrary to *in vivo* animal toxicity tests, *in vitro* bioassays are conducted at the molecular or cellular stages in the laboratory. While molecular level tests contain attachment of enzymes or receptors, cellular level tests monitor cell viability and growth. A benefit of *in vitro* tests is that their results can be used to predict the effect of chemicals on human cells, consequently taking out the inter-species dilemma of entire animal testing. *In vitro* tests identify the toxicity that occurs at much lower concentrations, generally under the detection limits of chemical analysis and *in vivo* testing (Onyango, 2015).

Aquatic toxicity data are required to evaluate the effects of chemical substances on aquatic organisms. For years, toxicity evaluation of aquatic environments has been conducted with test organisms such as algae, daphnia, fish, plants, earthworms, mussels and oysters (Niemirycz et al., 2007). According to standardize toxicity testing, OECD prepared three test guidelines (TGs) for different trophic levels. OECD TG 201 Freshwater Alga and Cyanobacteria, Growth Inhibition Test (72-h EC_{50}), OECD TG 202 Daphnia sp. Acute Immobilization Test (48-h EC_{50}) and OECD TG 203 Fish, Acute Toxicity Test (96-h LC_{50}) were published to measure toxicity (OECD, 2011; OECD, 2004; OECD, 1992). Especially, algae have a significant part in aquatic toxicity tests since, they have an important role in aquatic ecosystems as primary producers (DeLorenzo, 2009).

In vitro bioassays are performed not only to evaluate toxicity of substances (Sanchez-Meza et al., 2007) but also to monitor and benchmark the water quality (Escher et al., 2013), as they are more rapid and economical than *in vivo* toxicity tests (Latif and Licek, 2004). There are many studies that use *in vitro* bioassays for toxicity testing in the literature for instance, Bengston Nash et al. (2005) used phytotoxicity bioassays to monitor herbicide residues in water, Vermeirssen et al. (2005) performed yeast bioassay to characterize the estrogenicity, Escher and coworkers (2008) used umuC genotoxicity test to monitor sewage treatment efficiency and Tang and colleagues (2013) measured cytotoxicity by Microtox assay to monitor water quality.

Microtox assay is a sensitive, rapid and cost-effective toxicity bioassay that uses a bioluminescent bacteria *Aliivibrio fischeri* (*V. fischeri*) as a model organism. The Microtox organism, *Aliivibrio fischeri* was chosen because it shows the highest sensitivity across a broad range of toxicants. Inhibition of the luminescence of the *Aliivibrio fischeri* is commonly used for monitoring the treatment of water bodies (Marugan et al., 2012) and used to evaluate the toxicity of chemicals, mixtures and moreover to environmental samples, such as surface water, wastewater treatment plant effluents, groundwater and landfill leachates (Escher et al., 2017). Microtox test can also be applied to contaminated soil, drinking water monitoring, ecotoxicology, hazardous waste, industrial or municipal effluents, industrial process water, marine water, medical/pharmaceutical products, mining wastes, personal care products, households, recreational water, sediments, solid phase materials and storm water.

Aliivibrio fischeri is a nonpathogenic, marine bacterium that shows bioluminescence as a natural part of its metabolism. And since this bacterium emits light during its metabolic activities, any reduction in the intensity of this emission reflects the deterioration of cellular metabolism caused by one or more toxic substances in the environment. Toxicity is usually expressed as an EC_{50} value which is the effective concentration that causes 50% reduction in the intensity of light emission. While microtox test is performed within 15 or 30 minutes, other toxicity bioassays (such as fish, daphnia and shrimp) are usually take several days (Zadorozhnaya, 2015). In the microtox test, a unique bacterial strain of *Aliivibrio fischeri* is used as *Reagent*, 2% NaCl in ultrapure water solution is used as *Diluent*, a bifunctional device that operates as both incubator and luminometer is used as *Analyzer* and *MicrotoxOmni* software is used for data capturing and analyzing (Johnson, 2005).

2.4. Environmental Risk Assessment

European Union (EU) has published a regulation for Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) on 1 June 2007 to protect human health and the environment against the risks that can be caused by exposure of chemical substances into the environment. REACH gathers a broad dataset on single compounds (ecotoxicity, uses and exposure), that should be provided in material safety data sheet of each substance.

Environmental risk assessment for chemicals are commonly carried out based on the standardized laboratory tests that use organisms from major trophic levels and identification of the highest concentration, which the environment is preserved, is a substantial step in the environment risk assessment (Jin et al. 2012). In this context, Predicted No Effect Concentration (PNEC) is determined by choosing the most susceptible trophic level and performing a convenient assessment factor (AF). It is based on the assumption that all other groups of organisms are conserved by preserving the most sensitive trophic level (Backhaus and Faust, 2012).

An important step in the environmental risk assessment of chemicals is to determine the maximum concentration at which the ecosystem is protected. For the aquatic environment, if only short-term toxicity data is applicable PNEC is calculated by AF of 1000 used on the $L(E)C_{50}$ of the relevant toxicity data. In other words, $L(E)C_{50}$ values are measured for each chemical and these values are multiplied by AF of 1000 and the resulting value is specified as the concentration that should be the maximum for this chemical in surface waters. If a single long-term NOEC data is available for the most sensitive species, PNEC is derived by using AF of 100. AF of 50 is applied when two long-term No Observed Effective Concentration (NOEC) data is available for two most sensitive trophic levels and AF of 10 is used when at least three long-term NOEC data is available for at least three species represents three trophic levels (EU Commission, 2003).

Besides using AF, PNEC can also be calculated by using statistical extrapolation techniques such as Species Sensitivity Distribution (SSD). SSD assumes that sensitivity to chemicals within target species is random. SSD approach is promising but it is limited by the lack of data for most chemicals and the only existent data is based on the lethal responses of a small group of test laboratory species (EU Commission, 2003).

However, it is rare to find an aquatic environment that is contaminated by a single chemical substance. In water bodies, several chemical substances are usually present in significant amounts. The probability of living organisms be exposed to several chemicals at the same time requires consideration of the possible interactions between chemicals and their effects on organisms (van Leeuwen et al., 2007).

2.4.1. Interpretation of Mixture Toxicity

The potential risk from mixtures of chemicals in the environment has recently emerged in the scientific world as a result of the increasing concern over the potential impact on the environment from a ‘cocktail effect’ and the perception of current risk assessment procedures are inadequate. The toxicity of chemical mixtures is relatively well understood by the concepts of Concentration Addition (CA) and Independent Action (IA), and synergism is only a rare condition (van Leeuwen et al., 2007).

It is generally accepted that CA is used to predict combination effects of chemicals that have similar modes of toxic action while, IA is used to forecast mixture effects of chemicals that have different modes of toxic action. CA and IA both do not expect synergistic and antagonistic effects and they assume interactions between the components in the mixture do not alter the overall toxicity of the mixture (Neale et al., 2015; Backhaus and Faust, 2012).

According to CA, the EC_{50} of a mixture can be estimated based on the EC_{50} values of the individual substances. Since such values are highly reliable measures usually documented in published ecotoxicological studies and databases, the calculation of an EC_{50} for a mixture derived from CA generally does not pose any complication in ecotoxicology. On the contrary, the use of IA requires knowledge of the exact effects that each substance will provoke if found separately at the concentration present in the mixture (EU Commission, 2009).

In the early 1980s, Schuetzle and Lewtas have developed a different approach named effect-directed analysis (EDA) that relates chemical analysis and biological effect testing (Schuetzle and Lewtas, 1986). Ever since, EDA has perpetually enhanced and has commonly been used for identification of toxic substances in effluents, surface water, groundwater, soils and sediments. EDA is used to understand the association between the chemical mixtures and their related effects (Brack, 2003).

3. MATERIALS AND METHODS

3.1. Chemicals and Reagents

In this research, 222 micropollutants were selected from the chemicals that are listed as "contaminants of emerging concern (CECs)" by NORMAN Network or "priority pollutants" by Water Framework Directive or "specific pollutants for surface waters and environmental quality standards" by the Ministry of Forestry and Water Affairs of Turkey. These micropollutants are antibiotics, personal care products (PCPs), steroids, hormones, brominated flame retardants, nonylphenols, surfactants, antiseptics, disinfectants, pesticides, fungicides, plasticizers, UV blockers, fragrances and cyanotoxins that have mutagenic, carcinogenic, allergenic and toxic effects. Properties of all chemicals were shown in Table A.1. at APPENDIX A.

Table 4.1. Chemical groups and the number of chemicals in these groups.

Chemical Groups	No. of Chemicals
Antibiotics	17
Bleaching Agent	1
Combustion Byproducts	13
Corrosion Inhibitors	5
Cyanotoxins	3
Flame Retardants	15
Growth Promoters	1
Hormones	3
Industrial Chemicals	18
Pharmaceuticals	4
Preservatives	4
Personal Care Products	28
Pesticides	98
Plasticizers	2
Reaction byproduct	1
Surfactants	9
TOTAL	**222**

All chemicals were purchased from Sigma Aldrich Chemical Company at highest purity and the stock solutions (1000 ppm) of these chemicals were prepared in methanol or in water according to their solubilities and stored at -20 °C until use. Working solutions (1 – 100 ppb) for mass spectroscopic use were prepared by diluting stock solutions with methanol or water buffered with 0.1% formic acid. Chemical mixtures (0.01-200 ppb) for retention time determination and calibration curves were prepared by diluting the stock solutions with a 1:1 methanol:water mixture.

Methanol, water and formic acid used in both sample preparation and chromatography were obtained from Merck Chemicals at MS grade.

For Microtox toxicity analyses, Reconstitution Solution, Diluent (2% NaCl in ultra-pure water) and Microtox Acute Reagent (freeze-dried bacterial strain) were provided by the Enotek Company (Istanbul, Turkey).

3.2. Instrumentation

An AB SCIEX QTrap 4500 linear ion trap tandem mass analyzer system coupled with Eksigent UltraLC 110 ultra-high performance liquid chromatography (UHPLC) unit was used to develop the analytical technique for quantification of the micropollutants that have been chosen for the study.

QTrap 4500 tandem mass spectrometer has a detector that can detect mass with high sensitivity and resolution. Liquid samples can be introduced to the detector through syringe pump or UHPLC. Organic compounds are ionized either positive or negative ionization mode in an ionization cell that can operate in the electrospray (ESI) and chemical ionization (APCI) modes. To obtain optimum ionization, some parameters such as curtain gas flow (CUR), ion spray voltage (IS), orifice gases (GS1 and GS2) and temperature (TEM) must be optimized according to the flow rate of the sample. In addition to these parameters, optimization of the declustering potential (DP) which is the parameter that used to minimize the clustering of a chemical with solvent ions is required.

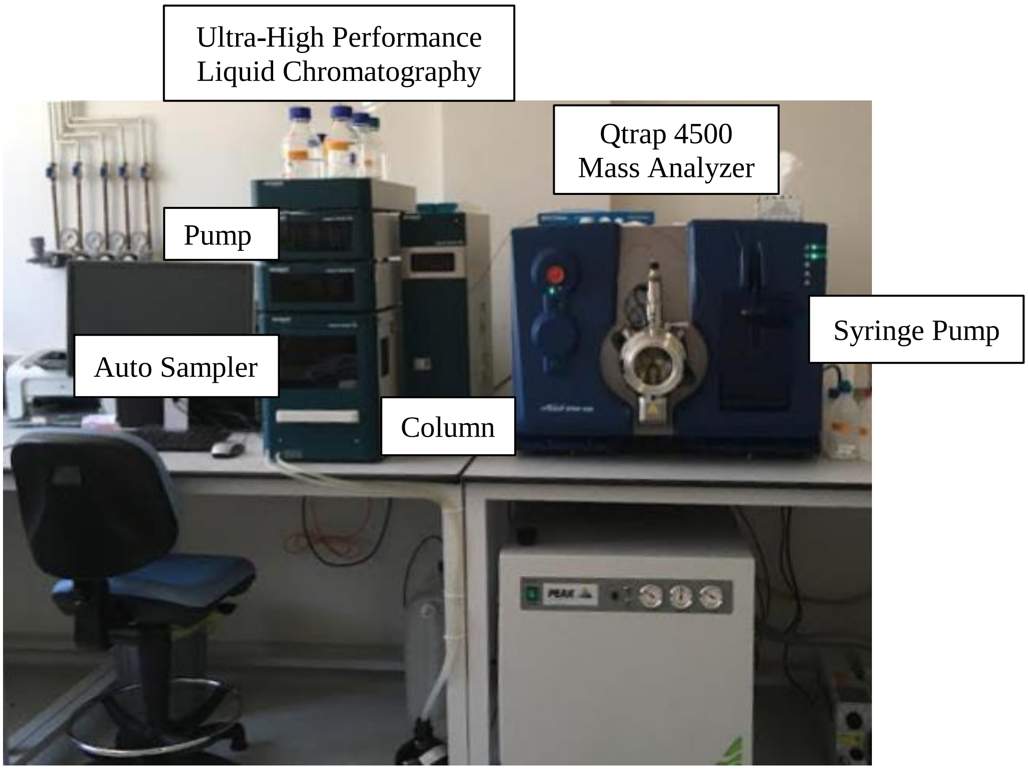

Figure 3.1. Display of the LC-MS/MS instrument system.

Ions that formed in the ionization chamber and separated from the matrix pass through the ion focuser (Q0) under high vacuum, which can be utilized as the first ion trap in QTrap 4500 system. Ions are then transferred to ion sorter (Q1) with respect to their entrance potential (EP), where the parent ions are aligned. Parent ions are associated with the molecular weight of the organics in the sample. When the collision chamber (Q2) and second ion sorter are not operated, the parent ions can directly reach to the detector and the parent ions of all ionizable organics in the sample can be determined. The first ion sorter is followed by the collision cell (Q2), where collision energy (CE) and nitrogen gas (CAD) are applied to the parent ions for fragmentation. During this collision, the parent ion is fragmented to daughter ions (Q3), aligned in the second ion sorter and detected in the detector. Since the CAD and CE parameters determine the level of the collision, they directly affect the distribution and density of the daughter ions. In addition, in QTrap 4500 system, second ion sorter can also be used as a trap and a second collision cell (AB Sciex, 2013; Eken et al., 2017).

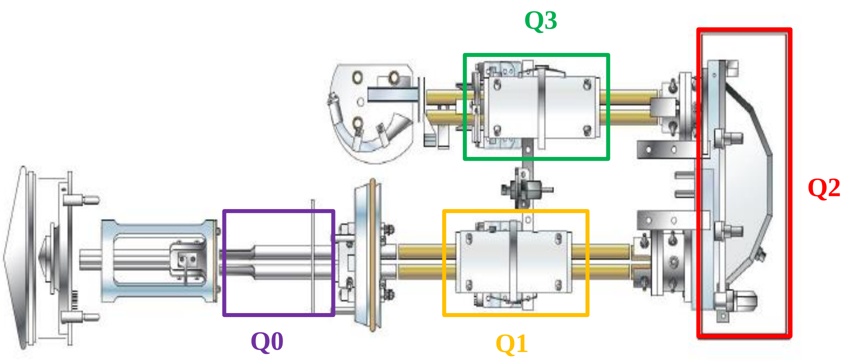

Figure 3.2. Structure of the AB SCIEX QTrap 4500 mass detector. Q0: Collisional focusing and ion trapping; Q1: Quadrupole; Q2: Curved collision cell; Q3: Linear trap (AB Sciex, 2013).

Microtox-500 Toxicity Analyzer (Azur, Environmental, USA) was used to determine acute toxicity of water samples and MicrotoxOmni© Software was used for collecting, analyzing and storing test data. Microtox-500 Toxicity Analyzer functions both as luminometer and as incubator.

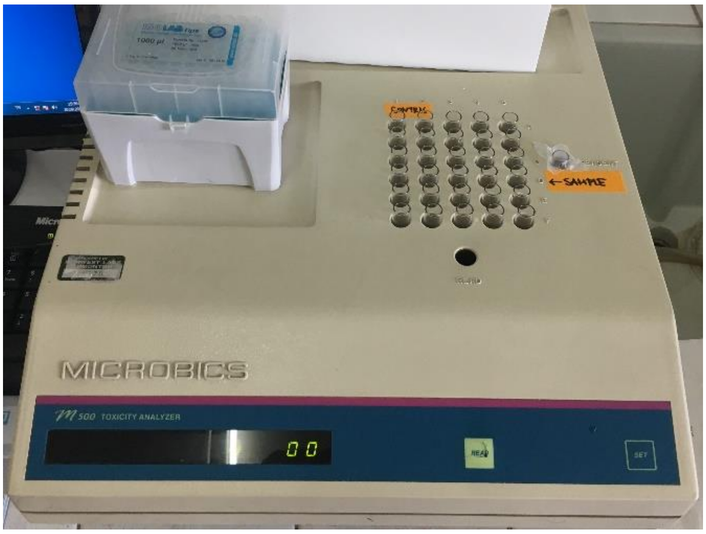

Figure 3.3. Microtox-500 Toxicity Analyzer.

3.3. Sampling

Sampling from Ergene River was performed by YABATAŞ Company (Ankara, Turkey) in August 2017. About a 1 L of sample was taken from 75 different points below 30 – 40 cm from the river surface and samples were kept in well cleaned glass containers that were rinsed at least twice with sample and transferred to the laboratory at 2±2 °C after parameters like temperature and pH measured in the field. Samples were stored at a cold room at 2±2 °C within few hours until the sample preparation.

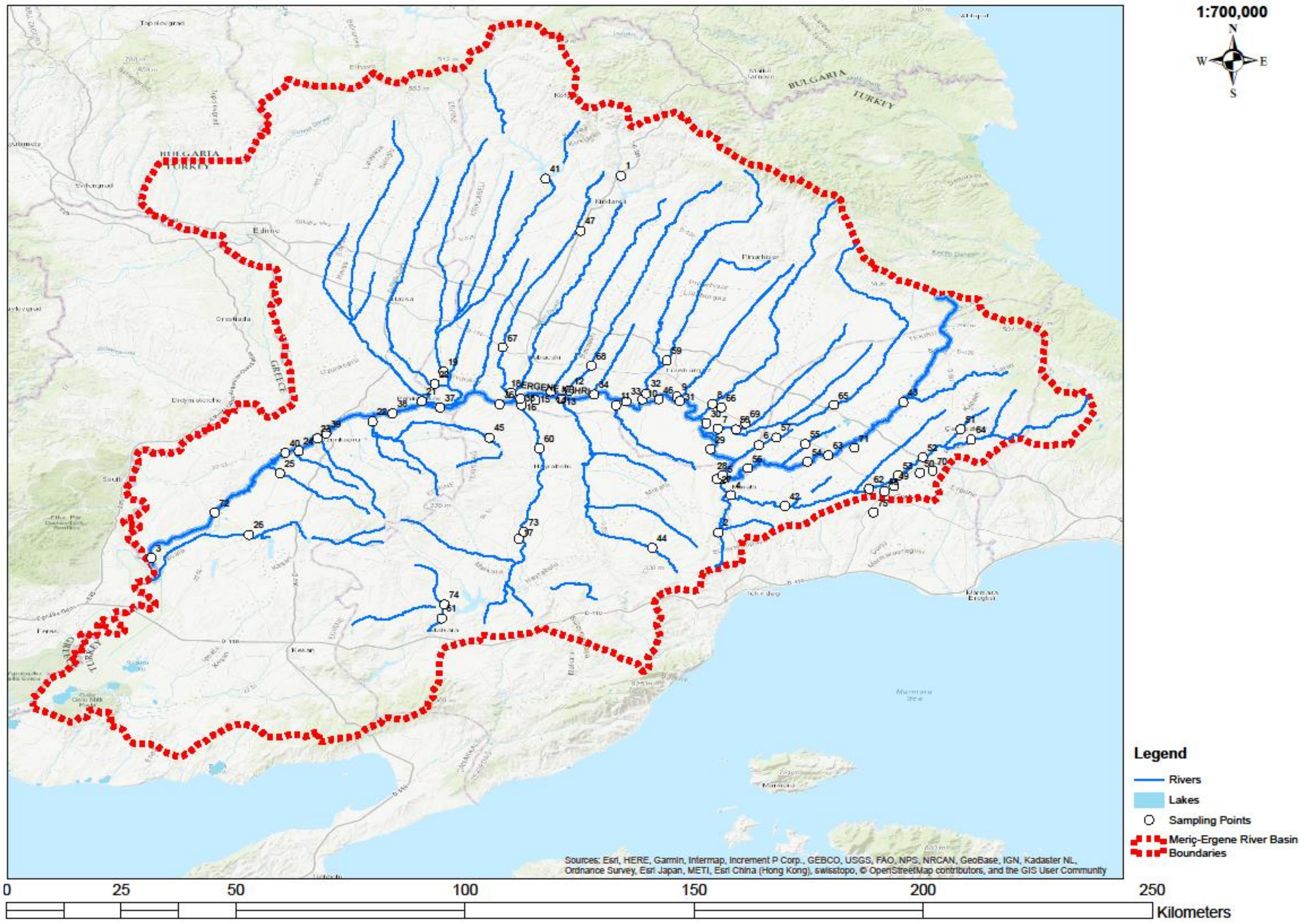

Figure 3.4. Sampling points along Ergene River.

3.4. Sample Analysis

3.4.1. Sample Preparation

Regenerated Cellulose (RC) Syringe Filters with 0.2 µm pore size were used to filter 20 mL of samples for Microtox toxicity tests and filtered samples were transferred to 20 mL amber glass vials with Teflon lined screw caps. Samples prepared for Microtox were kept at 2±2 ^oC. Since the pH range of the samples was 6.19 – 9.16, no pH adjustment was needed before the assay.

For MS analyses, 10 mL of samples were mixed with 10 mL of MS grade methanol and filtered from 0.2 µm RC syringe filter. Filtered samples were stored in 20 mL amber glass vials with Teflon lined screw caps at -20 ^oC.

3.4.2. Chemical Analysis

In order to identify a chemical using a mass spectrometry, first it must be ionized. Commonly, chemicals are ionized positively by gaining or negatively by losing protons. The ionized chemical, which has 1 Da heavier or lighter molecular mass than the mass of unionized chemical, is called the parent ion of the chemical. A workflow for targeted analysis of chemicals is shown in Figure 3.5. At first, to determine the parent ion of the selected chemical, working solution of the chemical was introduced into the mass detector (MSD) by an integrated syringe pump at a flow rate of 10 µL/min. MSD was operated at "Enhanced Mass Scanning (EMS)" mode which uses linear ion trap to enrich parent ions. ESI or APCI was used as ionization method. The working parameters were as follows: Curtain gas flow (CUR): 20, Declustering Potential (DP): +70V (for positive ionization) or -50V (for negative ionization), Ion Spray Voltage (IS): +5500 (for positive ionization) or -4500 (for negative ionization), Gas1 (GS1): 20, Gas2 (GS2): 0 Temperature (TEM): 0, Colissionally Activated Dissociation Gas Flow (CAD): Low, First Ion Trap (Q0): ON, Dynamic Fill Time: ON. The scanning range of EMS was ±50 of the exact molecular weight of the chemical. The mass range was scanned for 100 cycles and the mass intensities of each cycle was gathered (Multiple Channel Analyzer, MCA: ON).

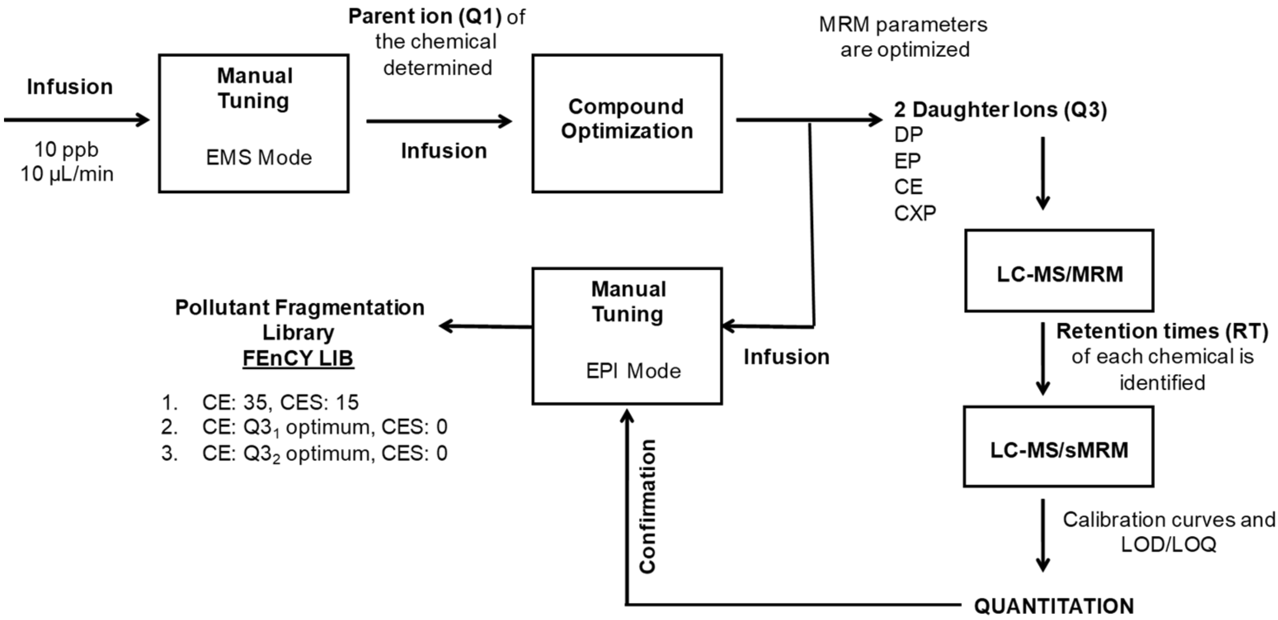

Figure 3.5. Workflow for targeted analysis of analytes in aqueous matrix (Eken et al., 2017).

After the parent ion (Q1) of each analyte was determined, 2 daughter ions (Q3s) and ideal declustering potential (DP), and collision energy (CE) conditions to get these daughter ions were obtained by working the MSD at “Compound Optimization” mode. By this run working solution was injected into MSD with a flow rate of 7 µL/min and 2 daughter ions (Q3s) that had the highest intensity among the other fragmented ions were determined. The ion that had the highest intensity among the fragmented ions was used for quantification while the second highest ion was used for confirmation.

For each analyte, three mass spectra were generated using specific “Multiple Reaction Monitoring (MRM)” transitions. When these mass spectra were generated, the MSD was worked at "Enhanced Product Ion (EPI)" scanning mode. The operating parameters were as follows: Curtain gas flow (CUR): 20, Declustering Potential (DP): the value obtained during the MRM optimization, Ion Spray Voltage (IS): +5500 (for positive ionization) or -4500 (for negative ionization), Gas1 (GS1): 20, Gas2 (GS2): 0 Temperature (TEM): 0, Colissionally Activated Dissociation Gas Flow (CAD): High, Q0: ON, Dynamic Fill Time: ON. The spectra were recorded in three CEs: (1) CE: 35 ± 15 eV, (2) optimum CE for the first daughter ion and (3) optimal CE for the second daughter ion. Each spectrum obtained for each analyte was recorded in the Mass Spectrometry Library and for the authentication of chemical substances this library was used. The workflow of the optimization method for targeted analysis was demonstrated in Figure 3.5.

MRM is performed to identify the target analytes by using the precursor ion (parent ion), its product ions (daughter ions) and the ionization conditions and mode. The highest ion intensity among the fragmented products is used for the quantitative analysis while the second highest ion is used for validation. The analytes that quantified are determined by matching the retention time (RT) of the equivalent standard. The MRM transitions and optimized conditions for each analyte were given in Table A.3. in APPENDIX A.

LC-MS/MS analysis was performed for separation and quantification of chemicals by using MS grade methanol (mobile phase A) and MS grade water (mobile phase B). The chemicals were optimally separated on a Phenomenex Kinetex C18 column (50 mm x 3 mm, 2.6 µm particle size) at 40 °C. The injected sample volume was 10 µL and 20 µL for ESI and APCI ionization modes, respectively. For best separation, following mobile phases were used in an overall 14+2 min (2 min initial equilibration time) run at a flow rate of 0.50 mL/min: positive ionization mode: (A) MS grade methanol plus 0.1% formic acid, (B) MS grade water plus 0.1% formic acid; negative ionization mode: (A) MS grade methanol plus 10 mM ammonium formate and 0.1% formic acid, (B) MS grade water plus 10 mM ammonium formate and 0.1% formic acid. To achieve the best separation gradient elution mode was used and performed gradient was given in Table 3.2.

Table 3.2. The gradient elution of chromatographic method.

Time	***Flow Rate (mL/min)***	***A (%)***	***B (%)***
0:00:01	0.50	0	100
0:01:30	0.50	0	100
0:02:00	0.50	50	50
0:04:00	0.50	50	50
0:08:01	0.50	100	0
0:14:00	0.50	100	0

3.4.3. Microtox Toxicity Test

Microtox is an acute toxicity test that uses the marine luminescent bacterium *Aliivibrio fischeri* (formerly known as *Photobacterium phosphoreum* or *Vibrio fischeri*) for toxicity evaluation. This bacterium emits light due to its normal metabolic processes. A reduction in luminescent ability during exposure to contaminants or pollutants is taken as a measure of toxicity. In this study, Microtox toxicity test is used to monitor acute toxicity of the water samples taken from the Ergene River using the change of bacterial luminescence.

Firstly, Microtox device is turned on and warmed up for 15 minutes. Type of the analysis is set to "ACUTE" from switch on the back of the device. MicrotoxOmni© Software is opened and type of test is also selected as "ACUTE" from Data Capture Test under the Options menu. Then clean unused glass cuvettes are placed in all incubation wells and reagent well. 1 mL of Reconstitution Solution is transferred into the cuvette in the reagent well and 0.5 mL of Diluent (2% NaCl in ultra-pure water) is transferred into cuvettes in wells B1-B5, C1-C5, E1-E5 and F1-F5 as shown in Figure 3.6. (A).

1.5 mL of Diluent (2% NaCl in ultra-pure water) is transferred into cuvettes in wells A1-A5, D1-D4 and 2.7 mL of filtered water sample is added into 0.3 mL of osmotic pressure adjustment solution (20% NaCl in ultra-pure water) in cuvette in well D5 as shown in Figure 3.6. (B).

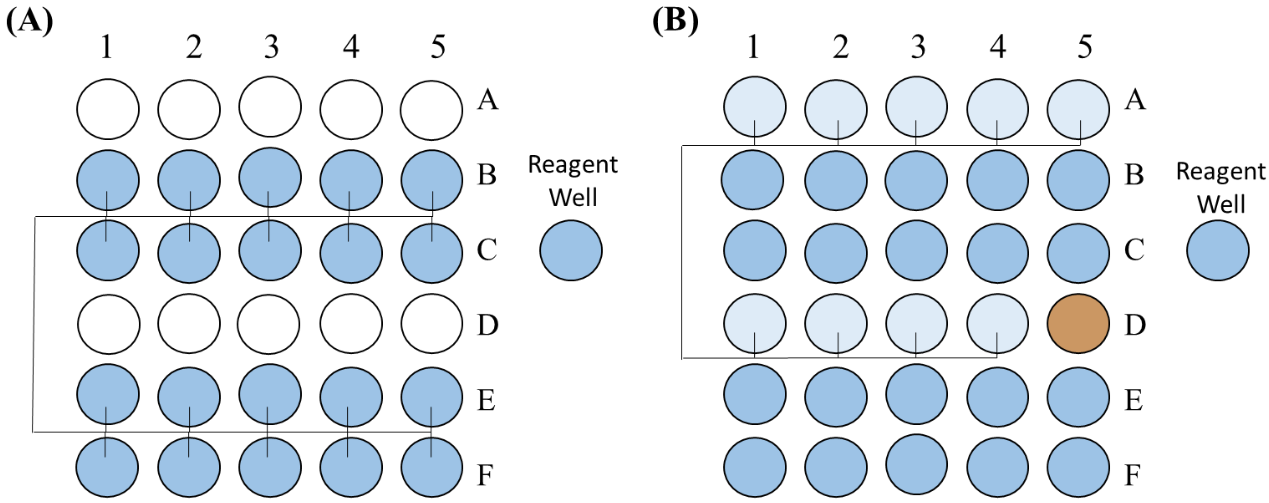

Figure 3.6. Microtox toxicity test setup.

Then filtered water samples is serially diluted with the dilution factor of 2 by transferring 1.5 mL from wells D5 to D4, D4 to D3, D3 to D2, D2 to D1, D1 to A5, A5 to A4, A4 to A3 and 1.5 mL from well A3 is discharged and nothing added to wells A1 and A2 since they are controls (Figure 3.7. (A)).

Microtox Acute Reagent, lyophilized (freeze-dried) *Aliivibrio fischeri* bacteria, is dissolved in a Reconstitution Solution that allows the optimum growth environment for bacteria and 10 µL of this reconstituted reagent is added into cuvettes in wells B1-B5, C1-C5, E1-E5 and F1-F5. After 15 minutes of stabilization period, 0.5 mL of water samples are added to cuvettes in wells B1-B5, C1-C5, E1-E5, F1-F5 (Figure 3.7. (B)) and the reduction of bacterial luminescence is measured in duplicate experiments as explained in the "Basic Test" procedure at 5th and 15th minutes.

Luminescence of each sample is recorded by a computer software and water ratio that shows 50% loss of luminescence is calculated and reported as effective concentration (EC_{50}). These EC_{50} (%) values were converted into dilution factors EC_{50} (df) to increase the meaningfulness of test results. This conversion was carried out by dividing hundred to the EC_{50} (%) value (equation 3.1).

$$EC_{50}(df) = \frac{100}{EC_{50}(\%)} \qquad (3.1)$$

EC_{50} (df): half maximal effective concentration as dilution factor

EC_{50} (%): half maximal effective concentration as percent

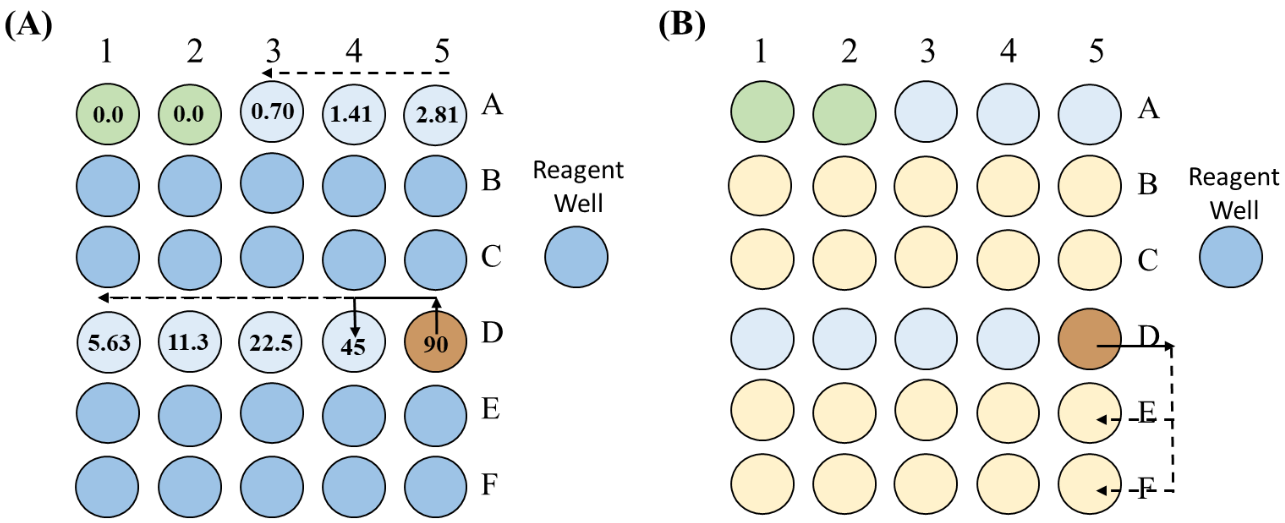

Figure 3.7. Microtox toxicity test setup (The numbers in the wells show the dilution factor of the sample in that well).

4. RESULTS AND DISCUSSION

4.1. Conventional Pollutants in Water Samples

When the water samples were examined, water temperature of the Ergene River varied between 19.5 and 35.4 ºC. Temperature was generally high in areas where organized industrial area discharges were high. The pH in the Ergene River and its branches was generally between 6.19 and 9.16. Ergene River is under the pressure of several sectors that containing colorants in their waste water. For the determination of industrial color pollution, color measurements were performed in the American Dye Manufacturer Index unit in all water samples. Color pollution in Ergene River reached up to 1300 ADMI units. The chemical oxygen demand (COD) value was between 45 and 1660 mg/L along the Ergene River and its branches. High COD concentrations were originated from food factories located in the basin. Phosphate, sulphate, bromide, fluoride, chloride, nitrite, nitrate and ammoniacal nitrogen were also measured in water samples. Among these, sulphate and chloride values were stand out. The ranges of conventional parameters are detected are given in the Table 4.1.

Table 5.1. Conventional pollutants and their ranges in Ergene River.

Conventional Pollutants	(Unit)	Range
pH		6.19 – 9.16
Temperature	(°C)	19.5 – 35.4
Color	(ADMI)	8 – 1269
TOC	(mg C/L)	0 – 532
COD	(mg COD/L)	45 – 1660
NH_3-N	(mg N/L)	0 – 271
NO_3	(mg/L)	0 – 98
NO_2	(mg/L)	0 – 4
Cl	(mg/L)	15 – 2428
Fl	(mg/L)	0 – 31
Br	(mg/L)	0 – 4
SO_4	(mg/L)	0 – 724
PO_4	(mg/L)	0 – 8

4.2. Method Validation for Micropollutant Analysis

All the analytes were detected within 10 minutes using the LC-MS/sMRM method developed in this study (Figure 4.1). The separation was mainly achieved with respect to hydrophobicity of compounds (Figure 4.2.).

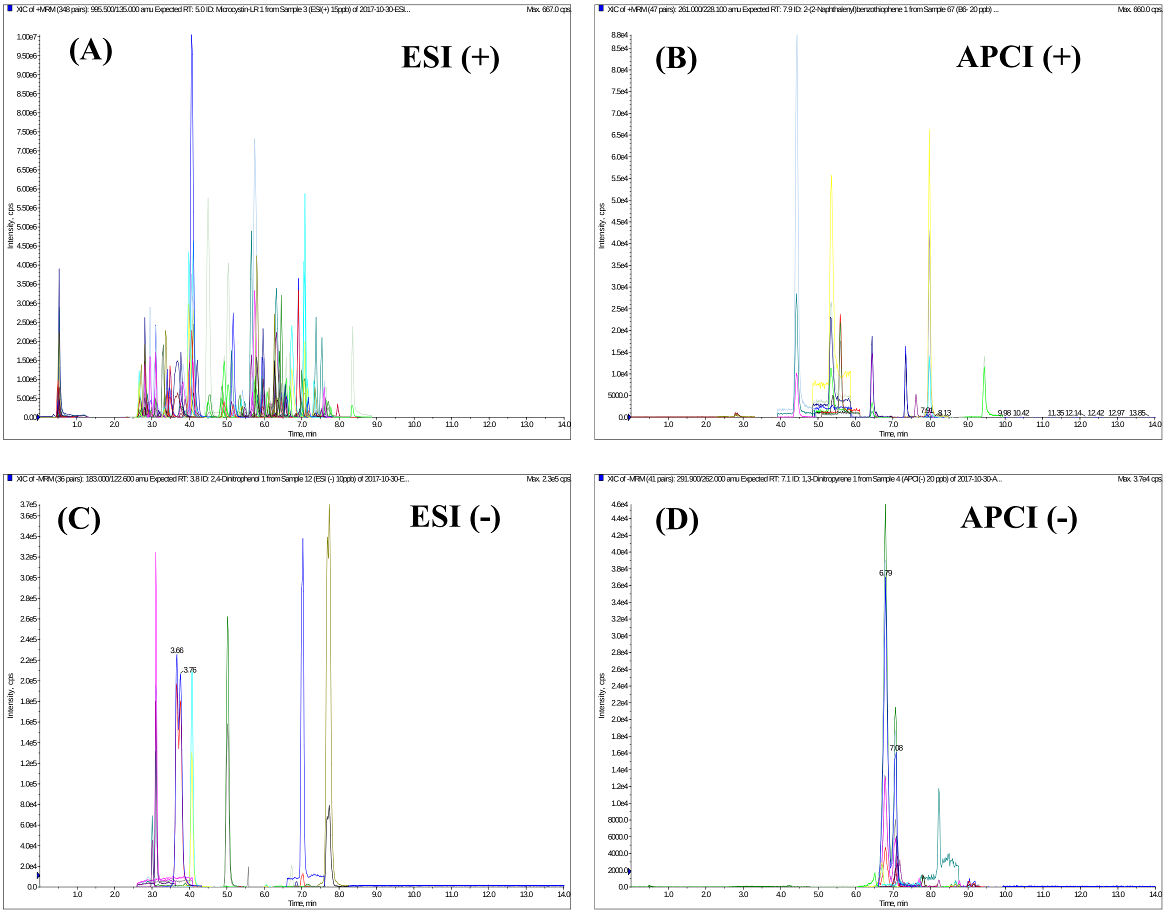

Figure 4.1. LC-MS/sMRM Chromatograms of selected analytes. Chromatogram of analytes (A) positively ionized by electrospray ionization (ESI (+)); (B) positively ionized by atmospheric pressure chemical ionization (APCI (+)); (C) negatively ionized by electrospray ionization (ESI (-)); (D) negatively ionized by atmospheric chemical ionization (APCI (-)).

Analytes that have lower octanol/water partition coefficient (LogP) values than 2 were mostly eluted from the column within first 4 minutes, while analytes that have LogP values between 2 and 5 were detected within 4 – 7 minutes and, analytes that have higher LogP values than 5 were eluted lastly from the column and monitored by the MS detector within 7 – 10 minutes (Figure 4.2).

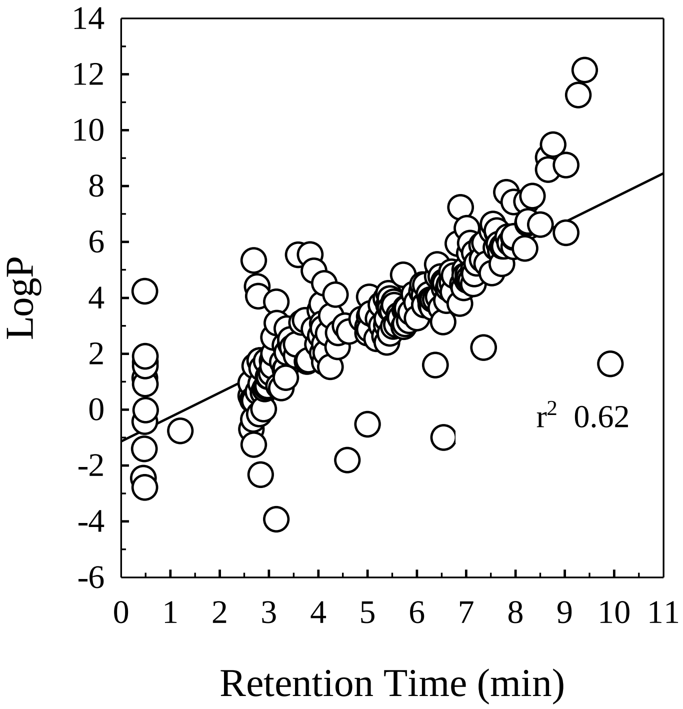

Figure 4.2. Relationship of retention time with LogP.

Calibration curves for each analyte were drawn within the concentration 0.01 to 200 µg/L. The concentration was linearly related with the peak area in the concentration range with a regression coefficient (r^2) greater than 0.99 for most of the analytes.

The limit of detection (LOD) is the lowest concentration of an analyte that can be accurately measured by an analytical instrument while, the limit of quantitation (LOQ) is the lowest concentration of an analyte that can be detected with an acceptable repeatability, precision and trueness. LOD and LOQ are two basic elements of method validation.

LOD and LOQ values for each analyte were calculated by using the slope of the calibration curves (S) and the standard deviation of the response of the lowest detectable concentration (S_y).

$$LOD = 3\left(\frac{Sy}{S}\right) \quad (4.1)$$

$$LOQ = 10\left(\frac{Sy}{S}\right) \quad (4.2)$$

The LOD of the method for analytes ranged between 0.8 to 21737 ng/L. Method was highly sensitive to pesticides and antibiotics than the other group of analytes.

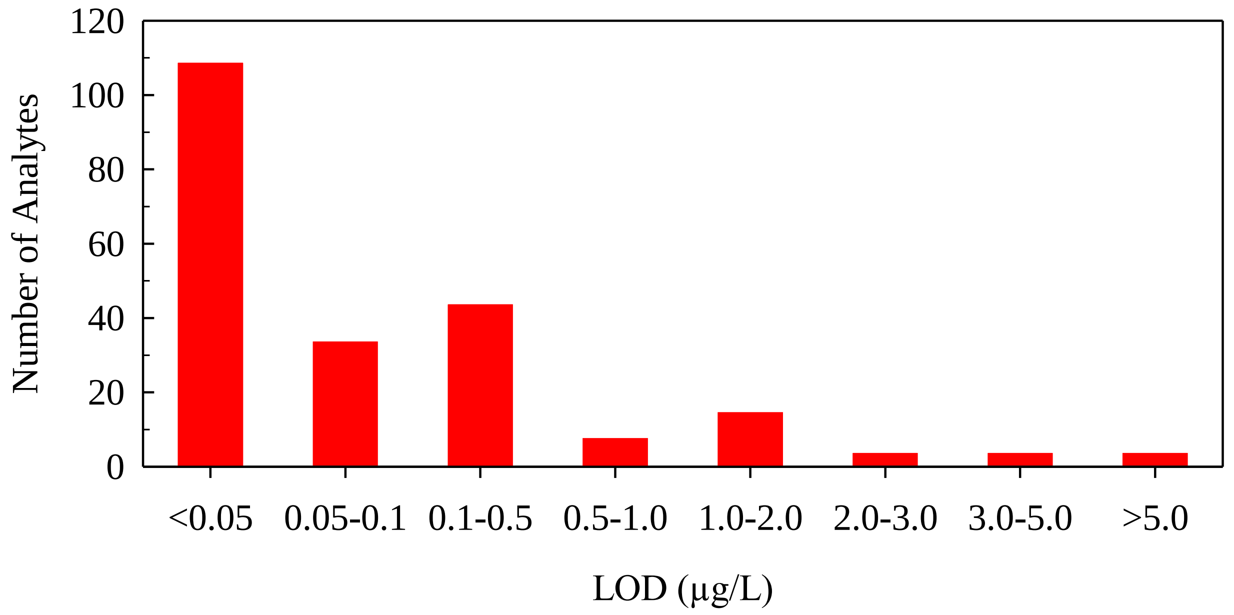

Figure 4.3. Distribution of LOD values of analytes.

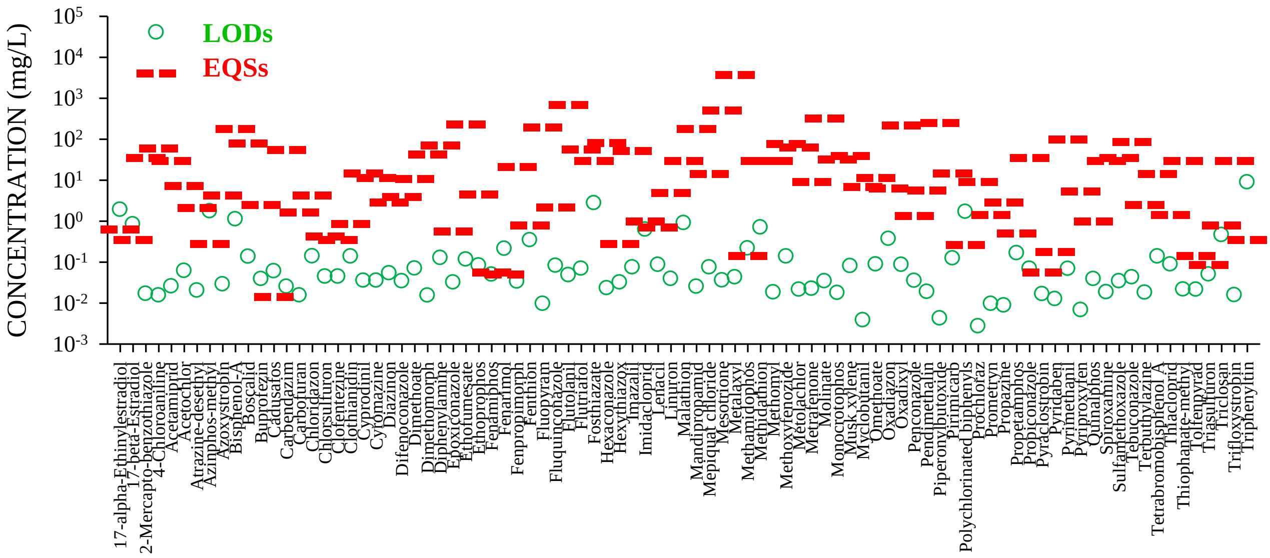

Figure 4.4. Comparison of Environmental Quality Standards (EQSs) and LODs of analytes.

As is clearly seen in Figure 4.4., for most of the analytes analyzed within the scope of this study, the LOD values are below the specified EQSs for these substances except for tris(1-chloro-2-propanyl) phosphate, triphenyltin, 17-alpha-ethinylestradiol, 17-alpha-estradiol, azinphos-methyl, PCB-169 and cadusafos.

4.3. Micropollutant Evaluation in Water Samples

About 222 micropollutants investigated in water samples, 131 micropollutants were detected in at least one sample. Among these contaminants are priority pollutants, antibiotics, brominated flame retardants, nonylphenols, disinfectants, pesticides, plasticizers, fragrances and even cyanotoxins. The maximum, minimum and mean concentrations of the detected chemicals, the number of detections among samples and the sampling points which the highest concentration of these chemicals have been observed are given in Table 4.2.

Table 4.2. Maximum, minimum and mean concentrations of detected micropollutants.

Compound Name	Max (µg/L)	Min (µg/L)	Median (µg/L)	No. of samples detected	Highest Conc. at
1,2,3-Benzotriazole	117.55	n.d.	2.66	68	SP48
1,3-Dinitropyrene	1.58	n.d.	0.00	1	SP50
1,6-Dinitropyrene	1.23	n.d.	0.00	2	SP50
1,8-Dinitropyrene	1.13	n.d.	0.00	3	SP50
1-Hydroxyibuprofen	95.60	n.d.	0.00	10	SP08
2-(2-Naphthalenyl) benzothiophene	22.87	n.d.	0.00	6	SP03
2,2',4,4',5,5'-Hexabromodiphenyl ether	7.13	n.d.	0.00	1	SP62
2,3,3',4,4',5,5',6-Octabromodiphenyl ether	3.12	n.d.	0.00	4	SP09
2,4-Dihydroxybenzophenone	2.53	n.d.	0.00	31	SP62
2-Mercapto-benzothiazole	3.46	n.d.	0.00	20	SP64
3-Chloroaniline	1.59	n.d.	0.00	29	SP48
3,3',4,4',5,5'-Hexachlorobiphenyl (PCB-169)	467.73	9.90	38.46	75	SP42
4,4'-Dichlorobenzophenone	3.68	n.d.	0.00	12	SP63
4-Aminomethyl-benzenesulfonamide	0.90	n.d.	0.00	8	SP66
4-Chloroaniline	2.05	n.d.	0.00	31	SP48
4-Methyl-1H-benzotriazole	36.19	n.d.	2.48	58	SP64
4-Methylbenzylidenecamphor	34.90	n.d.	0.00	16	SP09
4-tert-Octylphenol diethoxylate	0.28	n.d.	0.02	43	SP40
5,6-Dimethyl-1H-benzotriazole	20.86	n.d.	0.44	39	SP68
5-Methyl-1H-benzotriazole (5-Tolytriazole)	15.95	n.d.	1.72	63	SP64
7H-Benzo(de)anthracen-7-one (Benzanthrone)	30.31	n.d.	0.00	27	SP08
Acetaminophen (Paracetamol)	107.26	n.d.	0.66	49	SP57
Acetamiprid	1.93	n.d.	0.05	42	SP70
Aclonifen	0.75	n.d.	0.00	32	SP51
ADBI (Celestolide)	0.70	n.d.	0.00	20	SP49
AHDI (Phantolide)	3.44	n.d.	0.00	30	SP50
alpha-Terpineol	593.77	n.d.	0.00	10	SP52
Anthracene	851.00	n.d.	0.00	12	SP08
Atrazine	0.05	n.d.	0.00	20	SP57
Atrazine-desethyl	9.56	n.d.	0.00	29	SP08
Azithromycin	7.86	n.d.	0.28	71	SP02
Azoxystrobin	7.71	n.d.	0.00	6	SP25

Table 4.2. Maximum, minimum and mean concentrations of detected micropollutants (continued).

Compound Name	Max (μg/L)	Min (μg/L)	Median (μg/L)	No. of samples detected	Highest Conc. at
Benzenesulfonamide	71.87	n.d.	0.00	1	SP51
Benzo[a]anthracene	9.81	n.d.	0.00	6	SP57
Benzo[a]pyrene	0.98	n.d.	0.00	22	SP06
Benzo[b]fluoranthene	4.38	n.d.	0.00	3	SP57
Benzo[ghi]perylene	10.62	n.d.	0.00	4	SP09
Benzo[k]fluoranthene	3.01	n.d.	0.00	33	SP47
Benzothiazole	334.51	n.d.	0.00	1	SP51
Benzylamine	0.74	n.d.	0.00	18	SP50
Benzyldimethyldodecylammonium	23.89	0.05	0.64	75	SP42
Benzyldimethyltetradecylammonium	7.64	0.04	0.41	75	SP49
Benzyltrimethylammonium	0.33	n.d.	0.01	40	SP28
Bisphenol-A	48.98	n.d.	0.00	8	SP08
Boisvelone / Iso-Esuper	13.51	n.d.	0.00	34	SP09
Cadusafos	0.65	n.d.	0.00	3	SP09
Carbazole	1.66	n.d.	0.00	2	SP56
Carbendazim	6.33	n.d.	0.15	53	SP42
Carbofuran	0.13	n.d.	0.00	1	SP09
Chloramphenicol	0.11	n.d.	0.00	2	SP09
Chlorfenvinphos	0.44	n.d.	0.00	1	SP08
Chlorpyrifos	0.67	n.d.	0.00	10	SP11
Ciprofloxacin	51.62	n.d.	1.67	63	SP09
Clarithromycin	2.74	n.d.	0.10	58	SP08
Cyprodinil	0.29	n.d.	0.00	5	SP70
Damascone	814.20	n.d.	0.00	1	SP55
Di(2- ethylhexyl)phthalate (DEHP)	69.92	n.d.	0.00	33	SP47
Dicyclohexylamine	5.13	n.d.	0.10	62	SP50
Dimethoate	1.29	n.d.	0.00	1	SP14
Diuron	2.64	n.d.	0.23	49	SP28
Doxycycline	3.22	n.d.	0.00	6	SP49
Drometrizole	1.03	n.d.	0.00	21	SP29
Epoxiconazole	0.76	n.d.	0.00	18	SP24
Erythromycin	1.11	n.d.	0.00	11	SP08
Ethoprophos	0.21	n.d.	0.00	1	SP51
Ethylhexylmethoxycinnamate	13.86	n.d.	0.00	17	SP62
Fenamiphos	0.05	n.d.	0.00	1	SP05
Fluoranthene	19.44	n.d.	0.00	13	SP08
Flutolanil	0.20	n.d.	0.00	2	SP70
Flutriafol	0.33	n.d.	0.00	4	SP16
g-Methylionone	14.98	n.d.	0.00	30	SP06
Hexa(methoxymethyl)melamine	329166.95	n.d.	2482.03	66	SP48
Homosalate	124.42	n.d.	0.00	21	SP27
Imazalil	2.92	n.d.	0.00	4	SP09
Imazamox	0.76	n.d.	0.00	12	SP13
Imidacloprid	0.72	n.d.	0.00	1	SP69
Indeno[1,2,3-cd]pyrene	110.02	n.d.	0.00	8	SP09

Table 4.2. Maximum, minimum and mean concentrations of detected micropollutants (continued).

Compound Name	Max (µg/L)	Min (µg/L)	Median (µg/L)	No. of samples detected	Highest Conc. at
Lenacil	1.93	n.d.	0.00	2	SP09
Mepiquat chloride	0.64	n.d.	0.00	37	SP09
Metalaxyl	0.10	n.d.	0.00	5	SP05
Methyl -iso-propylcyclohexenone	3.84	n.d.	0.00	15	SP07
Methyl paraben	4.31	n.d.	0.00	8	SP50
Methyldihydrojasmonate	11.36	n.d.	0.00	9	SP49
Methylsalicylate	8.02	n.d.	0.00	8	SP50
Metolachlor	0.13	n.d.	0.00	19	SP08
Microcystin-LR	6.30	n.d.	0.00	1	SP48
Microcystin-RR	4.08	n.d.	0.00	19	SP69
Molinate	3.49	n.d.	0.00	13	SP21
Monocrotophos	0.05	n.d.	0.00	20	SP53
Myclobutanil	1.38	n.d.	0.00	13	SP35
N,N-Diethyl-m-toluamide	35.92	0.01	0.42	75	SP14
N-Benzyldimethylamine	3.79	n.d.	0.00	31	SP69
N-Benzylmethylamine	0.37	n.d.	0.00	29	SP48
N-Ethyl-2-tolysulfonamide	0.55	n.d.	0.04	39	SP05
Nonylphenol diethoxylate	11.99	n.d.	0.40	47	SP55
Norfloxacin	41.72	n.d.	2.94	69	SP09
Ofloxacin	530.39	0.04	0.55	75	SP69
Omethoate	1.46	n.d.	0.00	27	SP09
Oxadiazon	1.42	n.d.	0.00	9	SP25
Oxadixyl	2.72	n.d.	0.00	1	SP23
Oxybenzone	0.65	n.d.	0.02	39	SP62
Penconazole	0.06	n.d.	0.00	1	SP09
Pendimethalin	0.10	n.d.	0.00	10	SP27
Pentachlorobenzene	0.55	n.d.	0.00	3	SP30
Piperonylbutoxide	0.49	n.d.	0.05	65	SP27
Pirimicarb	1.61	n.d.	0.00	24	SP08
Prochloraz	0.52	n.d.	0.06	41	SP09
Propazine	0.01	n.d.	0.00	1	SP04
Propetamphos	0.47	n.d.	0.00	3	SP08
Propiconazole	10.08	n.d.	0.00	7	SP25
Propyl paraben	0.51	n.d.	0.00	1	SP09
Pyraclostrobin	0.18	n.d.	0.00	4	SP24
Pyridaben	0.03	n.d.	0.00	5	SP68
Pyriproxyfen	0.02	n.d.	0.00	10	SP48
Quinalphos	1.03	n.d.	0.00	28	SP08
Quinoxyfen	0.03	n.d.	0.00	1	SP26
Spiroxamine	0.24	n.d.	0.00	2	SP69
Sulfamethoxazole	3.27	n.d.	0.21	41	SP11
Tebuconazole	0.21	n.d.	0.00	2	SP58
Terbuthylazine	0.04	n.d.	0.00	3	SP22
Terbutryn	0.03	n.d.	0.00	36	SP28
Tetracycline	0.60	n.d.	0.00	13	SP09

Table 4.2. Maximum, minimum and mean concentrations of detected micropollutants (continued).

Compound Name	Max (µg/L)	Min (µg/L)	Median (µg/L)	No. of samples detected	Highest Conc. at
Thiacloprid	0.10	n.d.	0.00	1	SP11
Tonalide	0.50	n.d.	0.00	7	SP52
Triazophos	0.37	n.d.	0.00	4	SP48
Trifloxystrobin	0.20	n.d.	0.00	1	SP25
Trifluralin	2.16	n.d.	0.00	1	SP44
Trimethoprim	0.20	n.d.	0.00	4	SP64
Triphenylphosphineoxide	15.24	n.d.	0.00	4	SP71
Tris(2-butoxyethyl) phosphate	270.17	n.d.	0.43	51	SP48
Vancomycin	1.47	n.d.	0.00	1	SP48

21 out of 131 micropollutants were monitored in only one sampling point. These contaminants are including priority pollutants such as a brominated diphenyl ether (BDE-153), trifluralin, quinoxyfen and chlorfenvinphos; a cyanotoxin microcystin-LR (MC-LR); a synthetic fragrance damascone; pesticides as carbofuran, thiacloprid, trifloxystrobin, penconazole, oxadixyl, imidacloprid, dimethoate, ethoprophos, fenamiphos and propazine; antibiotics like vancomycin and benzenesulfonamide; a preservative agent propyl paraben; 1,3-dinitropyrene which is a combustion by product of PAHs and a flavoring agent benzothiazole.

Among priority pollutants, BDE-153 was observed fifty times above the environmental quality standards (EQS) at 7.13 µg/L in the SP62 which is close to discharge of Çorlu leather organized industrial site. Trifluralin was detected about seventy-five times above the EQS at 2.16 µg/L in the SP44 which is in an agricultural area and close to Tekirdağ solid waste landfill site. Chlorfenvinphos was also detected above the EQS at 0.44 µg/L in SP08 which is near to discharge of food, yeast and starch factories.

Microcystins (MCs) are very common hepatotoxins produced by a certain type of cyanobacteria and it is known as highly toxic and suspected as carcinogenic (Mrdjen, 2018). MC producing cyanobacteria are commonly encountered in eutrophic water bodies and cause serious problems in the context of water quality (Lawton et al., 1994). MC-LR was only monitored at 6.30 µg/L in SP48 that is near to Çorlu Leather organized industrial site. When sampling point is examined an algal bloom was observed. Another cyanotoxin MC-RR was observed at 19 of 75 sampling points. MC-RR was highly detected at 4.08 µg/L in SP69.

Benzyldimethyldodecylammonium (BAC 12), benzyldimethyltetradecylammonium (BAC 14), N,N-diethyl-m-toluamide (DEET), ofloxacin and 3,3',4,4',5,5'-hexachlorobiphenyl (PCB-169) were observed in all 75 sample points and, hexa(methoxymethyl)melamine, anthracene, damascone, PCBs, alpha – terpineol, tris(2-butoxyethyl) phosphate, di(2-ethylhexyl)phthalate (DEHP), homosalate, 1,2,3-benzotriazole and ofloxacin were detected at the highest mean concentrations.

BAC 12 and BAC 14 are known as quaternary ammonium compounds (QACs) and they are generally used as surfactant, disinfectant and biocide. QACs are widely used in both domestic and industrial purposes and they are known to cause antibiotic resistance and be toxic for aquatic environments (Tezel, 2009). The highest concentration of BAC 12 (23.89 µg/L) was monitored in SP42 while the highest concentration of BAC 14 (7.64 µg/L) was detected in SP49. Both sampling points are located near an agricultural area where SP49 is close to Sancak Boya Factory (Ervam Textile Factory) and SP42 is near to a poultry farm.

DEET is first produced by the US Army in the late 1940s. It is widely used as a main ingredient in insect repellents and directly applied to skin to repel mosquitos, bugs and ticks. According to US EPA, DEET has no toxic effects when used as described in the label directions. DEET was detected intensely in SP14 which is surrounded by residential area and close to an oil factory. DEET is a pollutant that is mostly caused by domestic activities.

Ofloxacin is a fluoroquinolone antibiotic used for treatment of many bacterial infections and it causes antibiotic resistance. Ofloxacin was highly found at 530.4 µg/L in SP69 which is right next to an industrial discharge of a pharmaceutical company named Zentiva.

PCBs are persistent organic pollutants that have been produced from the 1920s. They are extensively used for industrial applications (i.e., *production of electrical equipment*) since they are inflammable, stable and miscible with organic compounds. When they are released to environment, PCBs are not degraded easily and they bioaccumulate in higher trophic levels. Moreover, they cause carcinogenicity, neurotoxicity and endocrine disruption (Safe, 1994). PCB-169 were observed highly in SP42 above the EQS values.

In addition to these chemicals, antibiotics such azithromycin, norfloxacin, ciprofloxacin, clarithromycin, sulfamethoxazole, tetracycline and erythromycin; corrosion inhibitors like 1,2,3-benzotriazole, 5-tolytriazole, dicyclohexylamine, 4-methyl-1H-benzotriazole, 5,6-dimethyl-1Hbenzotriazole; a coating agent called hexa(methoxymethyl)melamine (HMMM); and pesticides like piperonylbutoxide, carbendazim, diuron, acetamiprid, prochloraz, terbutryn, aclonifen were also observed frequently in water samples.

Among the antibiotics detected, azithromycin was highly found at 7.86 µg/L in SP02 while, norfloxacin, ciprofloxacin and tetracycline were intensely observed in SP09. Domestic wastewater of Muratlı district is directly discharged to the Köy Stream (one of the tributaries of Ergene River) without treatment where SP02 is located therefore, it is obvious that azithromycin is sourced from this domestic discharge. Similarly, domestic wastewater of Lüleburgaz district is discharged directly without treatment to the Kavak Stream where SP09 is located on.

Pesticides were highly observed in SP27, SP42, SP28, SP70, SP09 and SP51. The common trait of these points is that they are all located in agricultural area. The reason for the presence of pesticides in these sampling points is the runoff from agricultural areas around them.

Bisphenol-A (BPA), a synthetic organic compound, is widely used for manufacturing of polycarbonate plastics. Moreover, it is frequently used as an ingredient of epoxy resins. Due to its' durability and high performance, BPA is used in different areas such as production of water bottles, sport equipment, compact disc, automotive parts and thermal paper (European Union, 2003). BPA was detected at 48.98 µg/L in SP08 which is near to Evrensekiz organized industrial site and food factories.

Alpha-terpineol is a fragrance used in cosmetic products, perfumery, shampoos, toiletries and in non-cosmetic products such as household cleaning products and washing agents (Bhatia et al., 2008). Alpha-terpineol was intensely monitored at 593.77 µg/L in SP52 which is located on the Çorlu Stream. SP52 is near to domestic wastewater discharges and it is surrounded by an agricultural area.

Tris(2-butoxyethyl) phosphate (TBEP) is an ingredient of floor waxes and it is used as a plasticizer in rubber and plastic industries. TBEP is introduced to the environment only by anthropogenic activities (Van Esch, 2000). TBEP is highly detected at 270.17 µg/L in SP48 which is near to Çorlu Leather organized industrial site.

Homosalate is frequently used as an active ingredient in sunscreens, personal care and cosmetic products. It degrades very quickly and produces harmful byproducts. Homosalate is intensely monitored in SP27 which is located on the Çorlu Stream and close to an agricultural stock farming (AKSA Tarım).

Dinitropyrenes (DNPs) are nitro-polycyclic aromatic hydrocarbons (nitro-PAH) that are not used commercially, yet they are detected in ambient atmospheric samples, diesel exhaust as a product of combustion and in water samples by wet precipitation from exhaust gas. DNPs are recognized as a human carcinogen and mutagen (Singletary and MacDonald, 2000; Djurid et al., 1988). 1,3-DNP, 1,6-DNP and 1,8-DNP were detected in SP50 which is near to carpet, textile and paint factories which apply high temperature fabric dyeing.

Acetaminophen (APAP) is an antipyretic and analgesic drug and it is used extensively worldwide. APAP is one of the most common anthropogenic micropollutants that is frequently detected in domestic and industrial wastewater effluents, surface waters and soils (Lancaster et al., 2015). APAP was monitored at 107.26 µg/L in SP57 which is near to Büyükkarıştıran Islah organized industrial site dominated by textile, dye and metal industries.

Among all chemicals HMMM was spotted in very high concentrations (avg. conc. = 28876.9 µg/L). HMMM is an emerging contaminant that is added to resins as an ingredient. HMMM containing resins are applied to coatings and plastics that are produced for cans, coils and automobiles (Dsikowitzky and Schwarzbauer, 2015). HMMM was detected in the extreme amounts in SP48 and SP57, 329166.9 µg/L and 254707.5 µg/L respectively and spread over from these points to the Maritsa River. An organized industrial site (Büyükkarıştıran Islah OSB), that is dominated by textile, dye and metal industries, is located right next to SP57.

Another chemical detected in high concentrations is anthracene. Anthracene is a priority pollutant that observed frequently in surface waters and bioaccumulates in aquatic organisms. It is a polycyclic aromatic hydrocarbon (PAH) and used as an ingredient in creosote, that is mainly used for preservation of wood materials. Anthracene is also used to produce anthraquinone, polymers, pigments and dyes. Since PAHs are commonly resulted from unfinished combustion, anthracene exists in tobacco smoke (WFD, 2000). Anthracene was monitored at 851.0 µg/L in the SP08 which is close to Evrensekiz organized industrial site and food factories.

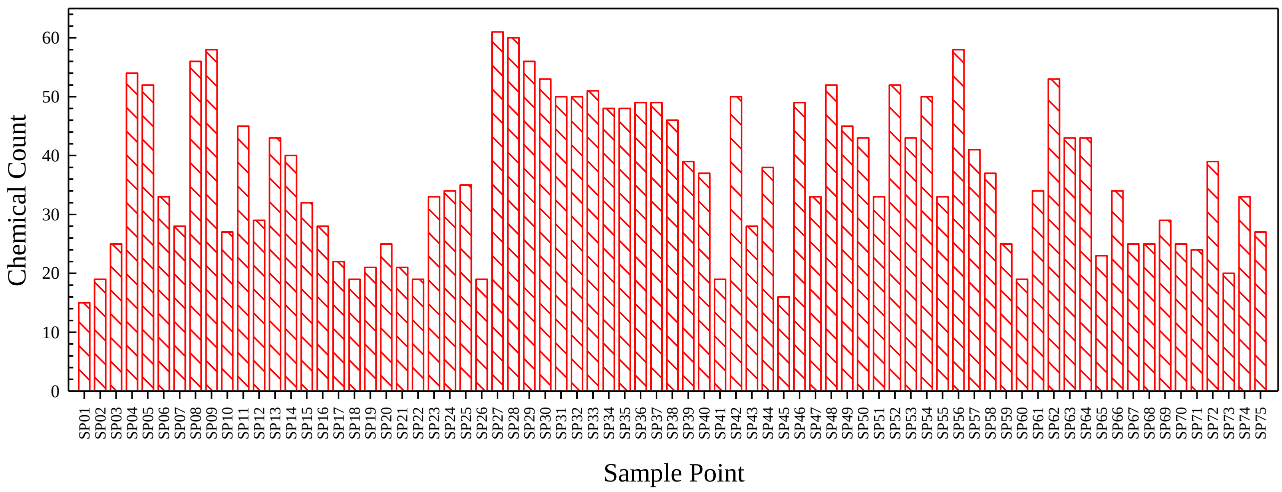

Figure 4.5. Number of chemicals detected at sample points.

The number of detected chemicals at each sample point is given in the Figure 4.5. and shown on the map in Figure 4.6. Most chemicals (61 micropollutants) were found in SP27 which was taken from one of the tributaries of Ergene River (Çorlu Stream) while, least chemicals (15 micropollutants) were detected in SP01 that was taken from one of the sources that feeds Ergene River.

The second most chemicals were detected at SP28 (60 micropollutants) which is surrounded by an agricultural area and close to İnanlı district. In SP28 domestic contaminants such as alpha-terpineol, homosalate, 1-hydroxyibuprofen, acetaminophen, BAC 12 and industrial chemicals like hexa(methoxymethyl)melamine, PCB-169, TBEP, BPA, indeno[1,2,3-cd]pyrene, 4 types of benzotriazoles were found at high concentrations. Additionally, diuron, benzyltrimethylammonium and terbutryn were detected in their highest concentrations at SP28.

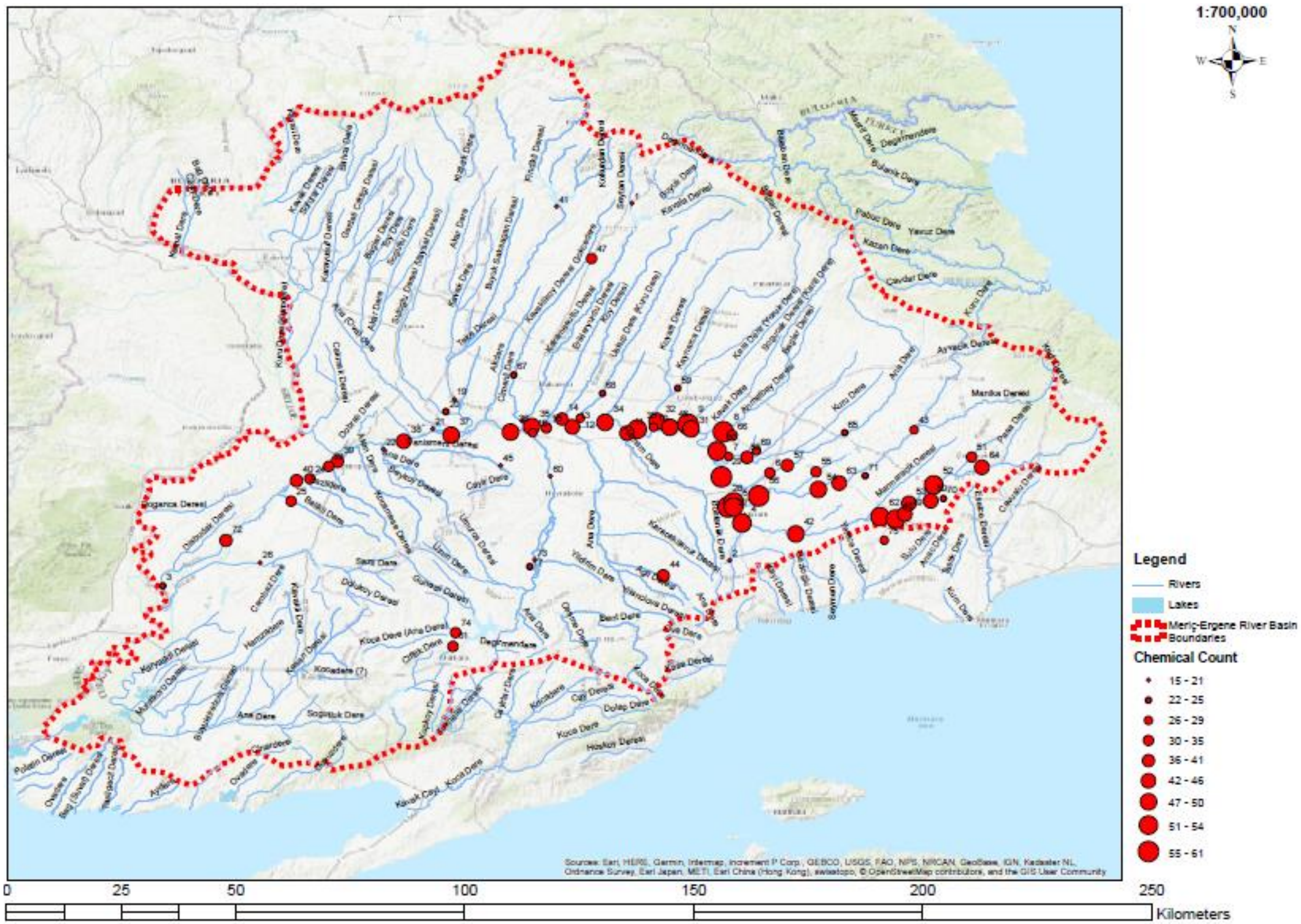

Figure 4.6. Distribution of the number of chemicals detected at sample points along the Ergene River.

4.4. Metals in Water Samples

All 18 heavy metals were detected in at least one water samples. While cadmium (Cd) was detected in only one sampling point, tin (Sn), boron (B), nickel (Ni), copper (Cu), aluminum (Al), cobalt (Co), vanadium (V), chromium (Cr), zinc (Zn) and barium (Ba) were monitored in every sampling point. 17 of 18 metals were observed in SP52 while 16 of 18 metals were detected in SP33, SP35, SP42 and SP49. The maximum, minimum and mean concentrations of the detected metals, the number of detections among samples and the sampling points where the highest concentration of these metals have been observed are given in the Table 4.3.

Table 4.3. Maximum, minimum and mean concentrations of detected heavy metals.

Metals	Max (µg/L)	Min (µg/L)	Median (µg/L)	No. of samples detected	Highest Conc. at
As	62.33	n.d.	0.69	43	SP57
Ba	534.47	6.46	99.82	75	SP09
Be	58.16	n.d.	0.00	22	SP11
Zn	1005.42	0.18	44.68	75	SP63
Cr	3628.89	0.24	8.75	75	SP44
V	50.43	1.75	11.74	75	SP09
Co	11.91	0.15	1.42	75	SP09
Al	12193.39	39.85	540.38	75	SP06
Cu	993.00	2.65	27.55	75	SP09
Pb	2937.36	n.d.	68.96	74	SP51
Ni	2395.52	22.46	151.75	75	SP48
Cd	0.56	n.d.	0.00	1	SP09
Ag	0.65	n.d.	0.00	9	SP51
B	2604.68	24.06	256.15	75	SP54
Sn	571.73	1.33	9.43	75	SP51
Ti	44.99	n.d.	4.02	61	SP55
Sb	50.13	n.d.	0.31	40	SP62
Hg	4.16	n.d.	0.00	12	SP36

Aluminum concentration is quite high throughout the Ergene River, but the highest Al concentration was detected as 12193.39 µg/L in SP06 which is located near to an aluminum factory and Büyükkarıştıran organized industrial area.

High concentrations of boron along the Ergene River were detected at 2604.7 µg/L, 2520.3 µg/L, 2018.0 µg/L in SP54, SP05 and SP56 respectively. All three sample points are located on the Ergene Creek which is under the pressure of several industrial discharges. SP08 is another point where Boron concentration is monitored highly (2525 µg/L). High concentrations of boron were not observed in the basin except for these SPs.

Nickel was also detected at high concentrations in all sampling points especially, on Ergene and Çorlu streams since these streams are dominated by direct domestic discharges and industrial discharges of metal processing factories and organized industrial areas.

Lead was observed in 74 of 75 SPs and lead concentrations in Ergene River were generally high. The highest concentration of Lead (2937.36 µg/L) was detected in SP51 which is close to Çerkezköy organized industrial area and Karaağaç residential area.

Along Ergene River, the concentration of Tin was observed in the range of 1 - 572 µg/L and the highest concentration of tin was detected at SP51 likewise the highest lead concentration was monitored in SP51. Tin and lead indicated a similar pollution profile since they are used together as an alloy to obtain solder. Therefore, automotive and metal industries in the region are accepted as pollution source of these two metals.

Chromium was detected intensely at 3628.9 µg/L and 2252.2 µg/L in SP44 and SP42, respectively. SP44 is located next to the Tekirdağ solid waste landfill site and the possibility of leachate from the field to the river is considered. A poultry farm and Çorlu Leather organized industrial site are close to SP42 and it is thought that leather processing wastes used as chicken feed and this appears as chromium pollution in the discharges of poultry farms.

4.5. Toxicity Analysis of Water Samples

The toxicity of each water sample was given as EC_{50} values in percentage, which shows the sample percent that causes a fifty percent decline in the activity of the test organism which is emitted light in Microtox Assay. EC_{50} values of nontoxic samples was indicated as EC_{50} (%) > 100 or "No Effect", while toxic samples expressed as 50 < EC_{50} (%) < 100 and very toxic samples displayed as EC_{50} (%) < 50. These EC_{50} (%) values were converted into dilution factors EC_{50} (df) to increase the meaningfulness of test results. This conversion was carried out by dividing hundred to the EC_{50} (%) value (equation 4.3). Microtox toxicity test results measured during 5- and 15-min exposure were given as both EC_{50} (%) and EC_{50} (df) in the Table 4.4. and dose-response curves of all samples derived for 5- and 15-minute exposure were given in APPENDIX B.

$$EC_{50}\,(df) = \frac{100}{EC_{50}\,(\%)} \tag{4.3}$$

EC_{50} (df): half maximal effective concentration as dilution factor

EC_{50} (%): half maximal effective concentration as percent

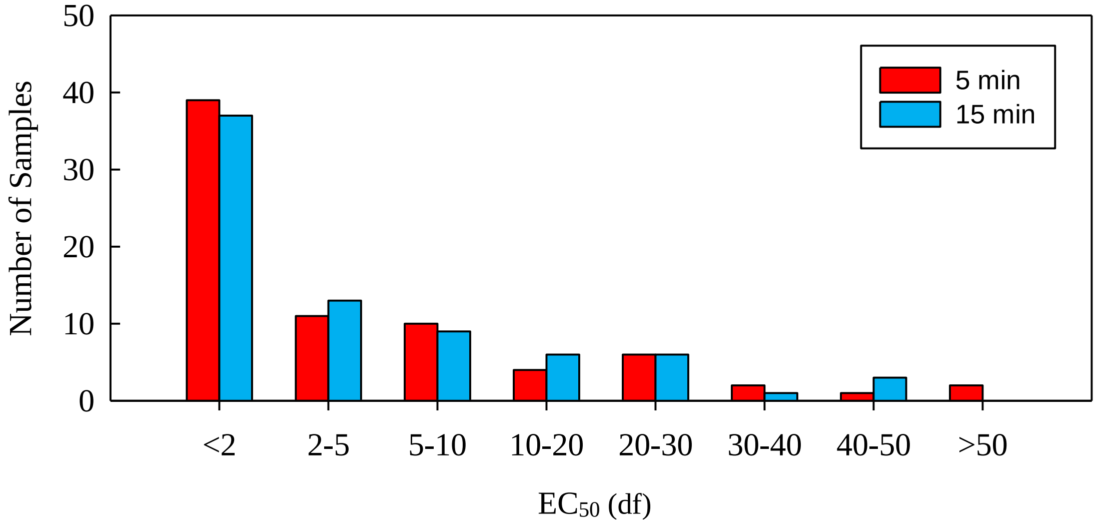

Figure 4.7. Toxicity values as dilution factor.

According to the results of toxicity tests, toxicity values as dilution factor are less than 2 in half of the samples and above 20 in 15% of the samples (Figure 4.7).

Table 4.4. Results of the Microtox toxicity test (5- and 15-min).

Sample Point	EC_{50} 5 min	EC_{50} 15 min
SP01	1.9	1.7
SP02	7.1	5.6
SP03	0.0	0.0
SP04	30.6	27.0
SP05	25.4	23.1
SP06	3.5	3.9
SP07	0.0	0.0
SP08	3.0	2.7
SP09	0.0	0.0
SP10	8.0	6.4
SP11	21.5	15.2
SP12	9.3	7.4
SP13	0.0	0.0
SP14	0.0	1.1
SP15	0.0	0.0
SP16	2.4	2.0
SP17	0.0	0.0
SP18	0.0	0.0
SP19	0.0	0.0
SP20	7.7	6.3
SP21	0.0	0.0
SP22	5.2	4.0
SP23	0.0	0.0
SP24	0.0	0.0
SP25	0.0	0.0
SP26	0.9	0.7
SP27	29.7	27.4
SP28	1.0	1.7
SP29	9.1	10.6
SP30	5.8	6.9
SP31	7.0	9.9
SP32	2.8	4.5
SP33	0.8	1.2
SP34	3.0	4.3
SP35	24.8	25.2
SP36	2.5	3.7
SP37	18.1	15.1
SP38	15.1	13.9
SP39	0.5	0.5
SP40	2.2	2.1
SP41	0.0	0.0
SP42	21.6	21.6
SP43	0.0	0.0
SP44	16.4	14.2
SP45	0.0	0.0
SP46	3.9	6.6
SP47	8.7	8.7
SP48	1.9	2.0
SP49	48.1	44.8
SP50	53.5	46.3
SP51	15.2	12.4
SP52	1.6	1.7
SP53	1.9	2.0
SP54	31.1	31.1
SP55	55.2	48.1
SP56	3.7	5.0
SP57	4.1	4.6
SP58	1.0	0.8
SP59	0.0	0.0
SP60	0.0	0.0
SP61	0.0	0.0
SP62	7.4	7.4
SP63	1.6	1.6
SP64	27.0	22.0
SP65	1.3	1.1
SP66	1.1	1.4
SP67	0.0	0.0
SP68	4.5	3.8
SP69	0.0	0.0
SP70	0.0	0.0
SP71	0.9	0.8
SP72	0.0	0.0
SP73	0.0	0.0
SP74	0.0	0.0
SP75	0.0	0.0

The Microtox tests performed on the water samples show that Ergene River has an important toxicity problem. Throughout the river, toxicity values were observed higher in the Ergene and Çorlu streams which are seriously polluted by several industrial and domestic discharges. On the other hand, there are also points where toxicity was not observed, and the common feature of these points is that they are in agricultural areas. Toxicity distribution along the Ergene River was demonstrated for 5- and 15-minute exposure on the maps given in Figure 4.9 and Figure 4.10, respectively.

The highest toxicity value was reported in the SP55 which is near to Ergene-1 organized industrial area that is dominated by textile, paint, plastic and metal industries. 33 micropollutants were detected in SP55 and especially, HMMM, damascone and PCB-169 were found at high concentrations; 38278.05 µg/L, 814.20 µg/L and 423.12 µg/L, respectively. Moreover, 15 heavy metals were monitored in SP55 and among these metals, aluminum, nickel, boron and zinc were detected at 1542.40 µg/L, 229.97 µg/L, 222.28 µg/L and 105.05 µg/L respectively.

In a previous study, HMMM was associated with acute toxicity effects on *daphnia*, which were used for online toxicity tests of Meuse River water. The results provided evidence that the toxic potential of HMMM is not fully understood and that synergistic toxic effects in combination with other contaminants are likely (de Hoogh et al., 2006).

The second and third highest toxicity results were detected in SP50 and SP49 which are close to each other and in the same branch of Ergene River. These SPs are under pressure of the discharge of Velimeşe organized industrial area that is dominated by textile, paint and metal industries. Among the micropollutants detected in these SPs HMMM, PCBs, TBEP, benzyldimethyldodecylammonium, nonylphenol diethoxylate, methylsalicylate, dicyclohexylamine, 1,2,3-benzotriazole, indeno[1,2,3-cd]pyrene and methyldihydrojasmonate had the highest concentrations while, among the metals monitored Al, B, Ni, Pb, Cu, Sn, Zn and Ba had the highest values.

To determine the pollution sources contributing to the toxicity in the Ergene River, toxicities were compared along the main stream. SP02 is located at the east of the Ergene River and is exposed to relatively less contaminants (19 micropollutants). From SP27 to SP03, which represents the point where the Ergene River connects to the Maritsa River, high toxicity values are observed throughout the main stream. Average of the measured EC_{50} (df) – 15 min values along the main stream was 7.7±8.1.

High toxicity values were detected on the tributaries that SP04 and SP05 were connected to the main stream. These tributaries are Çorlu Creek and Ergene Creek which are under the pressure of industrial discharges. In addition to these, the tributary that SP11 was connected to the main stream was also showed high toxicity. These three tributaries highly contribute to toxicity in the mainstream.

Çorlu Creek flows through Çerkezköy and Çorlu districts and merges with Ergene River in Muratlı district. Çorlu Creek is directly or indirectly under the pressure of Çerkezköy, Çorlu and Muratlı districts and Çerkezköy, Kapaklı, Yalıboyu, Velimeşe, Veliköy, Çorlu-1 and Çorlu Leather Organized Industrial Zones. SP02 was located the upstream of the point where Çorlu Creek connected to Ergene River and SP27 was located the downstream of this point. When the toxicity of Ergene River was considered before and after the Çorlu Creek joins, it was observed that Çorlu Creek significantly increased the toxicity of the Ergene River.

SP50, SP49, SP64, SP42 and SP04 had highest toxicity values along the Çorlu Creek. The sources of toxicity on these points were related to the discharges. SP64 was under the pressure of domestic and industrial discharges of Çerkezköy and Kapaklı districts. SP49 and SP50 were under the pressure of industrial discharge of Velimeşe OIZ while, SP42 was under the pressure of Çorlu Leather OIZ and a poultry farm.

Ergene Creek is the source of Ergene River. Ergene Creek flows from Saray to İnanlı districts and in the near of SP28 it merges with Ergene River. SP05 was taken before the Ergene Creek merges with the Ergene River and high toxicity was observed in SP05. High toxicity values observed along the Ergene Creek indicate that the creek is under pressure of major pollution sources. SP54, SP55 and SP05 had highest toxicity along Ergene Creek. SP54 was under the pressure of Ergene-2 OIZ and SP55 was under the pressure of Ergene-1 OIZ.

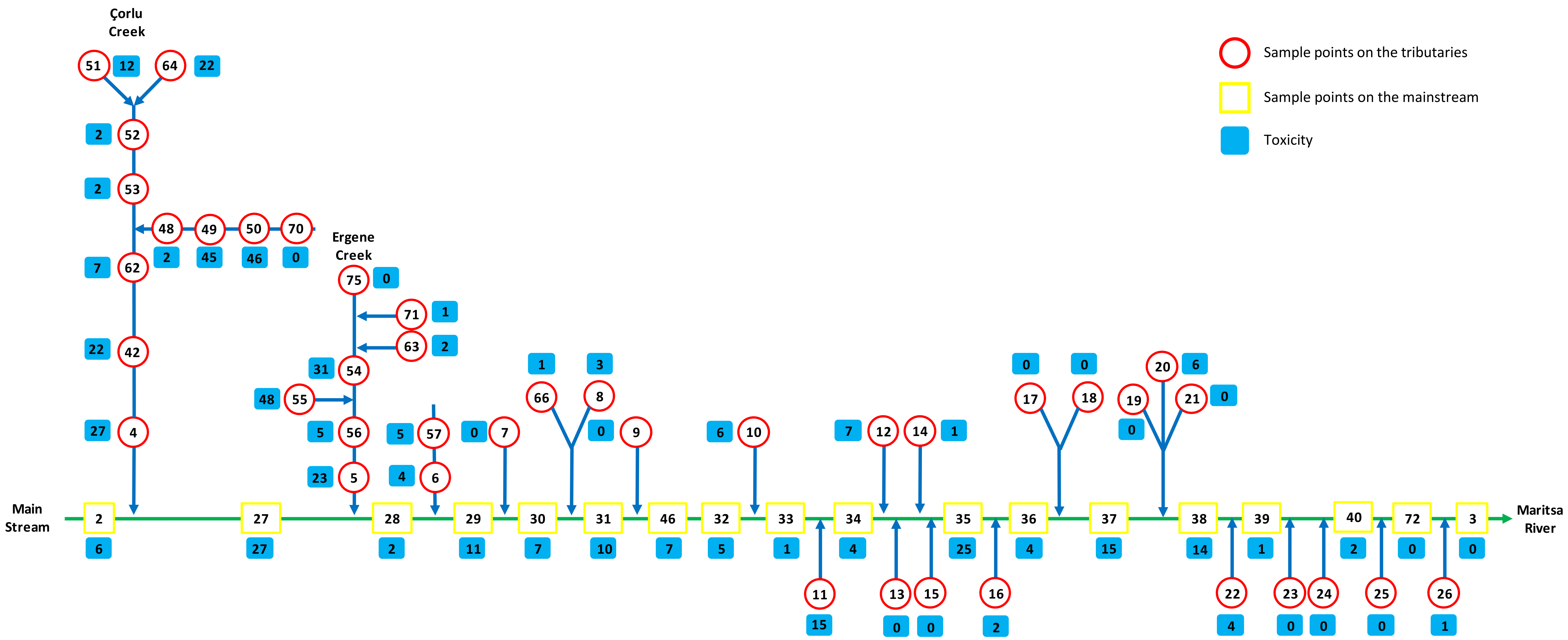

Figure 4.8. Toxicity (EC_{50} (df) – 15 min) flow of the mainstream and tributaries.

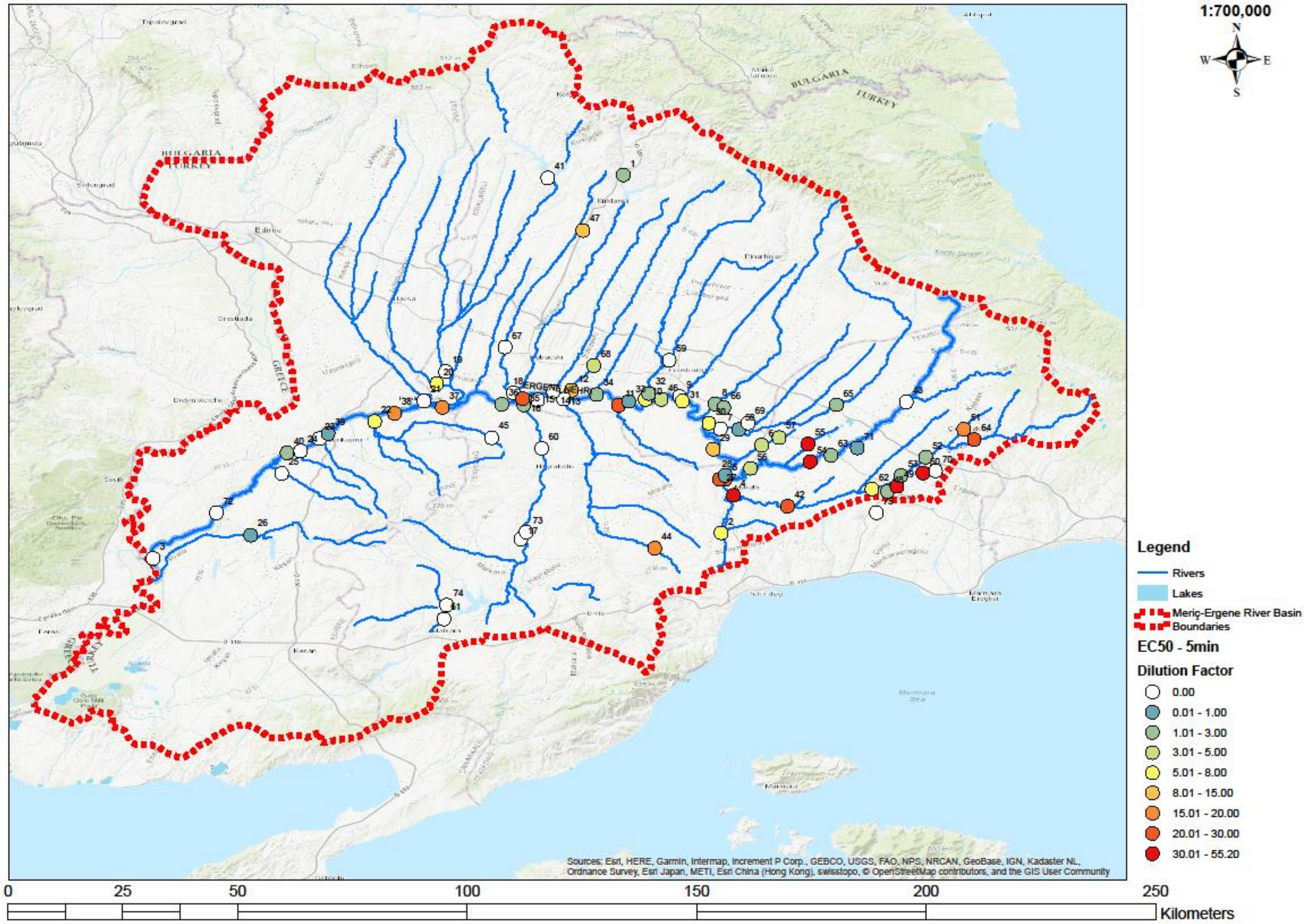

Figure 4.9. Microtox toxicity results as dilution factor along Ergene River during 5-minute exposure.

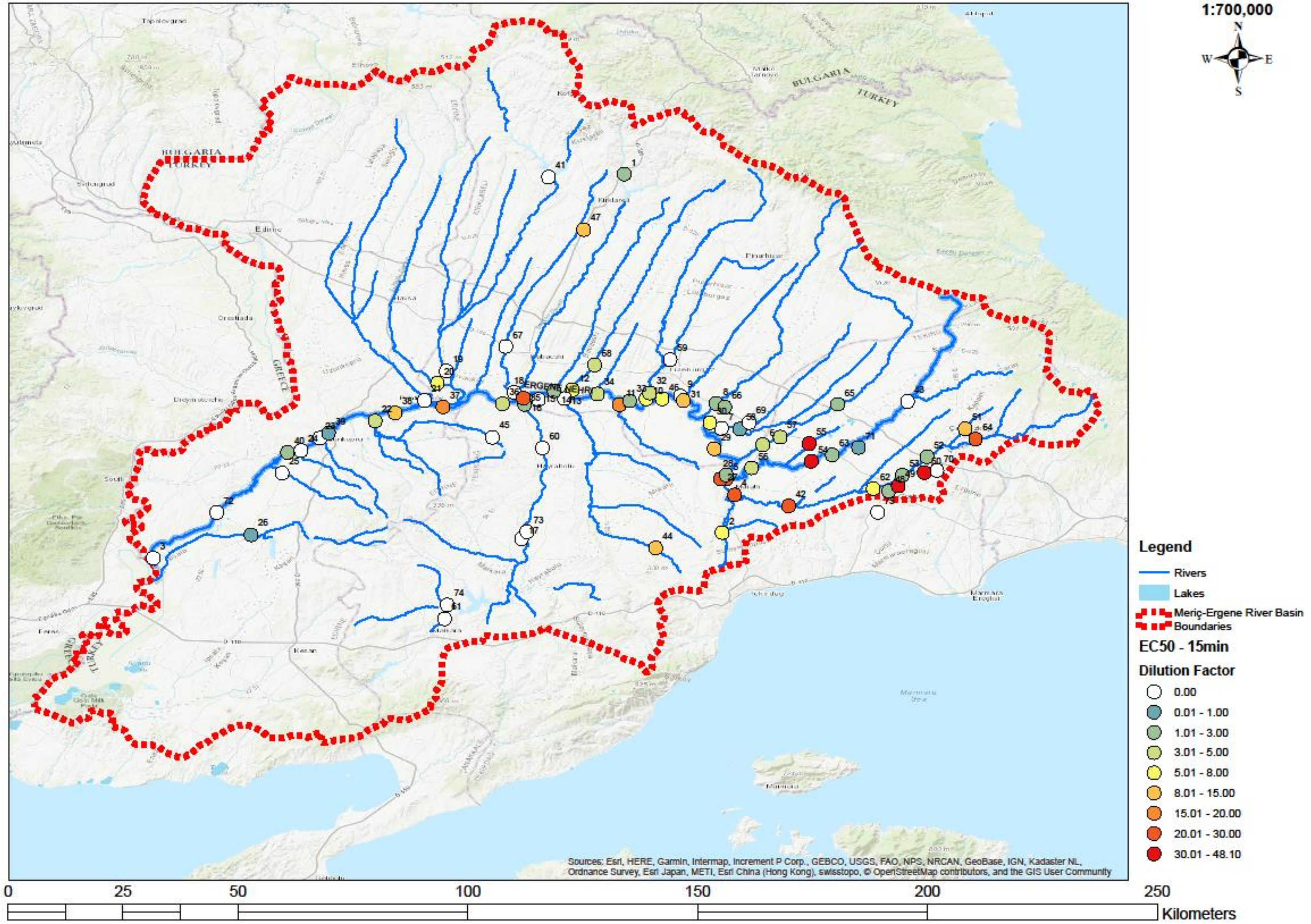

Figure 4.10. Microtox toxicity results as dilution factor along Ergene River during 15-minute exposure.

4.6. Prioritization of Pollution Source Zones

When the potential pollution sources in the region were examined, it was observed that the water samples taken from the Lüleburgaz, Muratlı, Çorlu and Çerkezköy districts were under the pressure of industrial discharges. Therefore, major source of pollution in Çorlu and Ergene creeks was industrial activities. On the other hand, it was determined that samples taken near Babaeski, Hayrabolu, Pehlivanköy districts are mainly under the pressure of domestic discharges. In addition to domestic and industrial pollutions, the impact of the agricultural runoff was observed in most of the water samples as the agricultural activities were widely applied in the region. Potential pollution sources affecting each point was explained in Table 4.5. and a map showing potential pollution sources was given in Figure 4.11.

Table 4.5. Potential Pollution Sources affecting sampling points.

Sample Point	Chemical Count	EC50 (df) 15 min	Location Near	Pollution Source Type
SP01	15	1.7	Kırklareli Dam/Kızılcıkdere village	Source of the river
SP02	19	5.6	Yeşilsırt village/Muratlı	Agricultural runoff
SP03	25	0.0	Adasarhanlı village/Meriç	Agricultural runoff
SP04	54	27.0	Muratlı/Tekirdağ	Domestic Discharge, Solid Waste Disposal Land Leachate
SP05	52	23.1	İnanlı village/Tekirdağ	Agricultural runoff
SP06	33	3.9	Büyükkarıştıran OIZ	Industrial Discharge
SP07	28	0.0	Çiftlikköy village/Lüleburgaz	Domestic Discharge
SP08	56	2.7	Evrensekiz OIZ/Lüleburgaz	Industrial Discharge
SP09	58	0.0	Eskibedir village/Lüleburgaz	Agricultural runoff
SP10	27	6.4	Durak village/Lüleburgaz	Agricultural runoff and Domestic Discharge
SP11	45	15.2	Düğüncübaşı village/Lüleburgaz	Agricultural runoff
SP12	29	7.4	Düğüncülü village/Babaeski	Agricultural runoff
SP13	43	0.0	Sinanlı town/ Babaeski	Agricultural runoff
SP14	40	1.1	Alpullu town/Babaeski	Domestic and Industrial (oil factory) discharge
SP15	32	0.0	Mandıra town/Babaeski	Domestic Discharge
SP16	28	2.0	Karakavak town/Hayrabolu	Agricultural runoff
SP17	22	0.0	Nadırlı village/Babaeski	Agricultural runoff
SP18	19	0.0	Katranca village/Babaeski	Agricultural runoff
SP19	21	0.0	Kumköy and İmampazarı/Pehlivanköy	Agricultural runoff
SP20	25	6.3	Hıdırca village/Pehlivanköy	Domestic Discharge and Agricultural runoff
SP21	21	0.0	Sazlımalkoç village/Uzunköprü	Agricultural runoff
SP22	19	4.0	Bayramlı village/Uzunköprü	Agricultural runoff
SP23	33	0.0	Uzunköprü/Edirne	Domestic Discharge and Agricultural runoff
SP24	34	0.0	Uzunköprü/Edirne	Domestic (Uzunköprü WWTP) Discharge and Agricultural runoff
SP25	35	0.0	Kavacık village/Uzunköprü	Agricultural runoff
SP26	19	0.7	Balaban village/Uzunköprü	Agricultural runoff
SP27	61	27.4	İnanlı village/Tekirdağ	Agricultural runoff, stock farming (AKSA Tarım)

Table 4.5. Potential Pollution Sources affecting sampling points (continued).

Sample Point	Chemical Count	EC50 (df) 15 min	Location Near	Pollution Source Type
SP28	60	1.7	İnanlı village/Tekirdağ	Domestic Discharge
SP29	56	10.6	Seyitler village/Lüleburgaz	Domestic Discharge and Agricultural runoff
SP30	53	6.9	Karamusul village/Lüleburgaz	Agricultural runoff
SP31	50	9.9	Eskibedir village/Lüleburgaz	Domestic, unothorized land fill leachate
SP32	50	4.5	Durak/Lüleburgaz/Kırklareli	Agricultural runoff
SP33	51	1.2	Düğüncübaşı village/Lüleburgaz	Agricultural runoff, unothorized land fill leachate
SP34	48	4.3	Oklalı village/Lüleburgaz	Agricultural runoff
SP35	48	25.2	Mandıra town/Babaeski	Agricultural runoff
SP36	49	3.7	Hedeyli town/Hayrabolu	Agricultural runoff
SP37	49	15.1	Akarca village/Pehlivanköy	Agricultural runoff
SP38	46	13.9	Muhacırkadı village/Uzunköprü	Agricultural runoff
SP39	39	0.5	Demirtaş village/Uzunköprü	Agricultural runoff
SP40	37	2.1	Çiftlikköy village/Uzunköprü	Agricultural runoff
SP41	19	0.0	Kayalı village/Kırklareli	Kayalıköy Dam on Teke River
SP42	50	21.6	Balabanlı town/Muratlı	Agricultural runoff, poultary farm
SP43	28	0.0	Uzunhacı town/Çerkezköy	Domestic Discharge
SP44	38	14.2	Banarlı town/Süleymanpaşa	Agricultural runoff
SP45	16	0.0	Çerkezmüsellim town/Hayrabolu	Domestic Discharge and Agricultural runoff
SP46	49	6.6	Durak village/Lüleburgaz	Domestic (Lüleburgaz WWTP) Discharge and Agricultural runoff
SP47	33	8.7	Merkez/Kırklareli	Domestic (Kırklareli WWTP) Discharge and Agricultural runoff
SP48	52	2.0	Çorlu /Tekirdağ	Domestic and Industrial Discharge
SP49	45	44.8	Çorlu /Tekirdağ	Agricultural runoff and industrial (textile)
SP50	43	46.3	Misinli town/Çorlu	Domestic and Industrial Discharge, Agricultural runoff
SP51	33	12.4	Karaağaç town/Çerkezköy	Domestic Discharge and unothorized land fill leachate
SP52	52	1.7	Velimeşe town/Çorlu	Domestic Discharge and Agricultural runoff
SP53	43	2.0	Yulaflı town/Çorlu	Industrial Discharge and Agricultural runoff
SP54	50	31.1	Esenler town/Çorlu	Domestic Discharge and Agricultural runoff
SP55	33	48.1	Vakıflar village/Ergene	Agricultural runoff and industrial (textile sector, Ergene-1 OIZ)
SP56	58	5.0	Aşağısevindikli town/Muratlı	Industrial (metal sector) Discharge
SP57	41	4.6	Büyükkarıştıran/Lüleburgaz	Agricultural runoff and industrial (textile sector, Büyükkarıştıran OIZ)
SP58	37	0.8	Büyükkarıştıran/Lüleburgaz	Agricultural runoff
SP59	25	0.0	Lüleburgaz/Kırklareli	Agricultural runoff
SP60	19	0.0	Çıkrıkçı village/Hayrabolu	Agricultural runoff
SP61	34	0.0	Gönence town/Malkara	Agricultural runoff and Domestic Discharge
SP62	53	7.4	Marmaracık town/Çorlu	Industrial (Çorlu Leather OIZ) Discharge
SP63	43	1.6	Kırkgöz and Ulaş town/Çorlu	Agricultural runoff and industrial (paper, textile industry, combustion plant)

Table 4.5. Potential Pollution Sources affecting sampling points (continued).

Sample Point	Chemical Count	EC50 (df) 15 min	Location Near	Pollution Source Type
SP64	43	22.0	Çerkezköy OIZ/Çerkezköy	Domestic and Industrial (metal, plastic sectors) Discharge
SP65	23	1.1	Beyazköy village/Saray	Agricultural runoff and industrial (beverage factory, textile factory)
SP66	34	1.4	Evrensekiz/Kırklareli	Industrial (textile) Discharge
SP67	25	0.0	Oruçlu village/Babaeski	Agricultural runoff
SP68	25	3.8	Kırıkköy village/Kırklareli	Agricultural runoff and food industry discharge
SP69	29	0.0	Büyükkarıştıran/Lüleburgaz	Industrial (chemical sector) Discharge
SP70	25	0.0	Velimeşe town/Çorlu	Industrial (spinning factory) Discharge
SP71	24	0.8	Ulaş town/Çorlu	Agricultural runoff
SP72	39	0.0	Yenicegörüce village/Meriç	Agricultural runoff
SP73	20	0.0	Kurtdere and Hacılı village/Hayrabolu	Agricultural runoff
SP74	33	0.0	Karaidemir Dam/Malkara	Agricultural runoff
SP75	27	0.0	Karamehmet and Bakırca town/Çorlu	Agricultural runoff

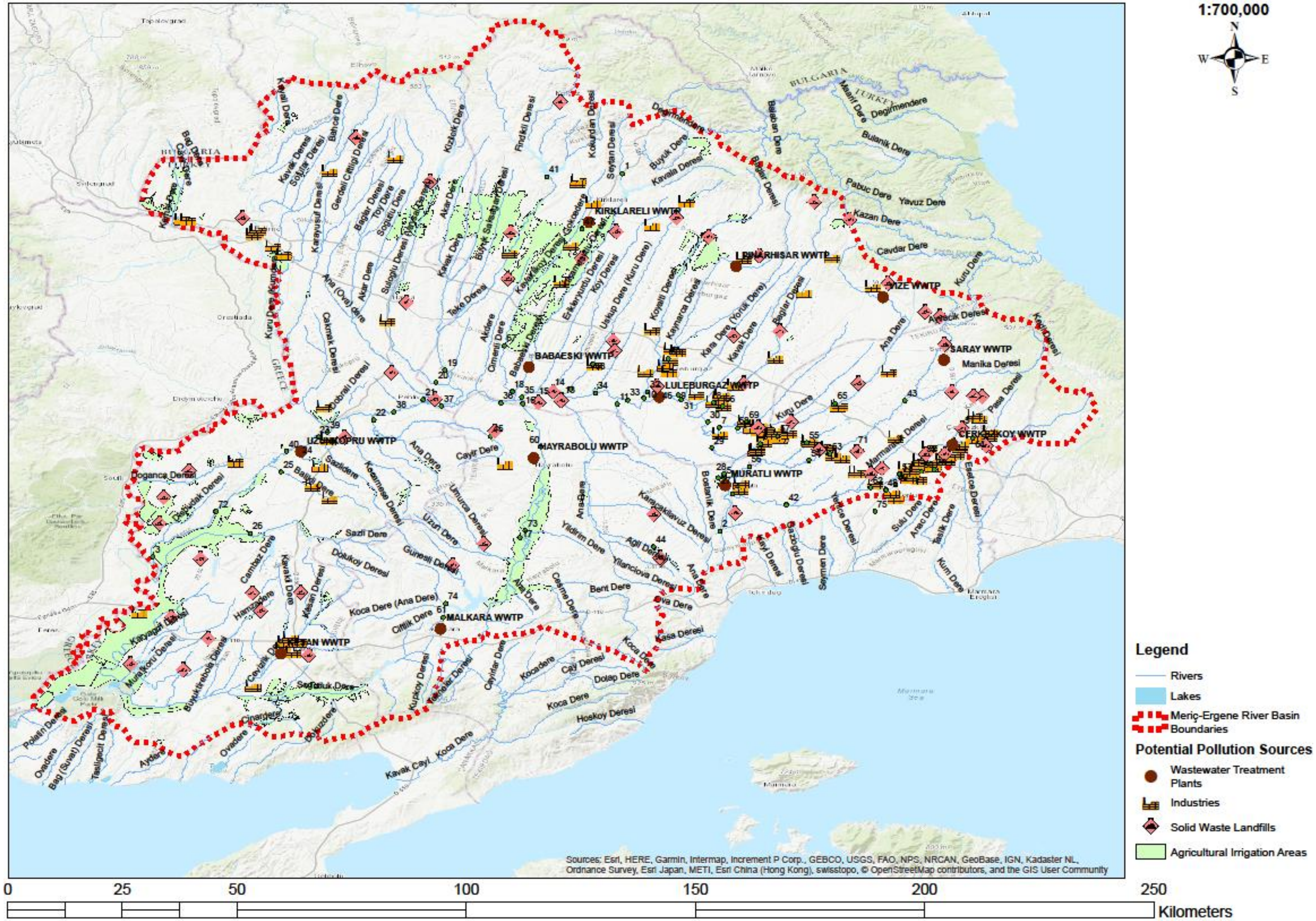

Figure 4.11. Illustration of potential pollution sources on a map

4.7. Pollution Source Clustering

To create a pollution tree of sampling points neighbor-joining (NJ) method based on Jaccard distance was used through MEGA software. First, the analysis results were converted to binary matrix by coding each compound as “1” or “0” respectively to their presence or absence. Then the converted data was used to obtain Jaccard distance and to construct a pollution tree by NJ method. The pollution tree and designated clusters of sampling points with a toxicity heatmap is illustrated in Figure 4.13. and a map is demonstrated in Figure 4.12. to evaluate relationship between locations of sampling points and clusters they belong.

Sample points were clustered according to the presence and absence of the chemical substances. Accordingly, although they were taken from different tributaries of Ergene River, the members of Cluster 4 showed similar toxicity and were clustered together since they were all under the pressure of agricultural activities. The sample points in the remaining clusters were mostly successive points. The sample points in the Cluster 5 were mainly under the pressure of industrial discharges of textile and paint industries while, the sample points in the Cluster 1, 2 and 3 were generally under the pressure of agricultural activities. The sample points in the Cluster 7 were located on the main stream and follow each other. The sample points in the Cluster 6 were also the downstream of each other and they were mainly under the pressure of domestic and industrial discharges.

When the toxicity distribution between clusters was examined, the highest toxicity was observed in water samples belonged to Cluster 5 while the lowest toxicity was determined in water samples belonging Cluster 3, Cluster 2 and Cluster 1, respectively. The sample points in the Cluster 5 are in the area that organized industrial zones are located and therefore, they are expected to show highly toxic effects.

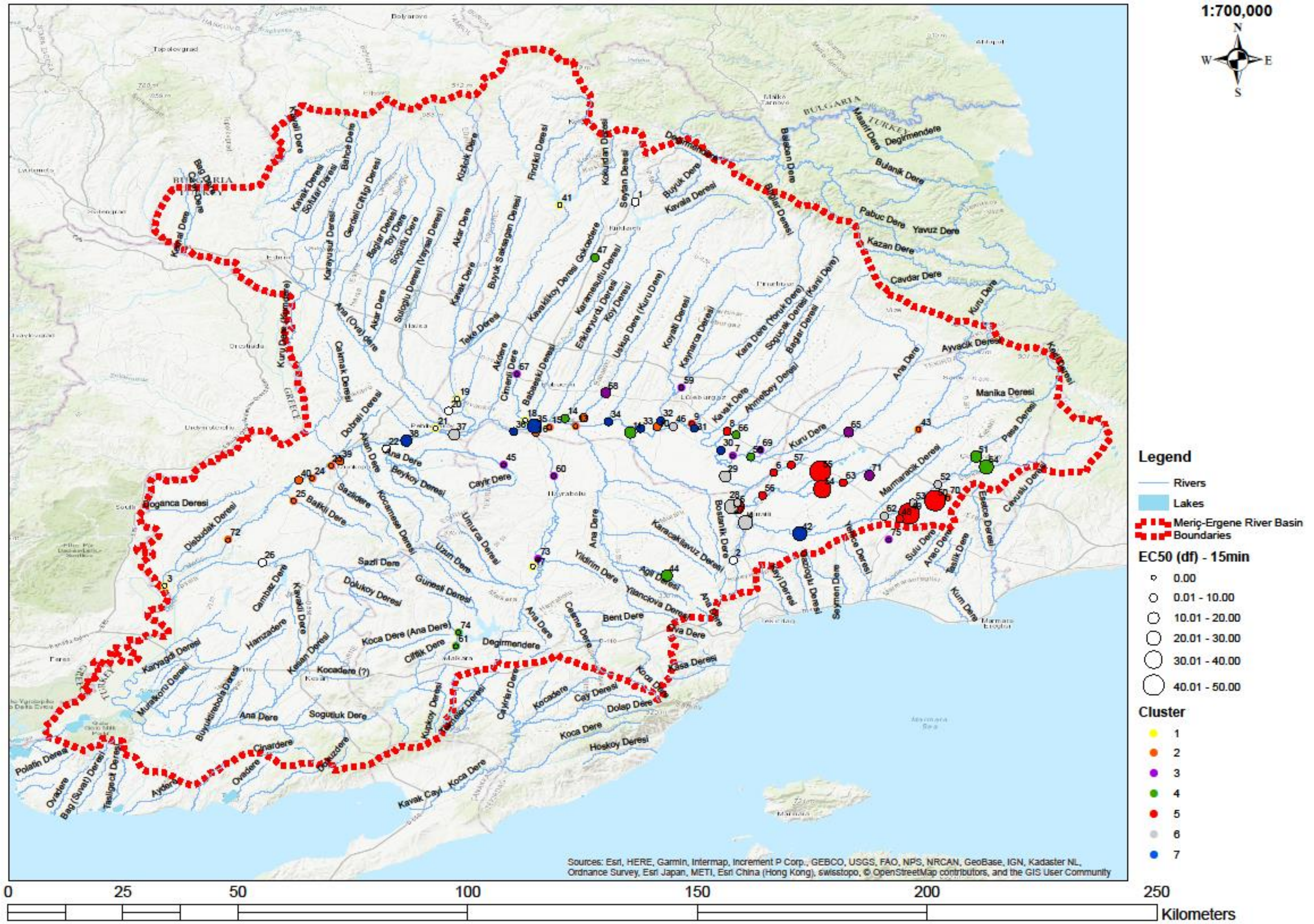

Figure 4.12. Toxicity distribution along Ergene River by cluster analysis.

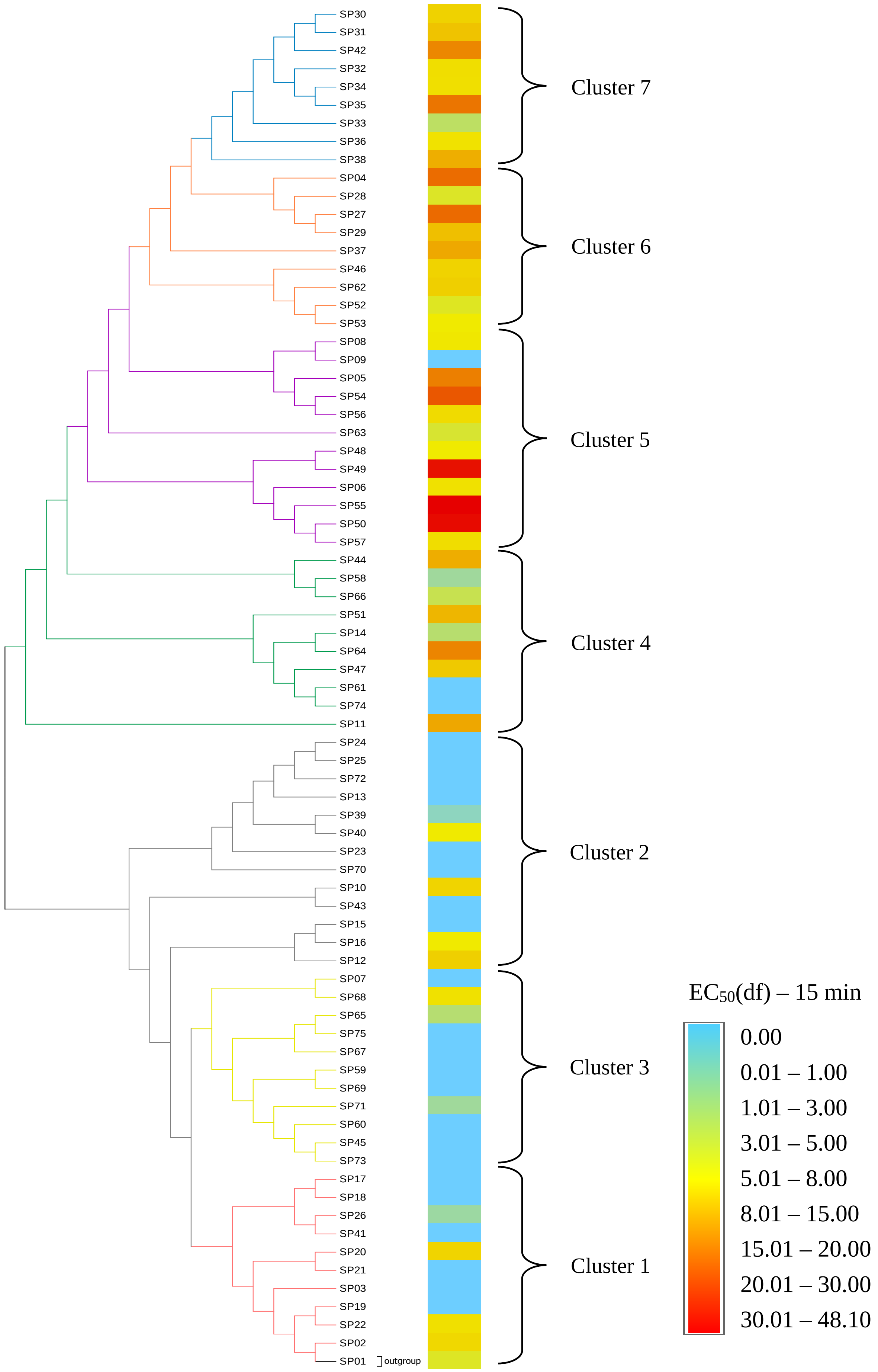

Figure 4.13. Pollution Tree constructed by NJ method.

4.8. Toxicity – Pollutant Relationships

4.8.1. Contribution of Micropollutants to Toxicity

To evaluate the relationship between toxicity and micropollutants regression curves were developed for each chemical. Regression of each contaminant with toxicity showed that benzyldimethyltetradecylammonium (BAC 14) (r^2=0.402), benzylamine (r^2=0.367), nonylphenol diethoxylate (NP2EO) (r^2=0.357), benzyldimethyldodecylammonium (BAC 12) (r^2=0.351), PCB-169 (r^2=0.346), dicyclohexylamine (r^2=0.259), celestolide (ADBI) (r^2=0.258) and 3-chloroaniline (r^2=0.226) were most probably related to toxicity.

Among these micropollutants, BAC 12 and BAC 14 are generally used as surfactant, disinfectant and biocide. They are widely used in both domestic and industrial purposes and they are known to cause antibiotic resistance and be toxic for aquatic environments. According to study done by Tezel (2009) 15-min Microtox toxicity values of BAC 12 and BAC 14 were measured as 0.14 mg/L and 0.27 mg/L, respectively. The maximum concentration of BAC 12 (23.89 µg/L) and BAC 14 (7.64 µg/L) measured in the water samples are lower than these EC_{50} values.

Benzylamine is used in synthetic textiles, in paints, and as corrosion inhibitor. It is also used as an intermediate in the manufacture of pharmaceutically active substances and compounds for crop protection (Heuer,2006). Vighi and coworkers (2009) measured Microtox toxicity value of benzylamine as 42.9 mg/L and this EC_{50} value is higher than the maximum concentration (0.74 µg/L) of benzylamine.

NP2EO is widely used in detergents, emulsifiers, solubilizers, wetting and dispersing agents in households and chemicals. Mode of toxicity for NP2EO is narcosis (TenEyck and Markee, 2007).

PCBs are generally used in several industrial applications, including lubricants, dielectric fluids, and plasticizers since they offer high chemical and physical stability and high dielectric constant (Bhalla et al., 2016).

DCHA is broadly used in chemical processes. It is a hydrophobic amine used in insecticides, plasticizers, in the metal industry, as a fuel oil additive and as a chemical intermediate (Munthe, 2011).

Celestolide (ADBI) is a synthetic polycyclic musk fragrance. It is used to embalm cleansers and cosmetics. Mode of toxic action for ABDI is non-polar narcosis in aquatic organisms (Brausch and Rand, 2011).

Chloroanilines (CAs) are widely used in the production of polyurethanes, rubber, dyes, pharmaceutics, photographic chemicals, varnishes, and pesticides. In a previous study by Aruoja and coworkers, the Microtox toxicity value of 3-CA was measured as 64.3 mg/L (Aruoja et al., 2011) which is 40-times higher than the maximum concentration of 3-CA.

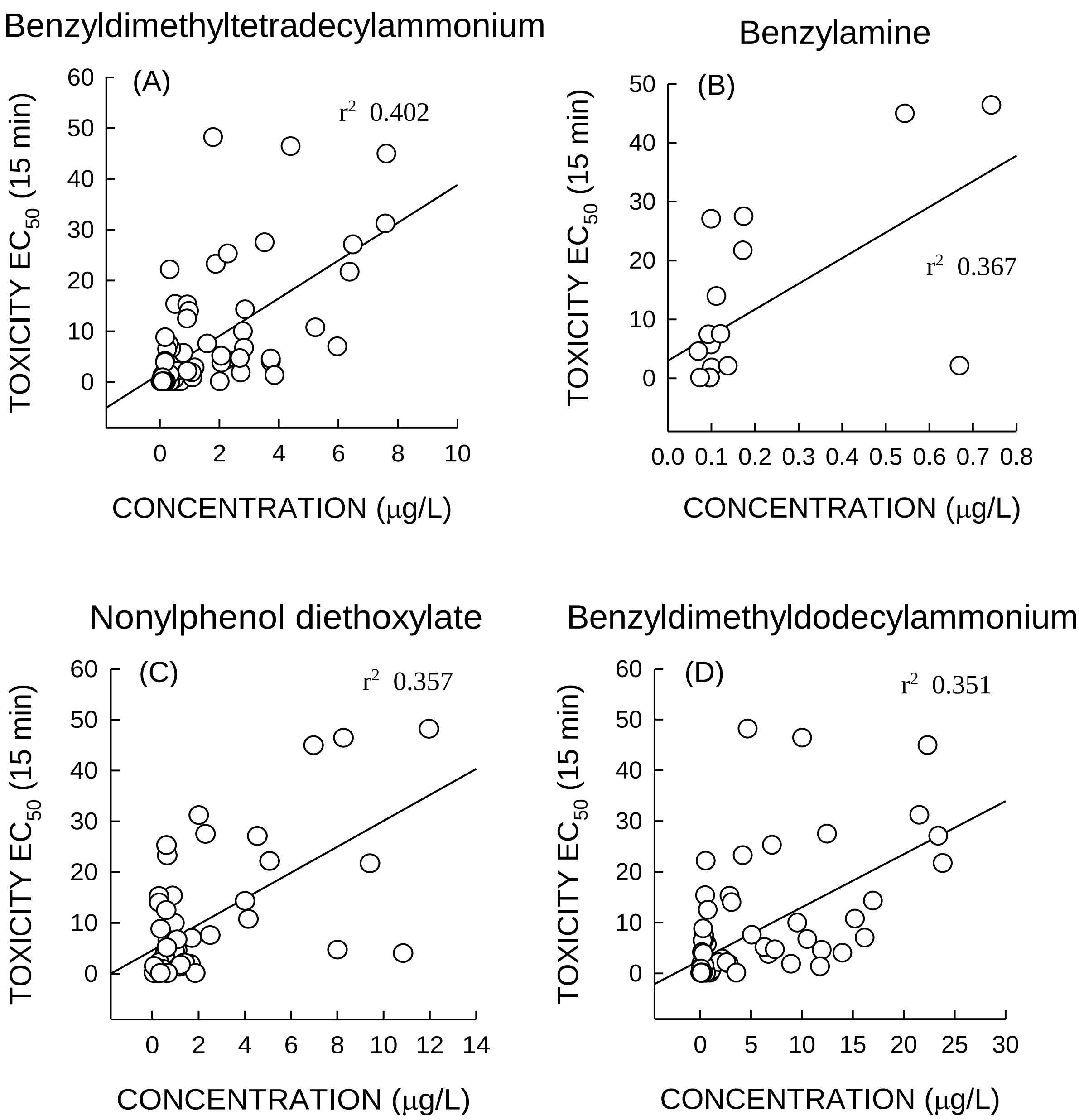

Figure 4.14. Toxicity vs. Concentration linear regression curves for highly correlated micropollutants.

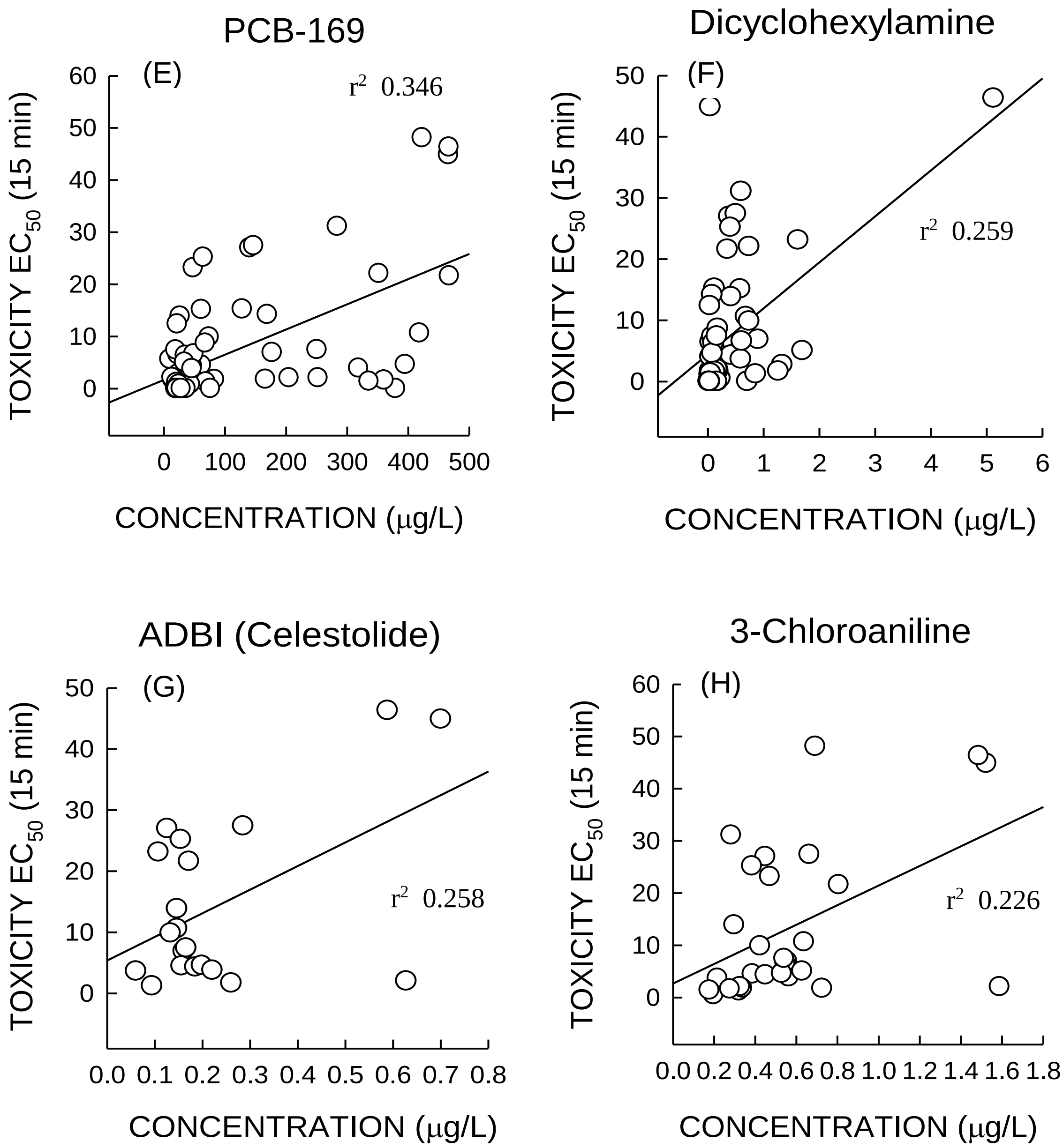

Figure 4.14. Toxicity vs. Concentration linear regression curves for highly correlated micropollutants (continued).

4.8.2. Mixture Toxicity Prediction

The joint toxicity of the chemical mixtures was predicted by Concentration Addition (CA) and Independent Action (IA) models. There are several studies to determine which model is better in predicting the toxicity for chemical mixtures. For instance, Gao and coworkers (2018) used both CA and IA models to predict the toxicity for metal mixtures on zebrafish larvae and found that the both models offered variable predictive capabilities for different metal combinations. However, in the study conducted by Di Nica and colleagues (2017), both models made similar predictions for the toxicity of the mixtures of Quaternary Ammonium Compounds (QACs).

4.8.2.1. Concentration Addition (CA). CA or dose addition describes the joint action of chemicals that have same mode of toxic action and it is based on the idea that all chemicals in the mixture act as if they are simple dilutions of each other and have same mechanism of action. CA is mathematically formulated as following:

$$ECx_{Mix} = \left[\sum_{i=1}^{n} \frac{p_i}{ECx_i} \right]^{-1} \quad (4.4)$$

n: the number of chemicals in mixture
p_i: the relative fraction of chemical i in the mixture
x: the common effect level

To estimate the toxicity of a mixture, single toxicity values of each component in the mixture should be known. Therefore, EC_{50} values for all detected chemicals were collected from ECOSAR database. Since Microtox toxicity data were not available for all chemicals in the database, algal toxicity values were used in the calculations. EC_{50} (algae) values taken from ECOSAR were shown in Table C.1. at APPENDIX C.

In order to compare measured toxicity data with predicted mixture toxicity, EC_{50} (mix) was calculated for algae based on the EC_{50} (algae) values and afterward, algal mixture toxicity data (EC_{50} (mix,algae)) was converted to predicted Microtox toxicity (EC_{50} (predicted)) according to the following equations derived by Neale and colleagues (2017):

$$\log\left(\frac{1}{EC_{50}(M)}\right) \text{(algal growth inhibition)} = 0.91 \times \log D_{lipw} + 0.63 \quad (4.5)$$

$$\log\left(\frac{1}{EC_{50}(M)}\right) \text{(Microtox)} = 0.75 \times \log D_{lipw} + 0.97 \quad (4.6)$$

D_{lipw}: liposome-water distribution ratio

Measured toxicity data were calculated by using Microtox toxicity test results (EC_{50} (df)) of water samples.

$$EC_{50}(\text{measured}) = \frac{1}{EC_{50}\,(df)} \cdot \Sigma Ci \quad (4.7)$$

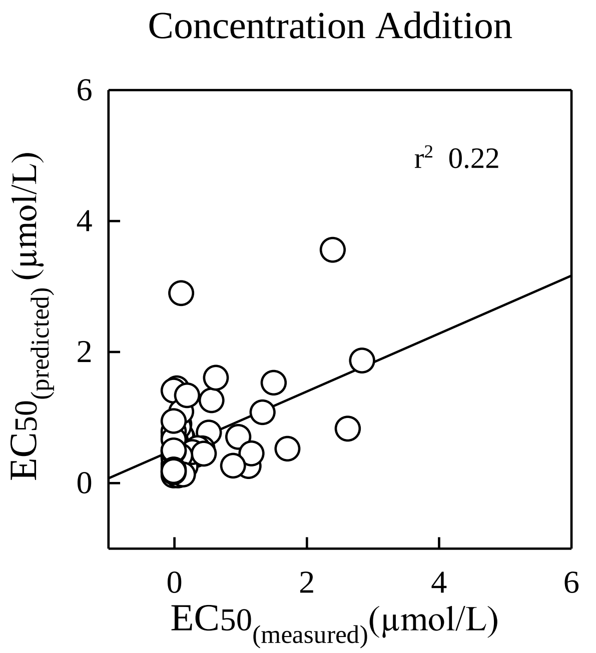

Figure 4.15. Comparison of measured and predicted mixture toxicity values by CA method.

__4.8.2.2. Independent Action (IA):__ IA or effect addition computes toxicity of mixtures when chemical components have different mode of action. IA is mathematically expressed as following:

$$E(C_{Mix})=1-\prod_{i=1}^{n}[1-E(C_i)] \tag{4.8}$$

$$C_{Mix}=\sum_{i=1}^{n} C_i \tag{4.9}$$

n: the number of chemicals in mixture

$E(C_{Mix})$: the effect provoked by the total mixture concentration

C_{Mix}: total concentration

Like CA method, first, $E(Cmix)_{algae}$ was calculated and converted to predicted Microtox toxicity (EC_{50} (predicted)) according to the equations 4.5 and 4.6. And measured toxicity data were calculated by using Microtox toxicity test results.

$$EC_{50}(\text{measured}) = \frac{\text{Cmix}/EC_{50}(\text{df})}{1+\frac{\text{Cmix}}{EC_{50}(\text{df})}} \tag{4.10}$$

Cmix: total concentration

EC_{50}(df): half maximal effective concentration as dilution factor

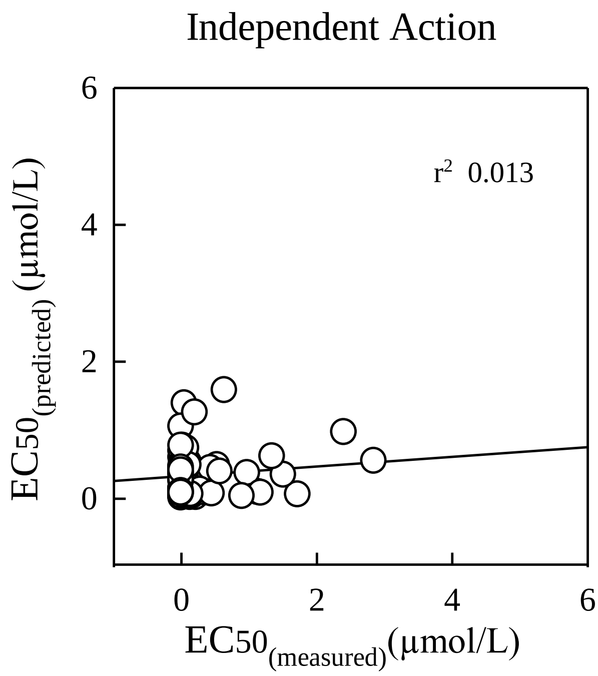

Figure 4.16. Comparison of measured and predicted mixture toxicity values by IA method.

When the mixture toxicity values predicted by the CA and IA models were compared with the actual toxicity results, it was observed that the CA model predicted more accurately than the IA model, but it was not perfect either. This can be explained by that many other chemicals, that are not analyzed in the scope of this study, are present in the water samples and they contribute to the mixture toxicity. Furthermore, ECOSAR toxicity values are derived from the LogP value and LogP varies between the measured and/or predicted values. It would be appropriate to re-examine the relationship with the toxicity data to be obtained with more reliable QSAR models.

4.9. PNEdf Calculations and Environmental Risk Maps

In the evaluation of surface waters with many contaminants as in this study, it is appropriate to develop a risk assessment parameter like the Predicted No Effect Dilution Factor (PNEdf). PNEdf values were derived in order to evaluate the harmful effects of the analyzed samples if they are discharged to receiving environments and to prevent these effects. PNEdf values calculated based on the results of the Microtox test and the highest EC_{50} (algae) ECOSAR values were given in the Table 4.6. and the risk maps obtained by using these values were shown in the Figure 4.17. and Figure 4.18. The EC_{50} (algae) values collected from ECOSAR were shown in Table C.1. at APPENDIX C.

$$\text{PNEdf(microtox)} = \text{EC}_{50}(\text{df}) \times \text{AF} \quad (4.11)$$

$$\text{PNEdf(algae)} = \text{EC}_{50}(\text{algae}) \times \text{AF} \quad (4.12)$$

AF: assessment factor of 1000

Table 4.6. PNEdf values for pollution sources based on EC_{50} (algae) values from ECOSAR and Microtox results.

Sample Point	PNEdf (Microtox)	PNEdf (algae)
SP01	1718.8	881.9
SP02	5614.8	616.8
SP03	0.0	1492.4
SP04	26976.0	36741.8
SP05	23121.4	10505.2
SP06	3886.5	276801.4
SP07	0.0	1488.2
SP08	2741.2	5132.3
SP09	0.0	23657.0
SP10	6426.7	8892.7
SP11	15243.9	8004.6
SP12	7369.2	1219.7
SP13	0.0	15957.3
SP14	1141.6	17596.8
SP15	0.0	25536.5
SP16	2003.2	8766.1
SP17	0.0	1638.8
SP18	0.0	1703.9
SP19	0.0	1302.7
SP20	6337.1	2194.3
SP21	0.0	7300.7
SP22	4027.4	2396.9
SP23	0.0	5533.6
SP24	0.0	31092.9
SP25	0.0	9032.1
SP26	733.1	22906.9
SP27	27397.3	41687.0
SP28	1703.0	34262.2
SP29	10604.5	77469.0
SP30	6887.1	82718.5
SP31	9852.2	55212.1
SP32	4468.3	43850.8
SP33	1227.0	53267.5
SP34	4297.4	52179.0
SP35	25188.9	25188.9

Table 4.6. PNEdf values for pollution sources based on EC_{50} (algae) values from ECOSAR and Microtox results (continued).

Sample Point	PNEdf (Microtox)	PNEdf (algae)
SP36	3655.0	37036.4
SP37	15128.6	33726.9
SP38	13850.4	31381.6
SP39	509.4	22668.5
SP40	2076.0	30093.4
SP41	0.0	4040.4
SP42	21598.3	77949.9
SP43	0.0	7033.9
SP44	14164.3	10554.0
SP45	0.0	1402.9
SP46	6596.3	48834.9
SP47	8695.7	44648.5
SP48	2024.7	377397.0
SP49	44843.0	234522.0
SP50	46296.3	130053.5
SP51	12376.2	1835.4
SP52	1737.6	28395.4
SP53	2009.2	28978.1
SP54	31055.9	17717.8
SP55	48076.9	43886.6
SP56	5025.1	28603.3
SP57	4580.9	292027.6
SP58	780.0	10933.0
SP59	0.0	1255.1
SP60	0.0	1422.2
SP61	0.0	4770.0
SP62	7423.9	65323.8
SP63	1622.3	22484.4
SP64	22041.0	21957.5
SP65	1121.1	10575.7
SP66	1380.1	20952.8
SP67	0.0	2248.4
SP68	3797.9	2871.7
SP69	0.0	15792.0
SP70	0.0	2188.2
SP71	789.3	29874.1
SP72	0.0	26102.4
SP73	0.0	2659.6
SP74	0.0	5031.6
SP75	0.0	5951.7

PNEdf values were observed at higher values in Çorlu and Çerkezköy regions where industrial wastewater load is high. For instance, $PNEdf_{(Microtox)}$ for SP55 and $PNEdf_{(algae)}$ for SP48 were calculated as highest among the river. According to these values, SP55 and SP48 should be diluted approximately fifty thousand times and three hundred seventy-five thousand times before discharged to any aquatic environment.

The PNEdf values for algae ranged from 617 to 377,397 and PNEdf values for Microtox from 0 to 48,077. According to PNEdf calculations, although the luminescent bacteria are more sensitive than algae, the environmental risk of water samples was observed higher for algae than for the bacteria. As seen in Figures 4.17. and 4.18., algae seem to be more sensitive to micropollutants than luminescent bacteria. At 25 of the water samples, environmental risk for luminescent bacteria was not observed, but was observed for algae. This is because the PNEdf values calculated for algae are not reliable, since these calculations were based on only the chemicals detected in the samples. On the other hand, PNEdf (microtox) values were calculated directly from the toxicity tests carried out through this study therefore they are reliable for demonstrating the environmental risks of water samples.

Among the water samples, SP55 has the most detrimental effect for luminescent bacteria and highest toxicity. SP55 is near to organized industrial area and dominated by textile, paint, plastic and metal industries’ chemicals. Similarly, high environmental risks were observed in Çorlu and Çerkezköy sub-regions where industrial activities were concentrated.

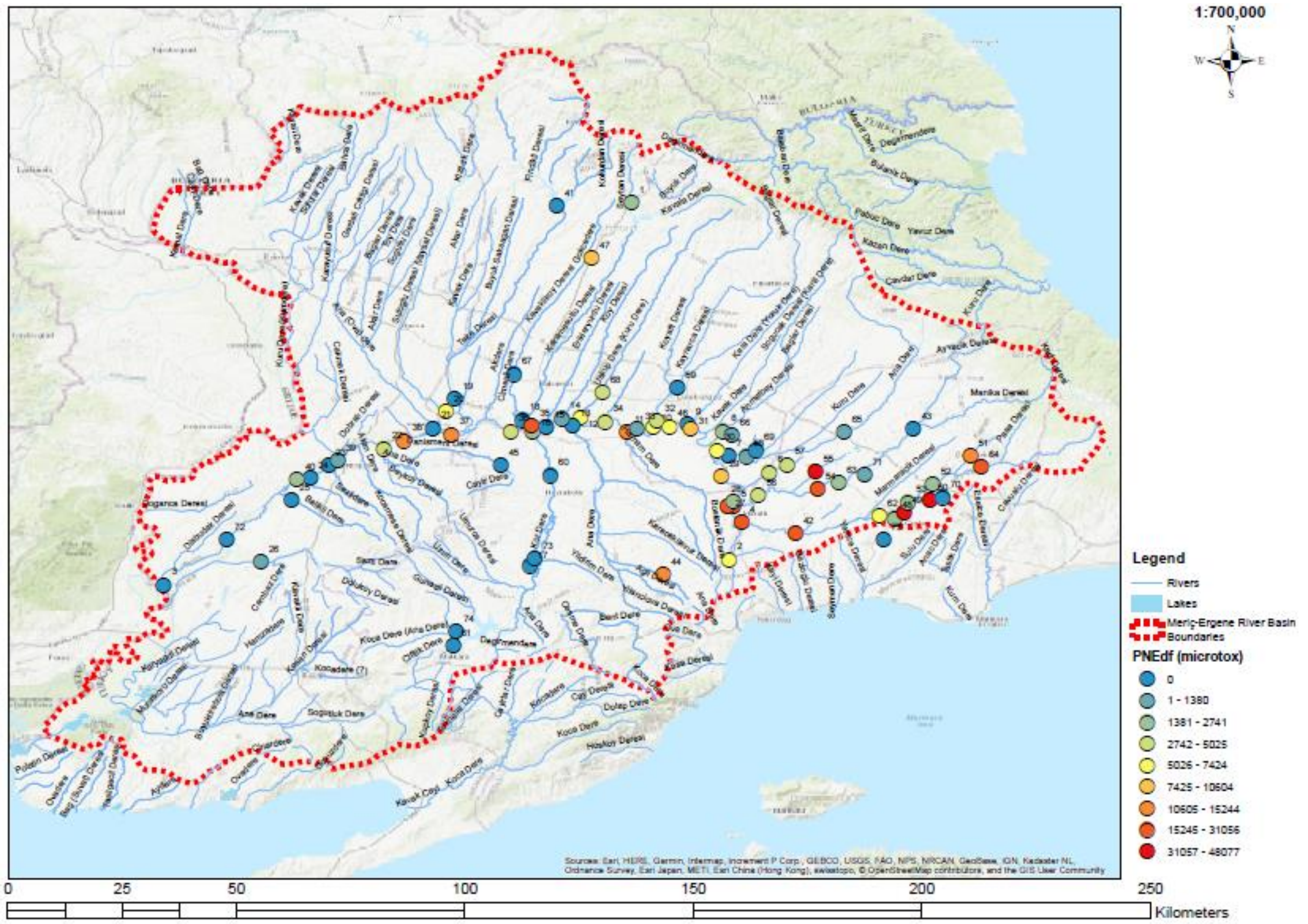

Figure 4.17. Environmental risk maps based on PNEdf (microtox).

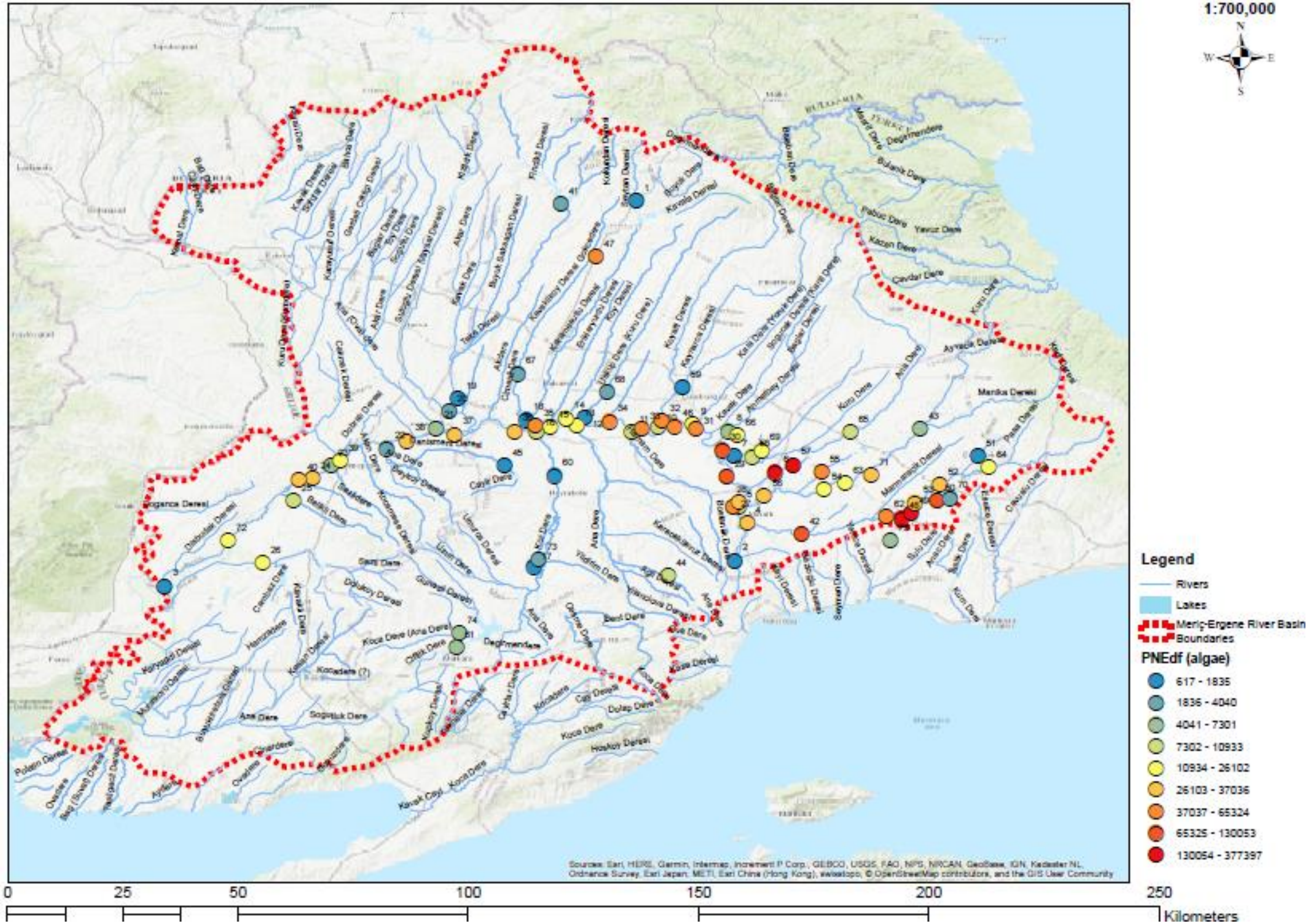

Figure 4.18. Environmental risk maps based on PNEdf (algae).

5. CONCLUSIONS AND RECOMMENDATIONS

For the past twenty years, Ergene River was highly polluted by both point sources like domestic and industrial discharges of many organized industrial sites and residential areas and non-point sources such as runoffs from agricultural areas. Unfortunately, pollution in Ergene River is easily visible and the region faces a very serious problem for many years.

In this study, 131 of 222 selected micropollutants were observed in at least one water sample. Priority pollutants, personal care products, antibiotics, brominated flame retardants, nonylphenols, disinfectants, pesticides, UV blockers, plasticizers, fragrances and even cyanotoxins were among these chemicals.

Benzyldimethyldodecylammonium, benzyldimethyltetradecylammonium, N,N-diethyl-m-toluamide, ofloxacin and PCB-169 were detected in every sampling point and, hexa(methoxymethyl)melamine, anthracene, damascone, alpha-terpineol, ofloxacin, PCB-169, benzothiazole, tris(2-butoxyethyl) phosphate, homosalate and 1,2,3-benzotriazole were observed at the highest concentrations.

Heavy metal pollution due to industrial discharges has been observed in large scale along the Ergene River. Most of metals have been monitored above the EQSs at many sampling points. The highest metal concentrations along the river were observed in sampling points near to discharges of metal factories, organized industrial sites. SP06, SP29, SP44, SP57, SP50, SP09 were the points with high metal concentration while most heavy metals (17 of 18) were observed in SP52.

When the quality and toxicity of Ergene River and its branches were examined, the highest toxicity values were observed in sampling points on Çorlu and Ergene Creeks which are under pressure of textile and leather organized industrial areas and domestic discharges. Leather industry wastewaters contains many organic and inorganic pollutants depending on the processes used. For this reason, leather industry is one of the most important industries that cause pollution of water resources and toxicity for many organisms (Júnior et al., 2007).

Organized industrial zones are mostly located around Çorlu and Çerkezköy districts in the Ergene region. In general, industries that have high wastewater volumes such as textile, chemical, paint, food, leather and metal sectors are dominant in the area and they discharge their wastewater with or without treatment into the Ergene River or its tributaries. Industrial wastewater discharges are major pollution sources on the Ergene River.

For better understanding of pollutant distribution over the Ergene River, a pollutant cluster analysis for sampling points was carried out and a pollution tree was constructed and their closeness to each other was determined. In this context, sample points were clustered into seven groups according to the chemicals they contain.

Regression of each micropollutant with toxicity was investigated and the results showed that benzyldimethyltetradecylammonium, benzylamine, nonylphenol diethoxylate, benzyldimethyldodecylammonium, PCB-169, dicyclohexylamine, celestolide (ADBI) and 3-chloroaniline were most probably related to toxicity. However, the correlation between toxicity and chemical substances was relatively low. Regression between actual toxicity and predicted mixture toxicity derived for detected chemicals for each sample points by using CA and IA toxicity prediction methods was also low suggesting that other chemicals that have not been measured in this study may also contribute to toxicity in Ergene River. To prevent this situation, all chemicals present in the water samples should be known however it is not possible for this study since only targeted analysis is performed.

Targeted chemical analysis is inadequate for detection of each chemical substance that exist in the aquatic environment because of the variety of micropollutants in water bodies. Thus, integration of chemical analyses with bioanalytical tools must be used to reveal the existence of undetected substances by targeted analysis and used for improved understanding about the biological effects of these chemical substances in the water samples.

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APPENDIX A: PHYSICOCHEMICAL PROPERTIES AND MRM TRANSITIONS OF SELECTED CHEMICALS

Table A.1. Properties of selected chemicals.

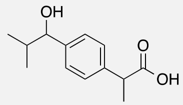
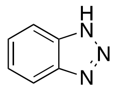
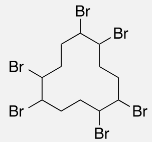
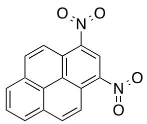
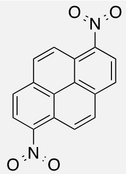
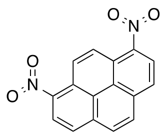
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
1-Hydroxyibuprofen	53949-53-4	$C_{13}H_{18}O_3$		3192	2.25	ECOSAR (estimated)
1,2,3-Benzotriazole	95-14-7	$C_6H_5N_3$		19800	1.44	Hansch et al., 1995
1,2,5,6,9,10-Hexabromocyclododecane	3194-55-6	$C_{12}H_{18}Br_6$		0.0086	7.74	ECOSAR (estimated)
1,3-Dinitropyrene	75321-20-9	$C_{16}H_8N_2O_4$		0.0541	4.57	ECOSAR (estimated)
1,6-Dinitropyrene	42397-64-8	$C_{16}H_8N_2O_4$		0.0540	4.57	ECOSAR (estimated)
1,8-Dinitropyrene	42397-65-9	$C_{16}H_8N_2O_4$		0.0540	4.57	ECOSAR (estimated)

Table A.2. Properties of selected chemicals (continued).

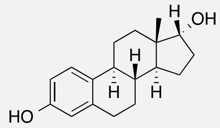
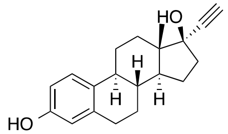
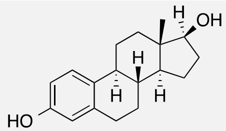
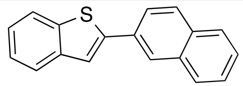
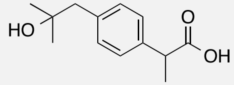
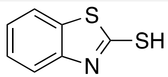
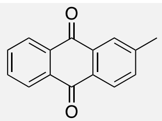
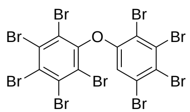
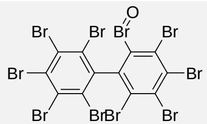
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
17-alpha-Estradiol	57-91-0	$C_{18}H_{24}O_2$		3.90	3.94	ECOSAR (estimated)
17-alpha-Ethinylestradiol	57-63-6	$C_{20}H_{24}O_2$		11.30	3.67	Hansch et al., 1995
17-beta-Estradiol	50-28-2	$C_{18}H_{24}O_2$		3.90	4.01	Hansch et al., 1995
2-(2-Naphthalenyl) benzothiophene	17164-77-1	$C_{18}H_{12}S$		0.014	5.93	ECOSAR (estimated)
2-Hydroxyibuprofen	51146-55-5	$C_{13}H_{18}O_3$		2974	2.29	ECOSAR (estimated)
2-Mercapto-benzothiazole	149-30-4	$C_7H_5NS_2$		120	2.42	Toxic Substances Control Act Test Submissions (TSCATS)
2-Methylanthraquinone	84-54-8	$C_{15}H_{10}O_2$		1.61	3.89	ECOSAR (estimated)
2,2',3,3',4,4',5,5',6-Nonabromodiphenyl ether	63936-56-1	$C_{12}HBr_9O$		5.63×10^{-10}	11.22	ECOSAR (estimated)
2,2',3,3',4,4',5,5',6,6'-Decabromodiphenyl ether	1163-19-5	$C_{12}Br_{10}O$		0.0001	12.11	ECOSAR (estimated)

Table A.3. Properties of selected chemicals (continued).

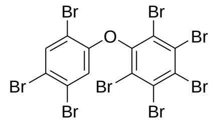
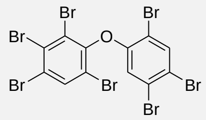
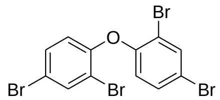
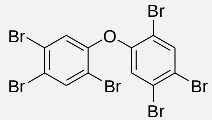
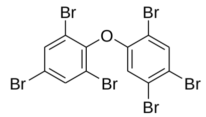
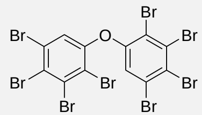
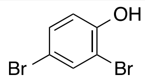
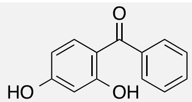
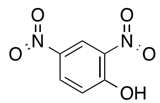
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
2,2',3,4,4',5,5',6- Octabromodiphenyl ether	337513-72-1	$C_{12}H_2Br_8O$		0.01	8.71	Geyer et al., 2000
2,2',3,4,4',5',6- Heptabromodiphenyl ether	207122-16-5	$C_{12}H_3Br_7O$		2.16×10^{-7}	9.44	ECOSAR (estimated)
2,2',4,4'-Tetrabromodiphenyl ether	5436-43-1	$C_{12}H_6Br_4O$		-	6.77	ECOSAR (estimated)
2,2',4,4',5,5'-Hexabromodiphenyl ether	68631-49-2	$C_{12}H_4Br_6O$		-	8.55	ECOSAR (estimated)
2,2',4,4',5,6'-Hexabromodiphenyl ether	207122-15-4	$C_{12}H_4Br_6O$		4.15×10^{-6}	8.55	ECOSAR (estimated)
2,3,3',4,4',5,5',6-Octabromodiphenyl ether	446255-56-7	$C_{12}H_2Br_8O$		-	10.33	ECOSAR (estimated)
2,4-Dibromophenol	615-58-7	$C_6H_4Br_2O$		1900	3.36	Sotomatsu et al., 1993
2,4-Dihydroxybenzophenone	131-56-6	$C_{13}H_{10}O_3$		235.64	2.96	ECOSAR (estimated)
2,4-Dinitrophenol	51-28-5	$C_6H_4N_2O_5$		2790	1.67	Hansch et al., 1995

Table A.4. Properties of selected chemicals (continued).

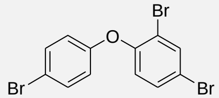
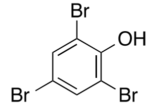
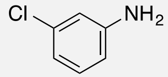
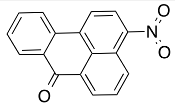
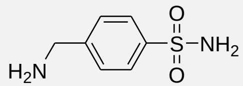
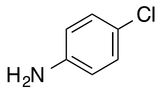
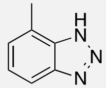
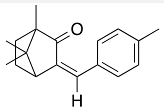
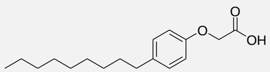
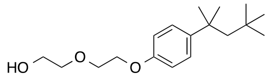
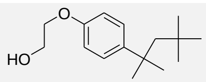
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
2,4,4'-Tribromodiphenylether	41318-75-6	$C_{12}H_7Br_3O$		0.03	5.88	ECOSAR (estimated)
2,4,6-Tribromophenol	118-79-6	$C_6H_3Br_3O$		70	4.13	Hansch et al., 1995
3-Chloroaniline	108-42-9	C_6H_6ClN		5400	1.88	Hansch et al., 1995
3-Nitrobenzanthrone	17117-34-9	$C_{17}H_9NO_3$		0.07	4.54	ECOSAR (estimated)
4-Aminomethyl-benzenesulfonamide	138-37-4	$C_7H_{10}N_2O_2S$		402910	-2.49	ECOSAR (estimated)
4-Chloroaniline	106-47-8	C_6H_6ClN		3900	1.83	Hansch et al., 1995
4-Methyl-1H-benzotriazole	29878-31-7	$C_7H_4D_3N_3$		1924.9	1.71	ECOSAR (estimated)
4-Methylbenzylidenecamphor	36861-47-9	$C_{18}H_{22}O$		0.20	5.92	ECOSAR (estimated)
4-Nonylphenoxy acetic acid	3115-49-9	$C_{17}H_{26}O_3$		2.19	5.80	ECOSAR (estimated)
4-tert-Octylphenol diethoxylate	2315-61-9	$C_{18}H_{30}O_3$		5.16	4.59	ECOSAR (estimated)
4-tert-Octylphenol monoethoxylate	2315-67-5	$C_{16}H_{26}O_2$		4.30	4.97	ECOSAR (estimated)

Table A.5. Properties of selected chemicals (continued).

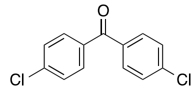
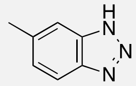
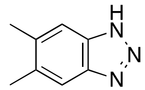
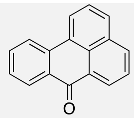
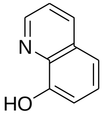
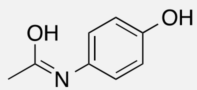
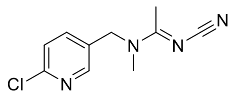
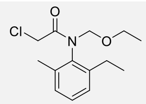
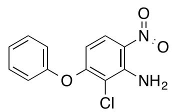
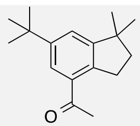
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
4,4'-Dichlorobenzophenone	90-98-2	$C_{13}H_8Cl_2O$		0.83	4.44	ECOSAR (estimated)
5-Methyl-1H-benzotriazole (5-Tolytriazole)	136-85-6	$C_7H_7N_3$		3069	1.71	ECOSAR (estimated)
5,6-Dimethyl-1H-benzotriazole	4184-79-6	$C_8H_9N_3$		914.20	2.26	ECOSAR (estimated)
7H-Benzo(de)anthracen-7-one (Benzanthrone)	82-05-3	$C_{17}H_{10}$		0.24	4.81	Chemicals Inspection and Testing Institute, 1992
8-hydroxyquinoline	148-24-3	C_9H_7NO		417	2.02	Hansch et al., 1995
Acetaminophen (Paracetamol)	103-90-2	$C_8H_9NO_2$		14000	0.46	Sangster, 1994
Acetamiprid	135410-20-7	$C_{10}H_{11}ClN_4$		4200	0.80	Tomlin, 1997
Acetochlor	34256-82-1	$C_{14}H_{20}ClNO_2$		223	3.03	Tomlin, 1994
Aclonifen	74070-46-5	$C_{12}H_9ClN_2O_3$		2.5	4.04	Nandihalli et al., 1993
ADBI (Celestolide)	13171-00-1	$C_{17}H_{24}O$		0.22	5.93	ECOSAR (estimated)

Table A.6. Properties of selected chemicals (continued).

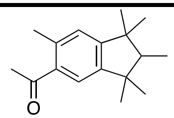
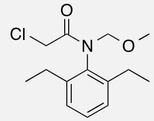
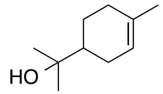
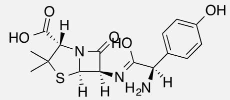
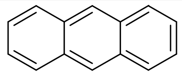
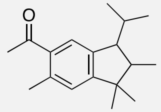
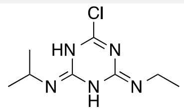
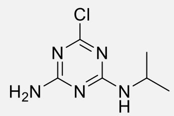
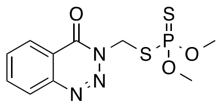
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
AHDI (Phantolide)	15323-35-0	$C_{17}H_{24}O$		0.25	5.85	ECOSAR (estimated)
Alachlor	15972-60-8	$C_{14}H_{20}ClNO_2$		240	3.52	Hansch et al., 1995
alpha-Terpineol	98-55-5	$C_{10}H_{18}O$		7100	2.98	Li and Perdue, 1995
Amoxicillin	26787-78-0	$C_{16}H_{19}N_3O_5S$		3430	0.87	Sangster, 1994
Anthracene	120-12-7	$C_{14}H_{10}$		0.04	4.45	Hansch et al., 1995
ATII (Traseolide)	68140-48-7	$C_{18}H_{26}O$		0.09	6.31	ECOSAR (estimated)
Atrazine	1912-24-9	$C_8H_{14}ClN_5$		34.70	2.61	Hansch et al., 1995
Atrazine-desethyl	6190-65-4	$C_6H_{10}ClN_5$		3200	1.51	Finizio et al., 1991
Azinphos-methyl	86-50-0	$C_{10}H_{12}N_3O_3PS_2$		20.90	2.75	Hansch et al., 1995

Table A.7. Properties of selected chemicals (continued).

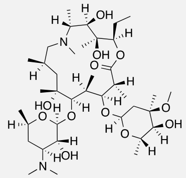
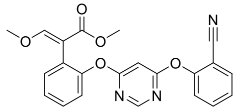
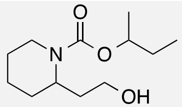
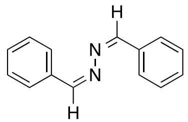
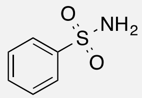
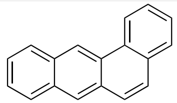
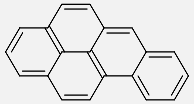
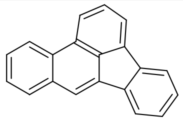
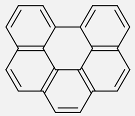
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Azithromycin	83905-01-5	$C_{38}H_{72}N_2O_{12}$		7.09	4.02	Mcfarland et al., 1997
Azoxystrobin	131860-33-8	$C_{22}H_{17}N_3O_5$		6.00	2.50	Tomlin, 1997
Bayrepel	658051-75-3	$C_{12}H_{23}NO_3$		8200	1.56	ECOSAR (estimated)
Banzaldehyde, (phenylmethylene)hydrazone	588-68-1	$C_{14}H_{12}N_2$		5.95	4.48	ECOSAR (estimated)
Benzenesulfonamide	98-10-2	$C_6H_7NO_2S$		4300	0.31	Hansch et al., 1995
Benzo(a)anthracene	56-55-3	$C_{18}H_{12}$		0.01	5.76	Wang et al., 1986
Benzo(a)pyrene	50-32-8	$C_{20}H_{12}$		0.001	6.13	De Maagd et al., 1998
Benzo(b)fluoranthene	205-99-2	$C_{20}H_{12}$		0.002	5.78	Wang et al., 1986
Benzo(ghi)perylene	191-24-2	$C_{22}H_{12}$		2.6×10^{-4}	6.63	Hansch et al., 1995

Table A.8. Properties of selected chemicals (continued).

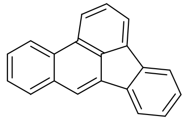
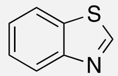
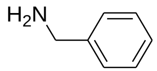
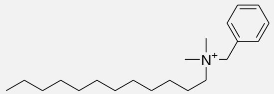
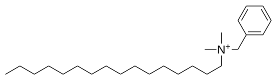
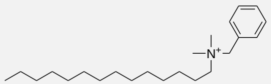
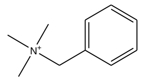
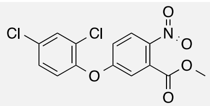
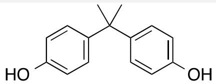
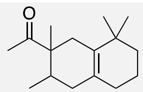
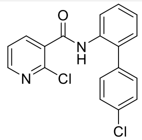
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Benzo(k)fluoranthene	207-08-9	$C_{20}H_{12}$		8.0×10^{-4}	6.11	De Maagd et al., 1998
Benzothiazole	95-16-9	C_7H_5NS		4300	2.01	Hansch et al., 1995
Benzylamine	100-46-9	C_7H_9N		1.0×10^{6}	1.09	Hansch et al., 1995
Benzyldimethyldodecylammonium	139-07-1	$C_{21}H_{38}ClN$		2.25	2.93	ECOSAR (estimated)
Benzyldimethylhexadecylammonium	122-18-9	$C_{25}H_{46}N$		1.09	4.89	ECOSAR (estimated)
Benzyldimethyltetradecylammonium	5285-67-6	$C_{23}H_{42}N$		1000	3.91	ECOSAR (estimated)
Benzyltrimethylammonium	14800-24-9	$C_{10}H_{16}N^{+}$		1000000	-0.47	ECOSAR (estimated)
Bifenox	42576-02-3	$C_{14}H_9Cl_2NO_5$		0.40	4.48	Hansch et al., 1995
Bisphenol-A	80-05-7	$C_{15}H_{16}O_2$		120	3.32	Hansch et al., 1995
Boisvelone / Iso-Esuper	54464-57-2	$C_{16}H_{26}O$		1.08	5.18	ECOSAR (estimated)
Boscalid	188425-85-6	$C_{18}H_{12}Cl_2N_2O$		4.6	2.96	Tomlin, 2003

Table A.9. Properties of selected chemicals (continued).

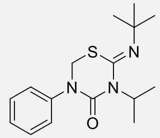
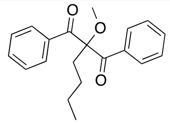
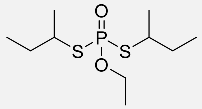
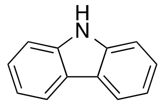
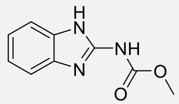
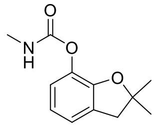
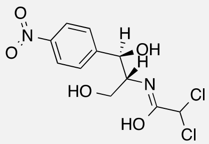
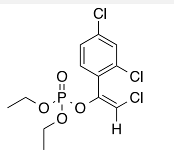
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Buprofezin	69327-76-0	$C_{16}H_{23}N_3OS$		0.9	4.30	Tomlin, 2003
Butylmethoxydibenzoylmethane	70356-09-1	$C_{20}H_{22}O_3$		2.20	4.51	ECOSAR (estimated)
Cadusafos	95465-99-9	$C_{10}H_{23}O_2PS_2$		248	3.90	Tomlin, 1997
Carbazole	86-74-8	$C_{12}H_9N$		1.8	3.72	Hansch et al., 1995
Carbendazim	10605-21-7	$C_9H_9N_3O_2$		29	1.52	Hansch et al., 1995
Carbofuran	1563-66-2	$C_{12}H_{15}NO_3$		320	2.32	Hansch et al., 1995
Chloramphenicol	56-75-7	$C_{11}H_{12}Cl_2N_2O_5$		2500	1.14	Hansch et al., 1995
Chlorfenvinphos	470-90-6	$C_{12}H_{14}Cl_3O_4P$		124	3.81	Sangster, 1994

Table A.10. Properties of selected chemicals (continued).

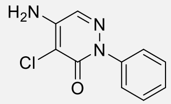
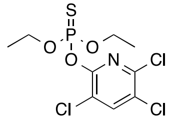
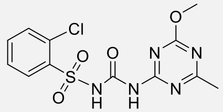
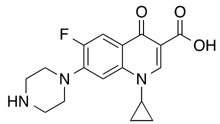
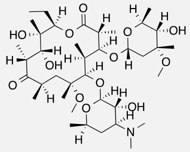
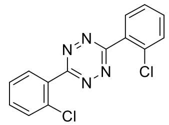
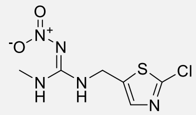
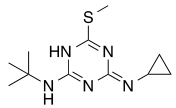
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Chloridazon	1698-60-8	$C_{10}H_8ClN_3O$		400	1.14	Braumann and Grimme, 1981
Chlorpyrifos	2921-88-2	$C_9H_{11}Cl_3NO_3PS$		1.12	4.96	Sangster, 1994
Chlorsulfuron	64902-72-3	$C_{12}H_{12}ClN_5O_4S$		31000	2.00	Ribo, 1988
Ciprofloxacin	85721-33-1	$C_{17}H_{18}FN_3O_3$		30000	0.28	Takacs-Novak et al., 1992
Clarithromycin	81103-11-9	$C_{38}H_{69}NO_{13}$		0.34	3.16	Mcfarland et al., 1997
Clofentezine	74115-24-5	$C_{14}H_8Cl_2N_4$		1.0	3.10	Tomlin, 1994
Clothianidin	210880-92-5	$C_6H_8ClN_5O_2S$		327	0.70	Tomlin, 2003
Cybutryne	28159-98-0	$C_{11}H_{19}N_5S$		7.52	4.07	ECOSAR (estimated)

Table A.11. Properties of selected chemicals (continued).

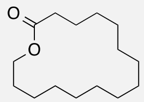
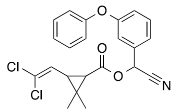
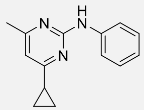
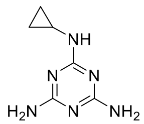
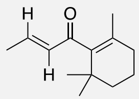
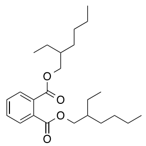
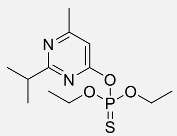
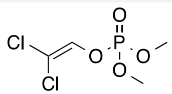
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Cyclopentadecanolide	106-02-5	$C_{15}H_{28}O_2$		0.22	6.15	ECOSAR (estimated)
Cypermethrin	52315-07-8	$C_{22}H_{19}Cl_2NO_3$		0.004	6.60	Macbean, 2010
Cyprodinil	121552-61-2	$C_{14}H_{15}N_3$		13.00	4.00	Tomlin, 1997
Cyromazine	66215-27-8	$C_6H_{10}N_6$		13000	-0.06	Tomlin, 2003
Damascone	23726-91-2	$C_{13}H_{20}O$		7.99	4.42	Meylan and Howard, 1995
Di(2- ethylhexyl)phthalate (DEHP)	117-81-7	$C_{24}H_{38}O_4$		0.27	7.60	Debruijn, 1989
Diazinon	333-41-5	$C_{12}H_{21}N_2O_3PS$		40.0	3.81	Hansch et al., 1995
Dichlorvos	62-73-7	$C_4H_7Cl_2O_4P$		8000	1.43	Hansch et al., 1995

Table A.12. Properties of selected chemicals (continued).

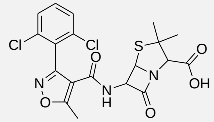
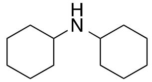
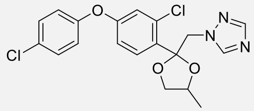
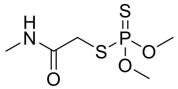
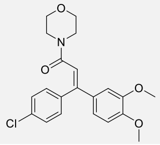
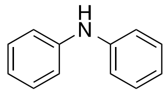
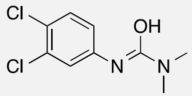
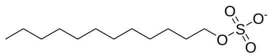
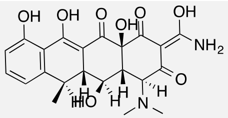
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Dicloxacillin	13412-64-1	$C_{19}H_{17}Cl_2N_3O_5S$		3.63	3.86	Meylan and Howard, 1995
Dicyclohexylamine	101-83-7	$C_{12}H_{23}N$		106.7	4.37	Meylan and Howard, 1995
Difenoconazole	119446-68-3	$C_{19}H_{17}Cl_2N_3O_3$		15.0	4.30	Biobyte, 1995
Dimethoate	60-51-5	$C_5H_{12}NO_3PS_2$		23300	0.78	Hansch et al., 1995
Dimethomorph	110488-70-5	$C_{21}H_{22}ClNO_4$		18.7	2.68	Tomlin, 1994
Diphenylamine	122-39-4	$C_{12}H_{11}N$		53.00	3.50	Hansch et al., 1995
Diuron	330-54-1	$C_9H_{10}Cl_2N_2O$		42.00	2.68	Hansch et al., 1995
Dodecyl Sulfate	151-21-3	$C_{12}H_{25}NaO_4S$		1.0×10^5	1.60	Hansch et al., 1995
Doxycycline	564-25-0	$C_{22}H_{24}N_2O_8$		630	-0.02	Sangster, 1994

Table A.13. Properties of selected chemicals (continued).

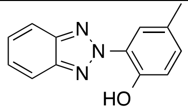
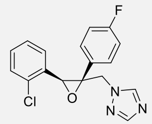
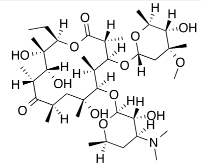
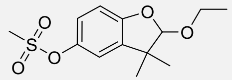
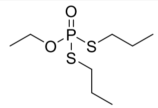
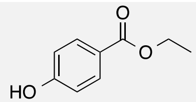
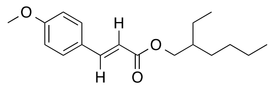
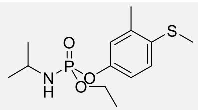
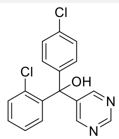
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Drometrizole	2440-22-4	$C_{13}H_{11}N_3O$		25.59	4.31	Hansch et al., 1995
Epoxiconazole	106325-08-0	$C_{17}H_{13}ClFN_3O$		6.63	3.44	Tomlin, 1994
Erythromycin	114-07-8	$C_{37}H_{67}NO_{13}$		1.44	3.06	Mcfarland, 1997
Ethofumesate	26225-79-6	$C_{13}H_{18}O_5S$		50	2.70	Tomlin, 2003
Ethoprophos	13194-48-4	$C_8H_{19}O_2PS_2$		750	3.59	Tomlin, 1994
Ethyl paraben	120-47-8	$C_9H_{10}O_3$		885	2.47	Hansch et al., 1995
Ethylhexylmethoxycinnamate	5466-77-3	$C_{18}H_{26}O_3$		0.15	5.80	Meylan and Howard, 1995
Fenamiphos	22224-92-6	$C_{13}H_{22}NO_3PS$		329	3.23	Hansch et al., 1995
Fenarimol	60168-88-9	$C_{17}H_{12}Cl_2N_2O$		14	3.60	Hansch et al., 1995

Table A.14. Properties of selected chemicals (continued).

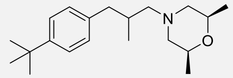
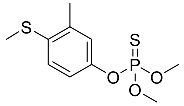
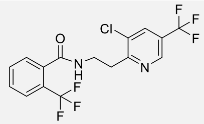
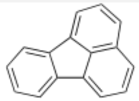
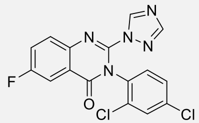
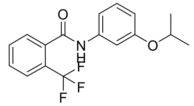
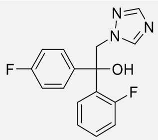
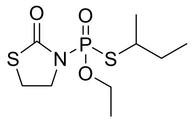
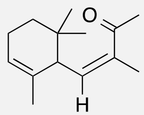
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Fenpropimorph	67306-03-0	$C_{20}H_{33}NO$		1000	5.50	Meylan and Howard, 1995
Fenthion	55-38-9	$C_{10}H_{15}O_3PS_2$		7.5	4.09	Hansch et al., 1995
Fluopyram	658066-35-4	$C_{16}H_{11}ClF_6N_2O$		0.61	4.78	ECOSAR (estimated)
Fluoranthene	206-44-0	$C_{16}H_{10}$		0.26	5.16	Hansch et al., 1995
Fluquinconazole	136426-54-5	$C_{16}H_8Cl_2FN_5O$		1.00	3.24	Tomlin, 1997
Flutolanil	66332-96-5	$C_{17}H_{16}F_3NO_2$		6.53	3.70	Biobyte, 1995
Flutriafol	76674-21-0	$C_{16}H_{13}F_2N_3O$		130	2.29	Patil et al., 1988
Fosthiazate	98886-44-3	$C_9H_{18}NO_3PS_2$		9850	1.68	Tomlin, 1997
g-Methylionone	127-51-5	$C_{14}H_{22}O$		2.98	4.84	ECOSAR (estimated)

Table A.15. Properties of selected chemicals (continued).

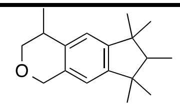
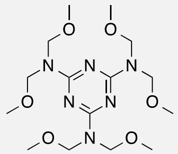
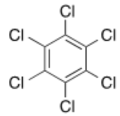
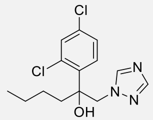
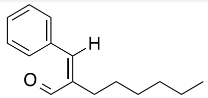
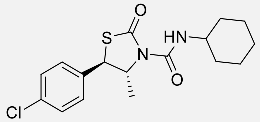
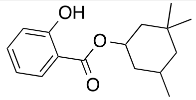
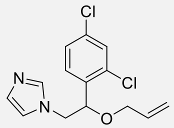
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Galaxolide	1222-05-5	$C_{18}H_{26}O$		1.75	5.90	US EPA, 2004
Hexa(methoxymethyl)melamine	68002-20-0	$C_{15}H_{30}N_6O_6$		149.30	3.07	ACD/Labs (predicted)
Hexachlorobenzene	118-74-1	C_6Cl_6		6.2×10^{-3}	5.73	Debruijn et al., 1989
Hexaconazole	79983-71-4	$C_{14}H_{17}Cl_2N_3O$		17	3.90	Tomlin, 1997
Hexylcinnamaldehyde	101-86-0	$C_{15}H_{20}O$		2.75	4.82	Meylan and Howard, 1995
Hexythiazox	78587-05-0	$C_{17}H_{21}ClN_2O_2S$		0.5	5.57	Meylan and Howard, 1995
Homosalate	118-56-9	$C_{16}H_{22}O_3$		0.42	6.16	Meylan and Howard, 1995
Imazalil	35554-44-0	$C_{14}H_{14}Cl_2N_2O$		180	3.82	Tomlin, 2003

Table A.16. Properties of selected chemicals (continued).

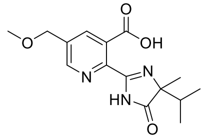
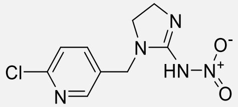
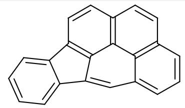
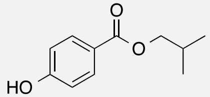
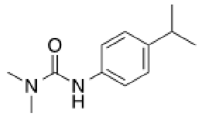
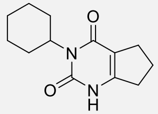
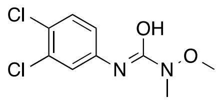
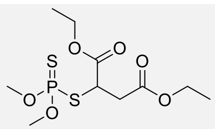
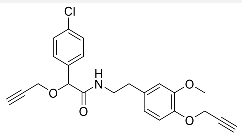
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Imazamox	114311-32-9	$C_{15}H_{19}N_3O_4$		4413	0.73	Tomlin, 1997
Imidacloprid	138261-41-3	$C_9H_{10}ClN_5O_2$		610	0.57	Tomlin, 2003
Indeno(1,2,3-cd)pyrene	193-39-5	$C_{22}H_{12}$		1.9×10^{-4}	6.70	Meylan and Howard, 1995
Isobutyl paraben	4247-02-3	$C_{11}H_{14}O_3$		223.70	3.40	Meylan and Howard, 1995
Isoproturon	34123-59-6	$C_{12}H_{18}N_2O$		65	2.87	Hansch et al., 1995
Lenacil	2164-08-1	$C_{13}H_{18}N_2O_2$		6	2.31	Tomlin, 1997
Linuron	330-55-2	$C_9H_{10}Cl_2N_2O_2$		75	3.20	Hansch et al., 1995
Malathion	121-75-5	$C_{10}H_{19}O_6PS_2$		143	2.36	Hansch et al., 1995
Mandipropamid	374726-62-2	$C_{23}H_{22}ClNO_4$		2.31	3.57	ECOSAR (estimated)

Table A.17. Properties of selected chemicals (continued).

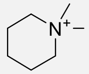
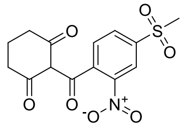
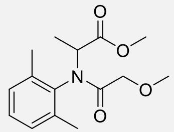
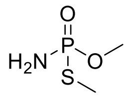
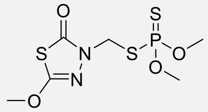
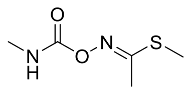
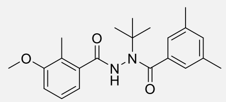
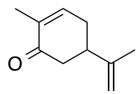
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Mepiquat chloride	24307-26-4	$C_7H_{16}ClN$		5.0×10^5	-2.82	Tomlin, 1997
Mesotrione	104206-82-8	$C_{14}H_{13}NO_7S$		1.5×10^4	1.49	ECOSAR (estimated)
Metalaxyl	57837-19-1	$C_{15}H_{21}NO_4$		8400	1.65	Hansch et al., 1995
Methamidophos	10265-92-6	$C_2H_8NO_2PS$		1.0×10^6	-0.80	Tomlin, 1997
Methidathion	950-37-8	$C_6H_{11}N_2O_4PS_3$		187	2.20	Tomlin, 1997
Methomyl	16752-77-5	$C_5H_{10}N_2O_2S$		5.8×10^4	0.60	Hansch et al., 1995
Methoxyfenozide	161050-58-4	$C_{22}H_{28}N_2O_3$		1.0	3.7	Tomlin, 1997
Methyl -iso-propylcyclohexenone	6485-40-1	$C_{10}H_{14}O$		1310	2.71	Griffin et al., 1999

Table A.18. Properties of selected chemicals (continued).

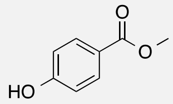
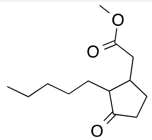
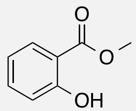
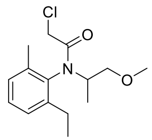
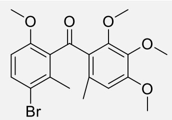
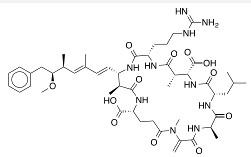
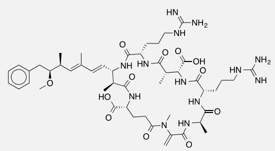
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Methyl Paraben	99-76-3	$C_8H_8O_3$		2500	1.96	Hansch et al., 1995
Methyldihydrojasmonate	24851-98-7	$C_{13}H_{22}O_3$		280	3.00	ECOSAR (estimated)
Methylsalicylate	119-36-8	$C_8H_8O_3$		700	2.55	Sangster, 1994
Metolachlor	51218-45-2	$C_{15}H_{22}ClNO_2$		530	3.13	Hansch et al., 1995
Metrafenone	220899-03-6	$C_{19}H_{21}BrO_5$		0.23	4.72	ECOSAR (estimated)
Microcystin-LR	101043-37-2	$C_{49}H_{74}N_{10}O_{12}$		-	-1.40	ACD/Labs (predicted)
Microcystin-RR	111755-37-4	$C_{49}H_{75}N_{13}O_{12}$		-	-3.96	ACD/Labs (predicted)

Table A.19. Properties of selected chemicals (continued).

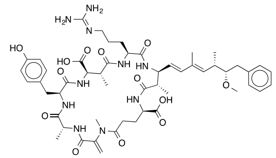
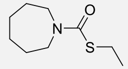
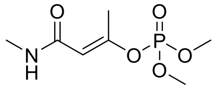
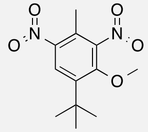
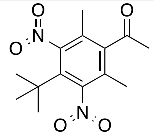
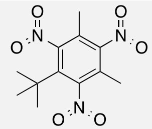
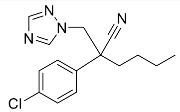
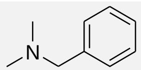
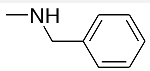
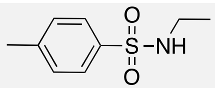
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Microcystin-YR	101064-48-6	$C_{52}H_{72}N_{10}O_{13}$		-	-1.85	ACD/Labs (predicted)
Molinate	2212-67-1	$C_9H_{17}NOS$		970	3.21	Hansch et al., 1995
Monocrotophos	6923-22-4	$C_7H_{14}NO_5P$		1.0×10^6	-0.20	Hansch et al., 1995
Musk ambrette	83-66-9	$C_{12}H_{16}N_2O_5$		1.67	4.17	Meylan and Howard, 1995
Musk ketone	81-14-1	$C_{14}H_{18}N_2O_5$		0.46	4.30	Tas et al., 1997
Musk xylene	81-15-2	$C_{12}H_{15}N_3O_6$		0.47	4.45	Meylan and Howard, 1995
Myclobutanil	88671-89-0	$C_{15}H_{17}ClN_4$		142	2.94	Biobyte, 1995
N-Benzyldimethylamine	103-83-3	$C_9H_{13}N$		1.2×10^4	1.98	Hansch et al., 1995
N-Benzylmethylamine	103-67-3	$C_8H_{11}N$		1.0×10^6	1.52	Hansch et al., 1995
N-Ethyl-2-tolysulfonamide	80-39-7	$C_9H_{13}NO_2S$		1106	1.87	ECOSAR (estimated)

Table A.20. Properties of selected chemicals (continued).

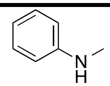
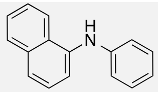
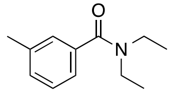
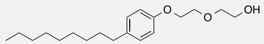
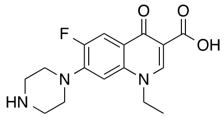
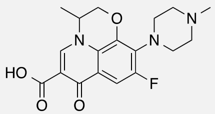
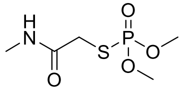
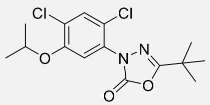
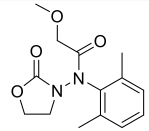
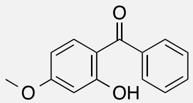
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
N-methyl aniline	100-61-8	C_7H_9N		5620	1.66	Hansch et al., 1995
N-phenyl-napthylamine	90-30-2	$C_{16}H_{13}N$		60	4.20	Hansch et al., 1995
N,N-Diethyl-m-toluamide	134-62-3	$C_{12}H_{17}NO$		912	2.18	Sangster, 1993
Nonylphenol diethoxylate	20427-84-3	$C_{19}H_{32}O_3$		1.05	5.30	ECOSAR (estimated)
Norfloxacin	70458-96-7	$C_{16}H_{18}FN_3O_3$		1.78×10^5	-1.03	Hansch et al., 1995
Ofloxacin	82419-36-1	$C_{18}H_{20}FN_3O_4$		2.83×10^4	-0.39	Hansch et al., 1995
Omethoate	1113-02-6	$C_5H_{12}NO_4PS$		1.0×10^6	-0.74	Tomlin, 1997
Oxadiazon	19666-30-9	$C_{15}H_{18}Cl_2N_2O_3$		0.70	4.80	Hansch et al., 1995
Oxadixyl	77732-09-3	$C_{14}H_{18}N_2O_4$		3400	0.80	Tomlin, 1997
Oxybenzone	131-57-7	$C_{14}H_{12}O_3$		69	3.79	Chemicals Inspection and Testing Institute, 1992

Table A.21. Properties of selected chemicals (continued).

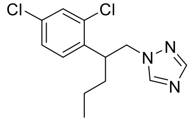
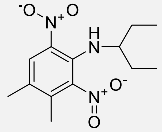
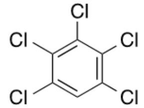
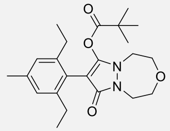
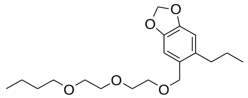
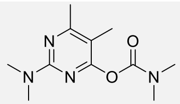
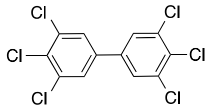
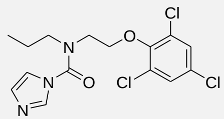
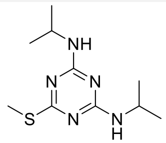
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Penconazole	66246-88-6	$C_{13}H_{15}Cl2N_3$		73	3.72	Tomlin, 1997
Pendimethalin	40487-42-1	$C_{13}H_{19}N_3O_4$		0.33	5.20	Tomlin, 2003
Pentachlorobenzene	608-93-5	C_6HCl_5		0.83	5.17	Hansch et al., 1995
Pinoxaden	243973-20-8	$C_{23}H_{32}N_2O_4$		2.59	3.6	ECOSAR (estimated)
Piperonylbutoxide	51-03-6	$C_{19}H_{30}O_5$		14.3	4.75	Tomlin, 1997
Pirimicarb	23103-98-2	$C_{11}H_{18}N_4O_2$		2700	1.70	Tomlin, 1994
3,3',4,4',5,5'-Hexachlorobiphenyl	1336-36-3	$C_{12}H_4Cl_6$		5.1×10^{-4}	7.41	Hansch et al., 1995
Prochloraz	67747-09-5	$C_{15}H_{16}Cl_3N_3O_2$		34	4.10	Baker et al., 1992
Prometryn	7287-19-6	$C_{10}H_{19}N_5S$		33	3.51	Hansch et al., 1995

Table A.22. Properties of selected chemicals (continued).

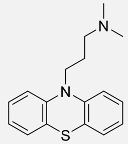
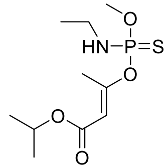
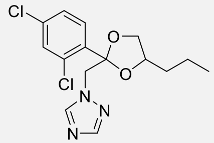
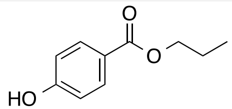
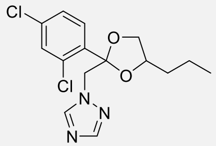
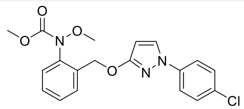
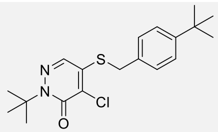
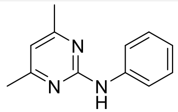
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Propazine	139-40-2	$C_9H_{16}ClN_5$		8.60	2.93	Hansch et al., 1995
Propetamphos	31218-83-4	$C_{10}H_{2}0NO_{4}PS$		110	3.82	Tomlin, 1997
Propiconazole	60207-90-1	$C_{15}H_{17}Cl_2N_3O_2$		110	3.72	Tomlin, 2003
Propyl paraben	94-13-3	$C_{10}H_{12}O_3$		500	3.04	Hansch et al., 1995
Prothioconazole	178928-70-6	$C_{14}H_{15}Cl_2N_3OS$		5.53	3.61	ECOSAR (estimated)
Pyraclostrobin	175013-18-0	$C_{19}H_{18}ClN_3O_4$		1.90	3.99	Tomlin, 2003
Pyridaben	96489-71-3	$C_{19}H_{25}ClN_2OS$		0.01	6.37	Tomlin, 1994
Pyrimethanil	53112-28-0	$C_{12}H_{13}N_3$		121	2.84	Tomlin, 1997

Table A.23. Properties of selected chemicals (continued).

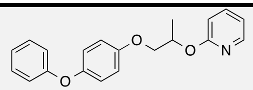
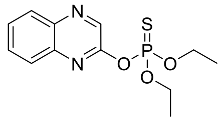
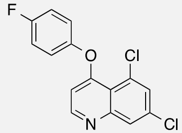
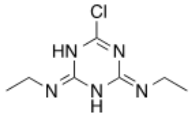
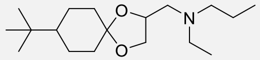
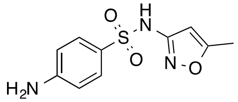
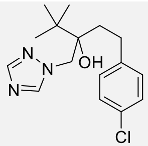
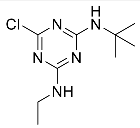
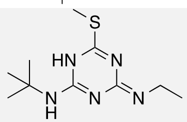
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Pyriproxyfen	95737-68-1	$C_{20}H_{19}NO_3$		0.47	5.55	Meylan and Howard, 1995
Quinalphos	13593-03-8	$C_{12}H_{15}N_2O_3PS$		22	4.44	Biobyte, 1995
Quinoxyfen	124495-18-7	$C_{15}H_8Cl_2FNO$		0.116	4.66	Tomlin, 2003
Simazine	122-34-9	$C_7H_{12}ClN_5$		6.20	2.18	Hansch et al., 1995
Spiroxamine	118134-30-8	$C_{18}H_{35}NO_2$		470	5.51	Meylan and Howard, 1995
Sulfamethoxazole	723-46-6	$C_{10}H_{11}N_3O_3S$		610	0.89	Hansch et al., 1995
Tebuconazole	107534-96-3	$C_{16}H_{22}ClN_3O$		36	3.70	Tomlin, 1997
Terbuthylazine	5915-41-3	$C_9H_{16}ClN_5$		8.5	3.21	Tomlin, 1997
Terbutryn	886-50-0	$C_{10}H_{19}N_5S$		25	3.74	Hansch et al., 1995

Table A.24. Properties of selected chemicals (continued).

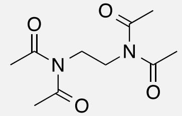
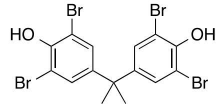
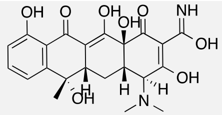
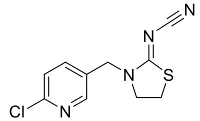
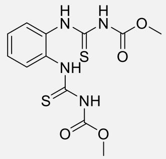
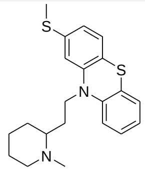
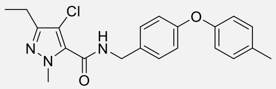
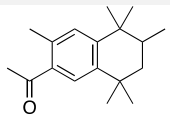
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Tetraacetylethylenediamine	10543-57-4	$C_{10}H_{16}N_2O_4$		200	-2.36	ECOSAR (estimated)
Tetrabromobisphenol A	79-94-7	$C_{15}H_{12}Br_4O_2$		0.24	7.20	Meylan and Howard, 1995
Tetracycline	60-54-8	$C_{22}H_{24}N_2O_8$		231	-1.30	Hansch et al., 1995
Thiacloprid	111988-49-9	$C_{10}H_9ClN_4S$		185	1.26	EPA Factsheet
Thiophanate-methyl	23564-05-8	$C_{12}H_{14}N_4O_4S2$		26.60	1.40	Hansch et al., 1995
Thioridazine	130-61-0	$C_{21}H_{26}N_2S_2$		0.14	4.93	Meylan and Howard, 1995
Tolfenpyrad	129558-76-5	$C_{21}H_{22}ClN_3O_2$		0.36	6.45	ECOSAR (estimated)
Tonalide	1506-02-1	$C_{18}H_{26}O$		1.25	6.35	ECOSAR (estimated)

Table A.25. Properties of selected chemicals (continued).

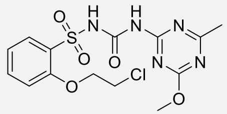
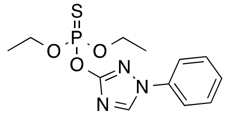
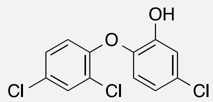
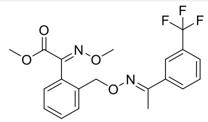
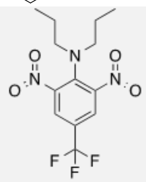
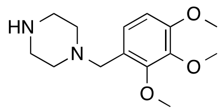
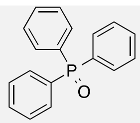
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Triasulfuron	82097-50-5	$C_{14}H_{16}ClN_5O_5S$		32.00	1.10	Tomlin, 1997
Triazophos	24017-47-8	$C_{12}H_{16}N_3O_3PS$		39.00	3.34	Tomlin, 1997
Triclosan	3380-34-5	$C_{12}H_7Cl_3O_2$		6.05	4.76	Chemicals Inspection and Testing Institute, 1992
Trifloxystrobin	141517-21-7	$C_{20}H_{19}F_3N_2O_4$		0.61	4.50	Tomlin, 2003
Trifluralin	1582-09-8	$C_{13}H_{16}F_3N_3O_4$		0.18	5.34	Hansch et al., 1995
Trimethoprim	738-70-5	$C_{14}H_{18}N_4O_3$		400	0.91	Hansch et al., 1995
Triphenylphosphineoxide	791-28-6	$C_{18}H_{15}OP$		62.8	2.83	Hansch et al., 1995

Table A.26. Properties of selected chemicals (continued).

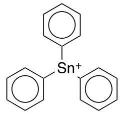
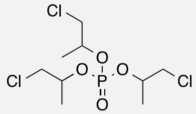
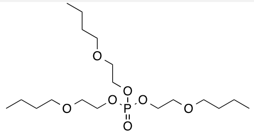
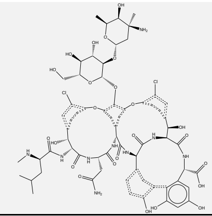
Chemical Name	CAS #	Molecular Formula	Molecular Structure	Solubility (mg/L)	LogP	LogP Reference
Triphenyltin	668-34-8	$C_{18}H_{15}Sn$		56.04	6.58	ECOSAR (estimated)
Tris(1-chloro-2-propanyl) phosphate	13674-84-5	$C_9H_{18}Cl_3O_4P$		1200	2.59	Chemicals Inspection and Testing Institute, 1992
Tris(2-butoxyethyl) phosphate	78-51-3	$C_{18}H_{39}O_7P$		1100	3.75	Chemicals Inspection and Testing Institute, 1992
Vancomycin	1404-93-9	$C_{66}H_{75}Cl_2N_9O_{24}$		50000	-1.44	ACD/Labs (predicted)

Table A.27. LOD and LOQ of each analyte and the goodness of fit of calibration curves.

Compound	LOD (ug/L)	LOQ (ug/L)	r^2
1-Hydroxyibuprofen	7.3887	24.6289	0.989
1,2,3-Benzotriazole	0.0831	0.2769	0.998
1,2,5,6,9,10-Hexabromocyclododecane	0.1374	0.4579	0.998
1,3-Dinitropyrene	0.0866	0.2885	0.997
1,6-Dinitropyrene	0.0296	0.0987	0.997
1,8-Dinitropyrene	0.0789	0.2628	0.995
17-alpha-Estradiol	1.5009	5.0031	0.997
17-alpha-Ethinylestradiol	1.8789	6.2630	0.994
17-beta-Estradiol	0.8303	2.7675	0.998
2-(2-Naphthalenyl) benzothiophene	0.4447	1.4822	0.993
2,2',3,3',4,4',5,5',6,6'-Decabromodiphenyl ether	0.5829	1.9430	0.991
2,2',3,3',4,4',5,5',6-Nonabromodiphenyl ether	0.3983	1.3278	0.999
2,2',3,4,4',5,5',6-Octabromodiphenyl ether	0.1882	0.6273	0.999
2,2',3,4,4',5',6-Heptabromodiphenyl ether	0.1221	0.4071	0.996
2,2',4,4',5,5'-Hexabromodiphenyl ether	0.0418	0.1392	0.998
2,2',4,4',5,6'-Hexabromodiphenyl ether	0.2806	0.9353	0.998
2,2',4,4'-Tetrabromodiphenyl ether	1.0936	3.6455	0.996
2,3,3',4,4',5,5',6-Octabromodiphenyl ether	0.1241	0.4136	0.999
2,4,4'-tribromodiphenylether	1.2483	4.1611	0.998
2,4,6-Tribromophenol	0.1736	0.5785	0.991
2,4-Dibromophenol	0.1393	0.4645	0.991
2,4-Dihydroxybenzophenone	0.0039	0.0129	0.999
2,4-Dinitrophenol	0.6569	2.1897	0.998
2-Hydroxyibuprofen	2.4138	8.0461	0.992
2-Mercapto-benzothiazole	0.0167	0.0556	0.993
2-Methylanthraquinone	0.0184	0.0614	0.999
3-Chloroaniline	0.0229	0.0762	0.998
3-Nitrobenzanthrone	0.3446	1.1488	0.997
4,4'-Dichlorobenzophenone	0.0470	0.1568	0.998
4-Aminomethyl-benzenesulfonamide	0.0186	0.0621	0.999
4-Chloroaniline	0.0152	0.0508	0.997
4-Methyl-1H-benzotriazole	0.0145	0.0482	0.999
4-Methylbenzylidenecamphor	0.0682	0.2275	0.999
4-Nonylphenoxy acetic acid	1.7505	5.8350	0.984
4-tert-Octylphenol diethoxylate	0.0120	0.0400	0.997
4-tert-Octylphenol monoethoxylate	1.3220	4.4067	0.989
5,6-Dimethyl-1H-benzotriazole	0.0055	0.0182	0.997
5-Methyl-1H-benzotriazole (5-Tolytriazole)	0.0224	0.0747	0.997
7H-Benzo(de)anthracen-7-one (Benzanthrone)	0.0377	0.1257	0.996
8-Hydroxyquinoline	0.0130	0.0433	0.999
Acetaminophen (Paracetamol)	0.0455	0.1516	0.998
Acetamiprid	0.0252	0.0841	0.994

Table A.28. LOD and LOQ of each analyte and the goodness of fit of calibration curves (continued).

Compound	LOD (ug/L)	LOQ (ug/L)	r^2
Acetochlor	0.0603	0.2008	0.995
Aclonifen	0.0569	0.1896	0.998
ADBI (Celestolide)	0.0114	0.0380	0.998
AHDI (Phantolide)	0.0668	0.2227	0.999
Alachlor	0.0769	0.2563	0.998
alpha-Terpineol	3.1507	10.5022	0.989
Amoxicillin	0.0991	0.3303	0.999
Anthracene	1.5064	5.0213	0.988
ATII (Traseolide)	0.1368	0.4561	0.997
Atrazine	0.0071	0.0237	0.999
Atrazine-desethyl	0.0201	0.0669	0.996
Azinphos-methyl	1.7247	5.7491	0.992
Azithromycin	0.0106	0.0352	0.997
Azoxystrobin	0.0284	0.0947	0.995
Bayrepel	1.3408	4.4693	0.992
Banzaldehyde, (phenylmethylene)hydrazone	0.0146	0.0488	0.998
Benzenesulfonamide	2.0702	6.9006	0.993
Benzo[a]anthracene	0.0140	0.0467	0.996
Benzo[a]pyrene	0.0041	0.0138	0.995
Benzo[b]fluoranthene	0.2545	0.8482	0.993
Benzo[ghi]perylene	0.0506	0.1685	0.997
Benzo[k]fluoranthene	0.0017	0.0056	0.995
Benzothiazole	4.0245	13.4150	0.987
Benzylamine	0.0201	0.0671	0.999
Benzyldimethyldodecylammonium	0.0059	0.0198	0.999
Benzyldimethylhexadecylammonium	0.0035	0.0116	0.993
Benzyldimethyltetradecylammonium	0.0032	0.0107	0.996
Benzyltrimethylammonium	0.0067	0.0224	1.000
Bifenox	0.0859	0.2863	0.996
Bisphenol-A	1.1017	3.6723	0.995
Boisvelone / Iso-Esuper	1.6544	5.5145	0.972
Boscalid	0.1340	0.4466	0.997
Buprofezin	0.0383	0.1278	0.997
Butylmethoxydibenzoylmethane	0.3144	1.0480	0.991
Cadusafos	0.0597	0.1992	0.997
Carbazole	0.0712	0.2375	0.994
Carbendazim	0.0248	0.0828	0.995
Carbofuran	0.0152	0.0506	0.997
Chloramphenicol	0.0542	0.1805	0.997
Chlorfenvinphos	0.0340	0.1132	0.999
Chloridazon	0.1374	0.4580	0.997
Chlorpyrifos	0.1251	0.4170	0.979

Table A.29. LOD and LOQ of each analyte and the goodness of fit of calibration curves (continued).

Compound	LOD (ug/L)	LOQ (ug/L)	r^2
Chlorsulfuron	0.0439	0.1462	0.995
Ciprofloxacin	0.3077	1.0258	0.995
Clarithromycin	0.0037	0.0124	0.999
Clofentezine	0.0438	0.1461	0.977
Clothianidin	0.1358	0.4528	0.994
Cybutryne	0.0008	0.0027	0.998
Cyclopentadecanolide	0.6776	2.2586	0.996
Cypermethrin	0.7397	2.4658	0.999
Cyprodinil	0.0348	0.1160	0.993
Cyromazine	0.0347	0.1156	0.844
Damascone	0.0811	0.2702	0.999
Di(2- ethylhexyl)phthalate (DEHP)	2.6823	8.9409	0.991
Diazinon	0.0527	0.1757	0.998
Dichlorvos	0.1708	0.5693	0.998
Dicloxacillin	0.0183	0.0609	0.997
Dicyclohexylamine	0.0129	0.0431	0.998
Difenoconazole	0.0338	0.1127	0.993
Dimethoate	0.0691	0.2303	0.991
Dimethomorph	0.0151	0.0503	0.997
Diphenylamine	0.1253	0.4177	0.993
Diuron	0.0218	0.0726	0.999
Dodecyl sulfate	3.4595	11.5317	0.998
Doxycycline	0.0403	0.1344	0.997
Drometrizole	0.0214	0.0713	0.993
Epoxiconazole	0.0314	0.1047	0.990
Erythromycin	0.0214	0.0713	0.993
Ethofumesate	0.1148	0.3828	0.996
Ethoprophos	0.0822	0.2740	0.993
Ethyl paraben	0.1053	0.3511	0.997
Ethylhexylmethoxycinnamate	0.1168	0.3893	0.979
Fenamiphos	0.0489	0.1630	0.991
Fenarimol	0.2104	0.7013	0.993
Fenpropimorph	0.0334	0.1114	0.991
Fenthion	0.3377	1.1256	0.990
Fluopyram	0.0095	0.0316	0.998
Fluoranthene	0.0803	0.2675	0.995
Fluquinconazole	0.0809	0.2698	0.986
Flutolanil	0.0476	0.1588	0.989
Flutriafol	0.0683	0.2275	0.993
Fosthiazate	2.7092	9.0306	0.906
Galaxolide	0.0648	0.2161	0.978
g-Methylionone	0.2221	0.7403	0.989

Table A.30. LOD and LOQ of each analyte and the goodness of fit of calibration curves (continued).

Compound	LOD (ug/L)	LOQ (ug/L)	r^2
Hexa(methoxymethyl)melamine	4.1916	13.9718	0.953
Hexachlorobenzene	1.5802	5.2675	0.992
Hexaconazole	0.0228	0.0760	0.989
Hexylcinnamaldehyde	0.1442	0.4808	0.996
Hexythiazox	0.0314	0.1046	0.998
Homosalate	5.8768	19.5892	0.981
Imazalil	0.0735	0.2451	0.992
Imazamox	0.0401	0.1338	0.996
Imidacloprid	0.6194	2.0647	0.995
Indeno[1,2,3-cd]pyrene	0.2066	0.6887	0.997
Isobutyl paraben	0.0202	0.0673	0.998
Isoproturon	0.0184	0.0612	0.998
Lenacil	0.0849	0.2829	0.991
Linuron	0.0386	0.1287	0.999
Malathion	0.8947	2.9824	0.985
Mandipropamid	0.0248	0.0827	0.995
Mepiquat chloride	0.0732	0.2439	0.997
Mesotrione	0.0355	0.1184	0.990
Metalaxyl	0.0423	0.1410	0.999
Methamidophos	0.2141	0.7135	0.993
Methidathion	0.6959	2.3197	0.985
Methomyl	0.0181	0.0605	0.987
Methoxyfenozide	0.1357	0.4524	0.989
Methyl -iso-propylcyclohexenone	0.0975	0.3252	0.994
Methyl paraben	0.0917	0.3056	0.997
Methyldihydrojasmonate	0.2457	0.8190	0.993
Methylsalicylate	0.1137	0.3789	0.998
Metolachlor	0.0210	0.0700	0.998
Metrafenone	0.0221	0.0735	0.998
Microcystin-LR	1.5059	5.0196	0.984
Microcystin-RR	0.0445	0.1485	0.997
Microcystin-YR	1.7014	5.6714	0.948
Molinate	0.0339	0.1129	0.988
Monocrotophos	0.0174	0.0581	0.998
Musk ambrette	0.1910	0.6366	0.996
Musk ketone	0.3823	1.2743	0.995
Musk xylene	0.0790	0.2632	0.996
Myclobutanil	0.0038	0.0126	0.987
N,N-Diethyl-m-toluamide	0.0042	0.0139	0.993
N-Benzyldimethylamine	0.0102	0.0341	0.999
N-Benzylmethylamine	0.0371	0.1237	0.988
N-Ethyl-2-tolysulfonamide	0.0243	0.0812	0.994

Table A.31. LOD and LOQ of each analyte and the goodness of fit of calibration curves (continued).

Compound	LOD (ug/L)	LOQ (ug/L)	r^2
N-methyl aniline	0.0270	0.0900	0.996
Nonylphenol diethoxylate	0.0175	0.0582	0.993
Norfloxacin	0.4866	1.6220	0.737
N-phenyl-2-napthylamine	0.0051	0.0171	0.995
Ofloxacin	0.0178	0.0593	0.969
Omethoate	0.0870	0.2901	0.994
Oxadiazon	0.3647	1.2157	0.992
Oxadixyl	0.0848	0.2828	0.986
Oxybenzone	0.0059	0.0196	0.997
Penconazole	0.0345	0.1149	0.995
Pendimethalin	0.0186	0.0620	0.996
Pentachlorobenzene	0.1066	0.3554	0.995
Pinoxaden	0.0068	0.0225	0.999
Piperonylbutoxide	0.0042	0.0141	0.997
Pirimicarb	0.1223	0.4075	0.992
Polychlorinated biphenyls	1.6739	5.5798	0.998
Prochloraz	0.0027	0.0082	0.984
Prometryn	0.0095	0.0317	0.997
Propazine	0.0087	0.0291	0.996
Propetamphos	0.1644	0.5479	0.994
Propiconazole	0.0680	0.2266	0.991
Propyl paraben	0.0357	0.1191	0.998
Prothioconazole	0.1367	0.4558	0.999
Pyraclostrobin	0.0163	0.0542	0.999
Pyridaben	0.0124	0.0412	0.997
Pyrimethanil	0.0679	0.2264	0.998
Pyriproxyfen	0.0067	0.0223	0.999
Quinalphos	0.0382	0.1274	0.995
Quinoxyfen	0.0105	0.0348	0.999
Simazine	0.0066	0.0219	0.999
Spiroxamine	0.0182	0.0607	0.993
Sulfamethoxazole	0.0340	0.1133	0.999
Tebuconazole	0.0423	0.1410	0.998
Terbuthylazine	0.0178	0.0595	0.996
Terbutryn	0.0038	0.0127	0.999
Tetraacetylethylenediamine	0.4478	1.4926	0.988
Tetrabromobisphenol A	0.1359	0.4531	0.999
Tetracycline	0.0168	0.0561	0.995
Thiacloprid	0.0868	0.2894	0.998
Thiophanate-methyl	0.0212	0.0706	0.994
Thioridazine	0.0042	0.0141	0.997
Tolfenpyrad	0.0209	0.0698	0.998

Table A.32. LOD and LOQ of each analyte and the goodness of fit of calibration curves (continued).

Compound	LOD (ug/L)	LOQ (ug/L)	r^2
Tonalide	0.0375	0.1251	0.997
Triasulfuron	0.0496	0.1654	0.998
Triazophos	0.0496	0.1652	0.999
Triclosan	0.4543	1.5144	0.992
Trifloxystrobin	0.0155	0.0517	0.999
Trifluralin	0.0219	0.0730	0.994
Trimethoprim	0.0053	0.0177	0.998
Triphenylphosphineoxide	0.1339	0.4464	0.999
Triphenyltin	8.7200	29.0665	0.983
Tris(1-chloro-2-propanyl) phosphate	21.7370	72.4567	0.942
Tris(2-butoxyethyl) phosphate	0.0256	0.0853	0.999
Vancomycin	0.0772	0.2573	0.999

Table A.3. MRM transitions and optimized MS/MS parameters.

Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
1,2,3-Benzotriazole	120.0	65.0 / 92.0	2.87	61	10	29 / 23	8 / 6	ESI (+)
1,3-Dinitropyrene	291.9	262.0 / 232.1	7.11	-40	-10	-24 / -40	-8 / -8	APCI (-)
1,6-Dinitropyrene	291.9	261.7 / 231.6	7.11	-18	-10	-24 / -32	-8 / -8	APCI (-)
1,8-Dinitropyrene	291.9	261.9 / 231.6	7.11	-35	-10	-24 / -36	-8 / -8	APCI (-)
17-alpha-Estradiol	271.0	144.8 / 142.5	5.47	-290	-10	-54 / -80	-11 / -7	ESI (-)
17-alpha-Ethinylestradiol	295.0	144.6 / 142.8	5.44	-180	-10	-54 / -84	-13 / -11	ESI (-)
17-beta-Estradiol	271.2	182.6 / 144.7	5.39	-155	-10	-56 / -58	-11 / -17	ESI (-)
1-Hydroxyibuprofen	220.9	158.7 / 176.4	3.57	-60	-10	-16 / -10	-9 / -5	ESI (-)
2-(2-Naphthalenyl) benzothiophene	261.0	228.1 / 260.0	7.90	66	10	40 / 40	8 / 8	APCI (+)
2,2',3,3',4,4',5,5',6,6'-Decabromodiphenyl ether	894.3	79.0 / 81.1	9.42	-55	-10	-108 / -108	-10 / -10	APCI (-)
2,2',3,3',4,4',5,5',6-Nonabromodiphenyl ether	816.5	79.0 / 80.9	9.29	-30	-10	-105 / -105	-10 / -10	APCI (-)
2,2',3,4,4',5,5',6- Octabromodiphenyl ether	736.5	78.6 / 80.5	9.04	-61	-10	-99 / -99	-10 / -10	APCI (-)
2,2',3,4,4',5',6- Heptabromodiphenyl ether	658.5	79.0 / 80.9	8.78	-55	-10	-100 / -100	-7 / -7	APCI (-)
2,2',4,4',5,5'- Hexabromodiphenyl ether	578.6	78.9 / 81.0	8.68	-60	-10	-110 / -110	-7 / -7	APCI (-)
2,2',4,4',5,6'- Hexabromodiphenyl ether	578.6	79.0 / 80.9	8.68	-50	-10	-85 / -85	-7 / -7	APCI (-)
2,2',4,4'-Tetrabromodiphenyl ether	420.8	78.7 / 80.6	7.98	-45	-10	-50 / -50	-7 / -7	APCI (-)
2,3,3',4,4',5,5',6- Octabromodiphenyl ether	736.6	78.9 / 81.0	9.04	-30	-10	-100 / -100	-10 / -10	APCI (-)
2,4,4'-tribromodiphenylether	343.0	78.8 / 80.5	7.68	-48	-10	-60 / -60	-10 / -10	APCI (-)
2,4,6-Tribromophenol	328.5	78.8 / 80.6	6.11	-45	-10	-64 / -64	-7 / -5	ESI (-)
2,4-Dibromophenol	250.6	80.5 / 78.6	5.05	-60	-10	-50 / -54	-5 / -11	ESI (-)
2,4-Dihydroxybenzophenone	215.0	136.9 / 80.9	4.56	61	10	27 / 51	8 / 6	ESI (+)
2,4-Dinitrophenol	183.0	122.6 / 152.4	3.82	-5	-10	-26 / -24	-3 / -15	ESI (-)
2-Hydroxyibuprofen	221.2	132.6 / 176.6	3.57	-60	-10	-12 / -14	-9 / -9	ESI (-)
2-Mercapto-benzothiazole	167.9	135.0 / 65.0	3.38	71	10	35 / 47	8 / 6	ESI (+)
2-Methylanthraquinone	223.1	152.0 / 165.0	6.29	71	10	41 / 47	6 / 8	ESI (+)
3-Chloroaniline	128.0	92.9 / 74.9	2.83	51	10	25 / 43	8 / 6	ESI (+)
3-Nitrobenzanthrone	276.0	202.0 / 230.0 / 246.0	6.56	100	10	44 / 33 / 26	7 / 10 / 8	APCI (+)

Table A.3. MRM transitions and optimized MS/MS parameters (continued).

Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
4,4'-Dichlorobenzophenone	251.0	139.0 / 110.8	6.67	71	10	27 / 55	6 / 8	ESI (+)
4-Aminomethyl-benzenesulfonamide	187.1	170.0 / 106.0	0.47	46	10	13 / 25	8 / 8	ESI (+)
4-Chloroaniline	128.0	93.0 / 74.8	2.83	56	10	25 / 43	8 / 6	ESI (+)
4-Methyl-1H-benzotriazole	134.0	76.9 / 78.9	3.09	46	10	37 / 27	8 / 6	ESI (+)
4-Methylbenzylidenecamphor	255.1	105.0 / 114.9	7.10	81	10	45 / 89	6 / 8	ESI (+)
4-Nonylphenoxy acetic acid	277.0	218.7 / 132.6	7.75	-80	-10	-24 / -60	-7 / -11	ESI (-)
4-tert-Octylphenol diethoxylate	312.2	183.1 / 120.9	7.04	61	10	17 / 29	10 / 8	ESI (+)
4-tert-Octylphenol monoethoxylate	268.1	113 / 251	6.99	46	10	11 / 9	6 / 12	ESI (+)
5,6-Dimethyl-1H-benzotriazole	148.1	76.9 / 92.9	3.34	81	10	39 / 27	6 / 8	ESI (+)
5-Methyl-1H-benzotriazole (5-Tolytriazole)	134.0	77.0 / 79.0	3.08	56	10	33 / 27	6 / 6	ESI (+)
7H-Benzo(de)anthracen-7-one (Benzanthrone)	230.8	202.0 / 150.0	6.43	40	10	45 / 89	14 / 5	APCI (+)
8-Hydroxyquinoline	146	128.0 / 74.9	0.51	61	10	33 / 57	6 / 6	ESI (+)
Acetaminophen (Paracetamol)	152	110.0 / 65.0	2.65	56	10	23 / 41	8 / 6	ESI (+)
Acetamiprid	223.1	126.0 / 99.0	2.99	76	10	31 / 55	11 / 9	ESI (+)
Acetochlor	270.2	224.0 / 148.0	5.78	46	10	11 / 29	15 / 11	ESI (+)
Aclonifen	265.0	248.0 / 182.1	6.16	61	10	25 / 39	8 / 12	ESI (+)
ADBI (Celestolide)	245.2	189.1 / 131.0	7.39	66	10	19 / 29	8 / 6	ESI (+)
AHDI (Phantolide)	245.2	175.1 / 119.0	7.33	71	10	25 / 47	8 / 6	ESI (+)
Alachlor	270.0	237.9 / 162.1	5.77	21	10	13 / 25	10 / 8	ESI (+)
alpha-Terpineol	137.2	80.8 / 136.9	5.40	10	10	16 / 19	6 / 10	APCI (+)
Amoxicillin	366.1	348.9 / 113.9	0.51	16	10	13 / 27	6 / 8	ESI (+)
Anthracene	178.0	152.0 / 176.0	6.94	152	10	45 / 51	8 / 8	APCI (+)
ATII (Traseolide)	259.1	189.1 / 147.1	7.64	81	10	21 / 33	8 / 6	ESI (+)
Atrazine	216.1	174.1 / 103.9	4.06	21	10	25 / 41	8 / 8	ESI (+)
Atrazine-desethyl	188.2	146.0 / 148.0	3.09	56	10	25 / 25	11 / 13	ESI (+)
Azinphos-methyl	318.0	131.9 / 76.9	4.64	46	10	19 / 61	10 / 6	ESI (+)
Azithromycin	749.5	591.3 / 82.8	2.80	86	10	43 / 89	6 / 6	ESI (+)

Table A.3. MRM transitions and optimized MS/MS parameters (continued).

Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
Azoxystrobin	404.1	372.0 / 344.1	5.20	76	10	21 / 35	13 / 25	ESI (+)
Banzaldehyde, (phenylmethylene)hydrazone	209.0	106.0 / 76.8	6.39	41	10	25 / 51	8 / 6	ESI (+)
Bayrepel	230.0	174.1 / 156	4.14	21	10	13 / 21	8 / 8	ESI (+)
Benzenesulfonamide	158.0	140.9 / 77.0	2.68	41	10	11 / 31	10 / 6	ESI (+)
Benzo[a]anthracene	228.0	226.0 / 222.0	7.62	160	10	51 / 51	10 / 10	APCI (+)
Benzo[a]pyrene	253.1	252.1 / 250.1	7.97	80	10	50 / 80	16 / 10	APCI (+)
Benzo[b]fluoranthene	252.1	250.1 / 224.1	7.98	100	10	64 / 85	16 / 13	APCI (+)
Benzo[ghi]perylene	276.0	274.0 / 272.0	8.26	281	10	77 / 105	42 / 14	APCI (+)
Benzo[k]fluoranthene	252.1	250.1 / 224.1	7.98	172	10	65 / 87	15 / 14	APCI (+)
Benzothiazole	136.0	108.9 / 64.9	3.38	71	10	33 / 45	6 / 6	ESI (+)
Benzylamine	108.1	90.9 / 65.0	0.50	36	10	17 / 35	6 / 8	ESI (+)
Benzyldimethyldodecylammonium	304.3	90.9 / 212.2	5.75	11	10	53 / 29	8 / 4	ESI (+)
Benzyldimethylhexadecylammonium	360.4	90.9 / 268.1	6.72	101	10	71 / 33	8 / 12	ESI (+)
Benzyldimethyltetradecylammonium	332.3	90.7 / 240.1	6.39	96	10	47 / 31	6 / 10	ESI (+)
Benzyltrimethylammonium	150.1	91.0 / 64.9	0.50	66	10	31 / 51	6 / 6	ESI (+)
Bifenox	359.0	309.8 / 341.9	6.59	21	10	15 / 9	12 / 6	ESI (+)
Bisphenol-A	226.9	211.1 / 132.7	4.28	-60	-10	-28 / -28	-10 / -10	APCI (-)
Boisvelone / Iso-Esuper	235.2	217.2 / 94.9	7.43	71	10	19 / 27	8 / 6	ESI (+)
Boscalid	343.0	307.0 / 140.0	5.30	101	10	27 / 27	18 / 14	ESI (+)
Buprofezin	306.0	201.0 / 115.9	6.65	61	10	11 / 17	10 / 10	ESI (+)
Butylmethoxydibenzoylmethane	311.0	161.1 / 135.0	7.71	91	10	35 / 33	8 / 6	ESI (+)
Cadusafos	271.1	158.9 / 214.9	6.62	66	10	21 / 13	13 / 17	ESI (+)
Carbazole	168.0	167.1 / 138.9	5.29	76	10	51 / 61	8 / 8	ESI (+)
Carbendazim	192.0	160.0 / 131.9	2.73	71	10	23 / 39	8 / 10	ESI (+)
Carbofuran	222.1	165.0 / 123.1	3.45	76	10	17 / 31	15 / 13	ESI (+)
Chloramphenicol	320.8	151.5 / 256.5	3.00	-70	-10	-24 / -18	-11 / -13	ESI (-)
Chlorfenvinphos	358.9	155.1 / 98.9	6.30	66	10	19 / 35	8 / 8	ESI (+)

Table A.3. MRM transitions and optimized MS/MS parameters (continued).

Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
Chloridazon	222.0	92.0 / 104.0	3.02	96	10	35 / 31	14 / 16	ESI (+)
Chlorpyrifos	349.9	96.8 / 197.9	7.16	56	10	55 / 35	8 / 6	ESI (+)
Chlorsulfuron	358.0	141.0 / 167.0	4.17	81	10	23 / 25	14 / 15	ESI (+)
Ciprofloxacin	332.2	314.0 / 230.9	2.72	76	10	29 / 51	12 / 10	ESI (+)
Clarithromycin	748.4	158.0 / 82.8	3.75	46	10	37 / 91	10 / 8	ESI (+)
Clofentezine	302.7	137.9 / 102.0	6.55	81	10	17 / 51	12 / 10	ESI (+)
Clothianidin	250.0	169.1 / 132.0	2.93	66	10	17 / 19	15 / 13	ESI (+)
Cybutryne	254.0	198.1 / 68.0	4.37	41	10	25 / 57	4 / 6	ESI (+)
Cyclopentadecanolide	241.2	223.2 / 205.3 / 55.1	7.86	42	10	13 / 15 / 39	6 / 9 / 7	APCI (+)
Cypermethrin	433.0	191.0 / 415.9	7.56	51	10	21 / 13	8 / 16	ESI (+)
Cyprodinil	226.1	93.1 / 77.0	5.05	91	10	49 / 65	9 / 7	ESI (+)
Cyromazine	167.0	85.0 / 68.0	0.52	66	10	23 / 45	8 / 6	ESI (+)
Damascone	193.0	146.8 / 137.0	6.19	41	10	15 / 17	8 / 6	ESI (+)
DEHP	391.3	120.8 / 148.9	8.36	61	10	69 / 35	8 / 8	ESI (+)
Diazinon	305.1	169.0 / 97.0	6.33	81	10	31 / 47	17 / 9	ESI (+)
Dichlorvos	220.9	108.9 / 78.9	3.36	61	10	25 / 49	8 / 6	ESI (+)
Dicloxacillin	470.1	159.9 / 310.8	6.62	71	10	17 / 21	12 / 14	ESI (+)
Dicyclohexylamine	182.2	83.0 / 100.0	2.78	61	10	29 / 27	6 / 6	ESI (+)
Difenoconazole	406.0	251.0 / 188.0	6.65	106	10	37 / 37	17 / 17	ESI (+)
Dimethoate	230.1	198.9 / 125.0	2.96	66	10	15 / 29	19 / 11	ESI (+)
Dimethomorph	388.1	301.1 / 165.1	5.47	56	10	31 / 43	11 / 17	ESI (+)
Diphenylamine	170.0	93.0 / 92.4	5.52	71	10	37 / 27	8 / 6	ESI (+)
Diuron	233.0	71.9 / 159.9	4.22	61	10	41 / 37	6 / 8	ESI (+)
Dodecyl sulfate	265.2	96.6 / 79.8	9.94	-85	-10	-38 / -98	-3 / -13	ESI (-)
Doxycycline	445.1	428.0 / 97.9	2.91	86	10	27 / 61	8 / 8	ESI (+)
Drometrizole	226.1	119.9 / 107.0	6.97	76	10	25 / 27	8 / 6	ESI (+)
Epoxiconazole	330.1	120.9 / 101.1	5.89	81	10	31 / 69	13 / 11	ESI (+)

Table A.3. MRM transitions and optimized MS/MS parameters (continued).

Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
Erythromycin	734.5	158.1 / 83.0	3.18	21	10	39 / 89	6 / 8	ESI (+)
Ethofumesate	304.1	121.1 / 121.1	5.02	56	10	31 / 31	11 / 11	ESI (+)
Ethoprophos	243.0	131.0 / 97.0	5.82	51	10	29 / 41	14 / 12	ESI (+)
Ethyl paraben	167.0	94.9 / 120.9	3.45	41	10	23 / 27	8 / 8	ESI (+)
Ethylhexylmethoxycinnamate	291.0	161.0 / 179.0	7.79	51	10	27 / 13	8 / 8	ESI (+)
Fenamiphos	304	217.0 / 202.0	6.02	71	10	31 / 45	15 / 15	ESI (+)
Fenarimol	331	268.0 / 81.1	5.79	76	10	33 / 49	23 / 17	ESI (+)
Fenpropimorph	304.0	147.0 / 117.0	3.61	76	10	39 / 71	14 / 14	ESI (+)
Fenthion	279.0	247.1 / 169.1	6.26	76	10	19 / 25	21 / 15	ESI (+)
Fluopyram	397.1	208.0 / 173.0	5.74	86	10	29 / 25	17 / 13	ESI (+)
Fluoranthene	202.1	200.0 / 150.0	6.43	160	10	55 / 65	8 / 8	APCI (+)
Fluquinconazole	376.0	307.0 / 349.0	5.68	86	10	33 / 25	20 / 22	ESI (+)
Flutolanil	324.0	262.1 / 282.0	5.44	86	10	25 / 19	23 / 25	ESI (+)
Flutriafol	302.0	123.0 / 109.0	4.00	71	10	39 / 43	14 / 14	ESI (+)
Fosthiazate	284.0	228.0 / 104.0	3.79	91	10	15 / 27	16 / 14	ESI (+)
Galaxolide	257.1	227.1 / 114.9	7.54	91	10	41 / 99	10 / 8	ESI (+)
g-Methylionone	207.1	111.0 / 68.9	6.85	41	10	17 / 27	8 / 6	ESI (+)
HBCDD	640.6	78.5 / 80.7	7.83	-39	-10	-62 / -44	-5 / -5	APCI (-)
Hexa(methoxymethyl)melamine	391.0	177.1 / 283.1	3.68	26	10	39 / 19	6 / 8	ESI (+)
Hexachlorobenzene	264.8	264.4 / 35.0	8.21	-15	-10	-14 / -47	-13 / -8	APCI (-)
Hexaconazole	314.0	70.0 / 159.0	6.34	66	10	39 / 37	12 / 14	ESI (+)
Hexylcinnamaldehyde	217.1	129.1 / 127.9	7.18	66	10	25 / 55	6 / 10	ESI (+)
Hexythiazox	353.1	228.0 / 168.0	7.18	76	10	23 / 37	19 / 15	ESI (+)
Homosalate	263.0	139.0 / 121.0	7.98	11	10	15 / 37	10 / 6	ESI (+)
Imazalil	297.0	159.0 / 201.0	3.17	56	10	31 / 23	14 / 15	ESI (+)
Imazamox	306.2	261.1 / 264.1	3.27	76	10	31 / 27	17 / 19	ESI (+)
Imidacloprid	256.1	175.1 / 209.1	2.90	71	10	29 / 21	17 / 19	ESI (+)

Table A.3. MRM transitions and optimized MS/MS parameters (continued).

Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
Indeno[1,2,3-cd] pyrene	276.0	274.1 / 272.1	8.27	291	10	71 / 97	24 / 26	APCI (+)
Isobutyl paraben	193.0	91.7 / 135.6	5.08	-75	-10	-34 / -24	-7 / -11	ESI (-)
Isoproturon	207.1	71.9 / 165.1	4.11	66	10	37 / 21	6 / 8	ESI (+)
Lenacil	235.1	153.1 / 136.1	4.14	66	10	19 / 43	13 / 11	ESI (+)
Linuron	249.0	159.9 / 132.9	4.90	61	10	27 / 47	8 / 8	ESI (+)
Malathion	331.1	127.0 / 285.0	5.41	81	10	19 / 11	13 / 11	ESI (+)
Mandipropamid	412.2	328.1 / 125.0	5.47	86	10	21 / 55	19 / 11	ESI (+)
Mepiquat chloride	113.9	58.1 / 98.1	0.50	46	10	29 / 29	6 / 10	ESI (+)
Mesotrione	340.0	228.0 / 104.0	4.26	91	10	23 / 41	21 / 21	ESI (+)
Metalaxyl	280.2	220.1 / 160.1	4.14	56	10	19 / 33	19 / 17	ESI (+)
Methamidophos	142.0	94.0 / 125.0	1.22	36	10	19 / 19	17 / 9	ESI (+)
Methidathion	303.0	145.0 / 85.0	4.41	46	10	15 / 27	14 / 12	ESI (+)
Methomyl	163.1	88.1 / 106.1	2.79	51	10	13 / 13	9 / 9	ESI (+)
Methoxyfenozide	369.0	149.0 / 133.0	5.56	66	10	23 / 31	14 / 14	ESI (+)
Methyl -iso-propylcyclohexenone	151.4	109.0 / 94.0 / 123.0	4.42	38	10	13 / 51 / 17	6 / 11 / 7	APCI (+)
Methyl paraben	151.0	135.6 / 91.6	3.11	-60	-10	-20 / -30	-13 / -5	ESI (-)
Methyldihydrojasmonate	227.4	209.1 / 153.0	5.60	30	10	14 / 19	9 / 7	APCI (+)
Methylsalicylate	151.1	135.7 / 91.6	3.11	-70	-10	-20 / -28	-9 / -13	ESI (-)
Metolachlor	284.1	252.0 / 176.1	5.86	61	10	23 / 37	23 / 15	ESI (+)
Metrafenone	409.1	209.2 / 227.0	6.50	71	10	19 / 23	19 / 15	ESI (+)
Microcystin-LR	995.5	135.0 / 106.9	5.02	181	10	111 / 127	6 / 6	ESI (+)
Microcystin-RR	519.8	135.0 / 102.9	3.17	96	10	35 / 91	6 / 8	ESI (+)
Microcystin-YR	1045.6	135.0 / 106.9	4.61	266	10	115 / 127	6 / 4	ESI (+)
Molinate	188.0	126.0 / 83.0	5.41	51	10	19 / 25	14 / 12	ESI (+)
Monocrotophos	224.2	192.9 / 126.9	2.82	56	10	13 / 21	17 / 11	ESI (+)
Musk ambrette	252.9	45.9 / 220.7	6.75	-35	-10	-60 / -38	-10 / -8	APCI (-)
Musk ketone	264.0	46.0 / 205.7	6.57	-66	-10	-60 / -30	-7 / -7	APCI (-)

Table A.3. MRM transitions and optimized MS/MS parameters (continued).

Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
Musk xylene	266.9	46.0 / 175.0	7.16	-33	-10	-52 / -35	-12 / -7	APCI (-)
Myclobutanil	289.0	70.0 / 125.0	5.54	66	10	33 / 41	12 / 14	ESI (+)
N,N-Diethyl-m-toluamide	192.1	118.9 / 90.9	4.10	71	10	25 / 43	6 / 6	ESI (+)
N-Benzyldimethylamine	136.1	91.0 / 65.0	0.51	41	10	25 / 47	6 / 6	ESI (+)
N-Benzylmethylamine	122.2	90.8 / 64.9	0.51	36	10	23 / 41	8 / 16	ESI (+)
N-Ethyl-2-tolysulfonamide	200.0	90.9 / 155.0	3.29	46	10	37 / 15	8 / 8	ESI (+)
N-methyl aniline	108.1	92.9 / 66.0	0.50	56	10	23 / 39	6 / 6	ESI (+)
Nonylphenol diethoxylate	326.2	183.1 / 121.0	7.37	61	10	15 / 31	10 / 6	ESI (+)
Norfloxacin	320.2	302.0 / 231.0	2.71	71	10	29 / 55	12 / 10	ESI (+)
N-phenyl-2-napthylamine	220.1	143 / 114.9	6.56	101	10	37 / 57	6 / 4	ESI (+)
Ofloxacin	362.2	318.0 / 261.0	2.70	46	10	27 / 37	6 / 10	ESI (+)
Omethoate	213.9	124.9 / 182.9	2.66	51	10	27 / 13	10 / 14	ESI (+)
Oxadiazon	362.1	303.0 / 220.1	7.05	56	10	23 / 35	19 / 19	ESI (+)
Oxadixyl	279.2	219.0 / 133.0	3.21	76	10	17 / 31	19 / 13	ESI (+)
Oxybenzone	229.1	151 / 104.8	6.01	61	10	27 / 25	8 / 12	ESI (+)
PCB-196	340.8	340.4 / 304.5	8.24	-60	-10	-19 / -36	-9 / -14	APCI (-)
Penconazole	284.2	158.9 / 70.2	6.17	81	10	37 / 35	15 / 7	ESI (+)
Pendimethalin	282.2	211.9 / 193.9	7.23	51	10	17 / 25	17 / 17	ESI (+)
Pentachlorobenzene	279.0	77.0 / 201.0	7.74	138	10	57 / 39	8 / 8	APCI (+)
Pinoxaden	401.2	317.1 / 57.1	6.50	81	10	29 / 53	27 / 11	ESI (+)
Piperonylbutoxide	356.2	177.0 / 118.9	6.99	16	10	17 / 47	8 / 12	ESI (+)
Pirimicarb	238.7	72.1 / 182.1	2.96	66	10	33 / 23	7 / 17	ESI (+)
Prochloraz	376.0	307.8 / 265.8	5.96	26	10	17 / 23	12 / 8	ESI (+)
Prometryn	242.2	158.1 / 200.0	4.05	76	10	33 / 27	13 / 15	ESI (+)
Propazine	229.9	145.9 / 188.0	5.02	46	10	27 / 21	10 / 10	ESI (+)
Propetamphos	282.2	138.0 / 156.0	5.55	56	8.5	23 / 17	14 / 14	ESI (+)
Propiconazole	342.1	159.0 / 69.1	6.30	96	10	43 / 35	15 / 7	ESI (+)

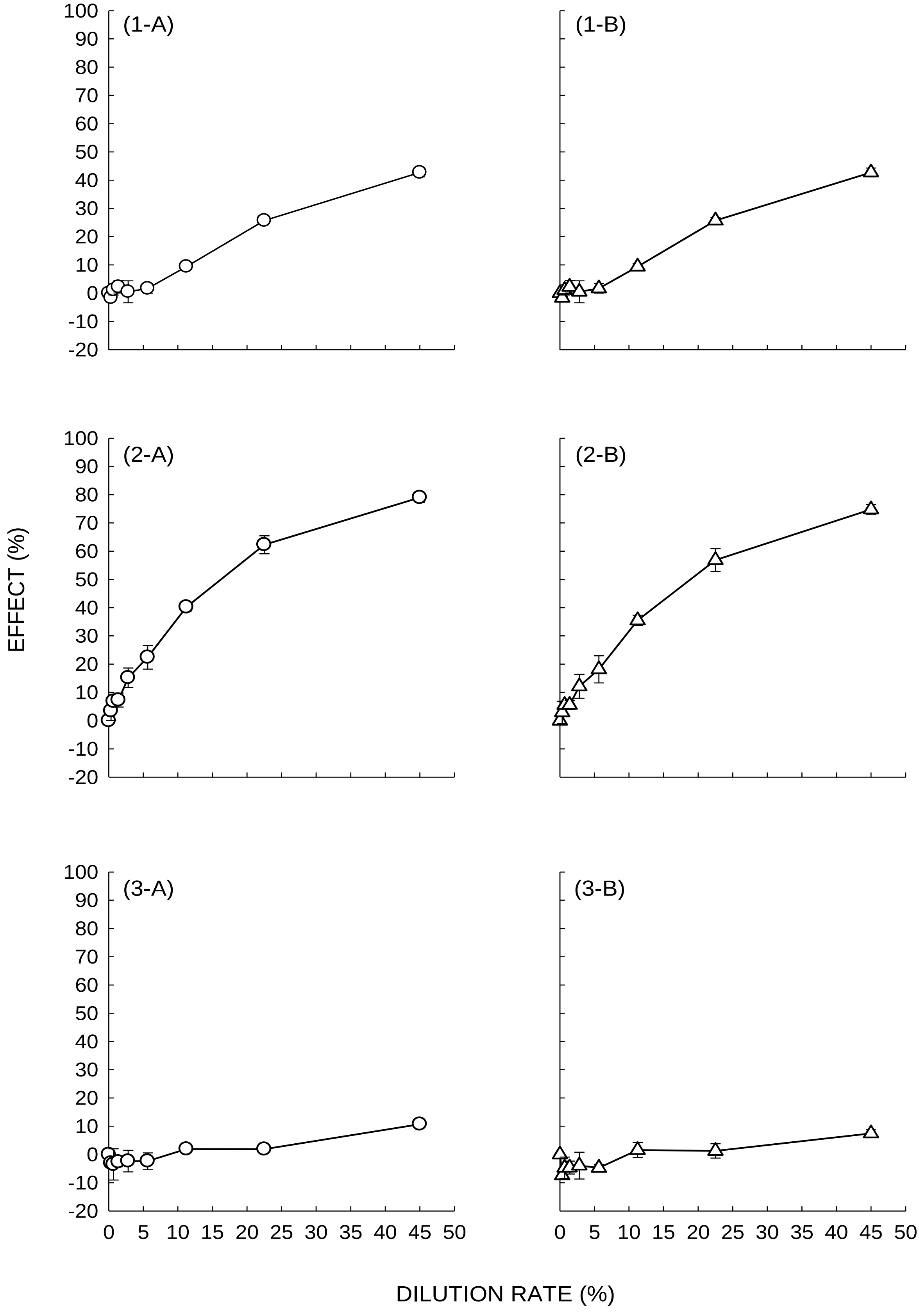
Table A.3. MRM transitions and optimized MS/MS parameters (continued).

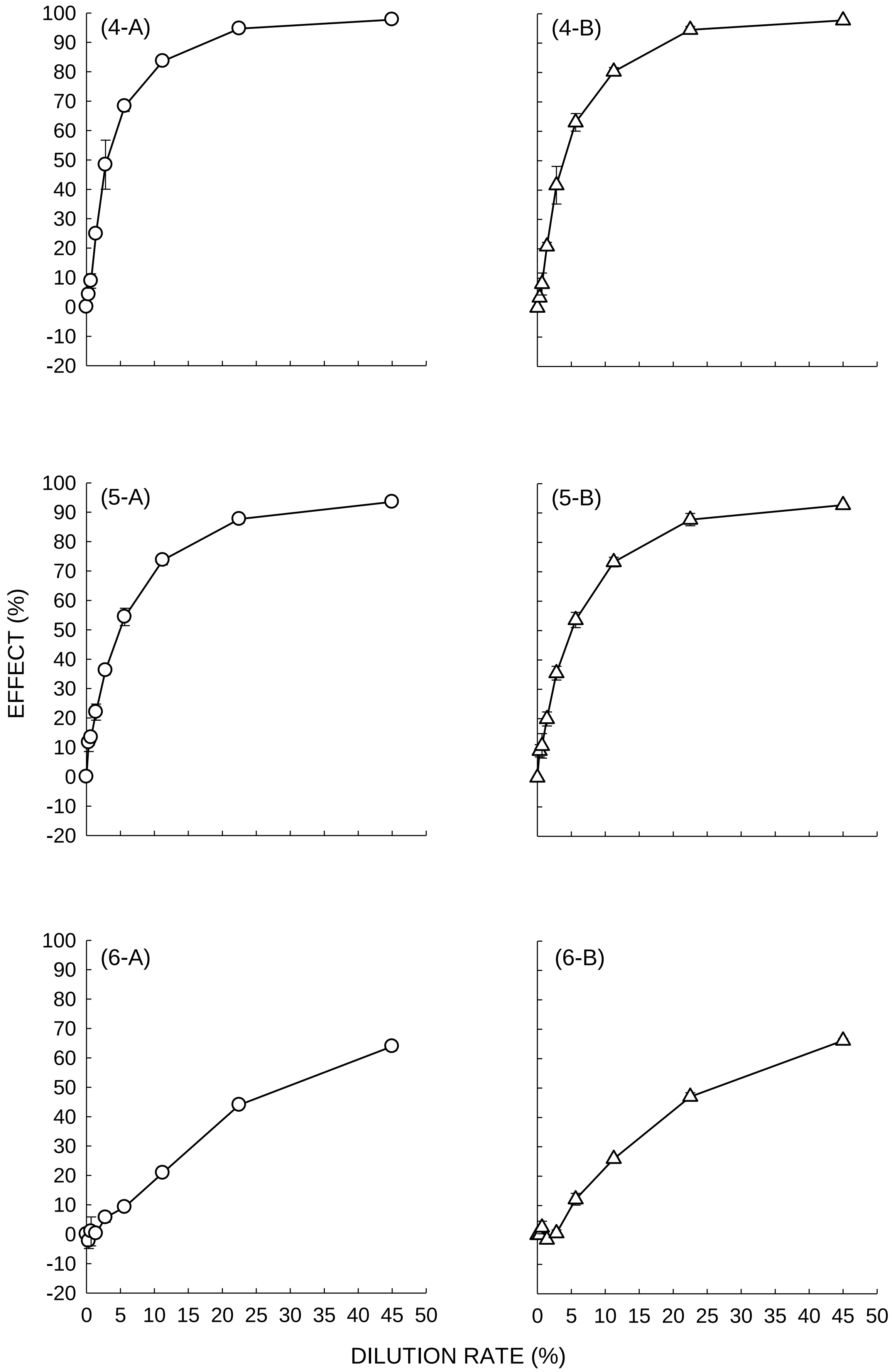
Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
Propyl paraben	179.0	91.7 / 135.7	4.10	-60	-10	-36 / -22	-9 / -11	ESI (-)
Prothioconazole	344.1	326.0 / 328.1	6.33	61	10	17 / 17	7 / 7	ESI (+)
Pyraclostrobin	388.0	194.0 / 163.0	6.45	36	10	19 / 29	15 / 15	ESI (+)
Pyridaben	365.1	309.1 / 147.1	7.64	66	10	19 / 37	11 / 13	ESI (+)
Pyrimethanil	200.2	82.1 / 107.2	3.93	81	10	37 / 35	17 / 11	ESI (+)
Pyriproxyfen	322.1	95.9 / 185.1	7.08	51	10	23 / 31	8 / 8	ESI (+)
Quinalphos	299.0	147.0 / 163.0	6.13	61	10	29 / 29	14 / 15	ESI (+)
Quinoxyfen	307.9	197.0 / 162.0	7.07	111	10	45 / 65	8 / 8	ESI (+)
Simazine	202.1	103.9 / 124.0	3.49	41	10	35 / 25	8 / 8	ESI (+)
Spiroxamine	298.0	144.0 / 100.0	3.85	71	10	27 / 41	14 / 14	ESI (+)
Sulfamethoxazole	254.0	91.9 / 107.8	2.85	46	10	35 / 35	6 / 8	ESI (+)
Tebuconazole	308.2	70.1 / 125.0	6.17	91	10	47 / 53	7 / 13	ESI (+)
Terbuthylazine	230.1	174.1 / 104.1	5.23	76	7.5	23 / 41	12 / 12	ESI (+)
Terbutryn	242.0	186.0 / 68.0	4.09	61	10	27 / 63	8 / 6	ESI (+)
Tetraacetylethylenediamine	229.1	145.1 / 85.9	2.85	36	10	15 / 37	8 / 8	ESI (+)
Tetrabromobisphenol A	538.8	78.5 / 288.5	6.90	-130	-10	-100 / -50	-7 / -1	ESI (-)
Tetracycline	445.1	409.9 / 153.9	2.71	71	10	27 / 35	6 / 8	ESI (+)
Thiacloprid	253.2	126.0 / 186.1	3.06	111	12	29 / 19	14 / 18	ESI (+)
Thiophanate-methyl	343.0	151.0 / 192.0	3.34	56	10	15 / 25	27 / 11	ESI (+)
Thioridazine	371.0	126.1 / 98.0	3.93	66	10	29 / 51	6 / 8	ESI (+)
Tolfenpyrad	384.2	197.1 / 91.0	7.03	131	10	37 / 37	15 / 15	ESI (+)
Tonalide	259.1	175.1 / 147.1	7.54	71	10	25 / 37	8 / 6	ESI (+)
Triasulfuron	402.0	167.0 / 141.0	3.36	76	10	25 / 29	14 / 14	ESI (+)
Triazophos	314.0	161.9 / 119.0	5.65	66	10	27 / 51	8 / 8	ESI (+)
Triclosan	286.7	35.1 / 218.5	6.77	-55	-10	-28 / -14	-5 / -7	ESI (-)
Trifloxystrobin	409.1	186.0 / 205.9	6.73	61	10	23 / 21	19 / 19	ESI (+)
Trifluralin	336.4	232.0 / 236.0 / 252.0	7.34	17	10	25 / 25 / 25	11 / 11 / 11	APCI (+)

Table A.3. MRM transitions and optimized MS/MS parameters (continued).

Analyte	Precursor ion (m/z)	Product ions (m/z)	RT (min)	DP (V)	EP (V)	CE (V)	CXP (V)	Ionization Mode
Trimethoprim	291.1	260.9 / 123.0	2.65	81	10	35 / 33	16 / 6	ESI (+)
Triphenylphosphineoxide	279.1	201.0 / 76.9	5.05	96	10	37 / 67	10 / 6	ESI (+)
Triphenyltin	351.0	119.8 / 196.9	8.52	126	10	73 / 37	6 / 6	ESI (+)
Tris(1-chloro-2-propanyl) phosphate	327.3	98.9 / 80.8 / 250.9 / 175.0	5.36	6	10	40 / 86 / 16 / 18	8 / 9 / 25 / 11	APCI (+)
Tris(2-butoxyethyl) phosphate	399.2	299.1 / 198.8	6.89	26	10	19 / 23	4 / 8	ESI (+)
Vancomycin	724.7	99.9 / 74.0	0.49	81	10	73 / 101	8 / 6	ESI (+)

APPENDIX B: DOSE-RESPONSE CURVES OF ALL SAMPLES FOR 5- AND 15- MIN EXPOSURE

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(6-B)
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-20
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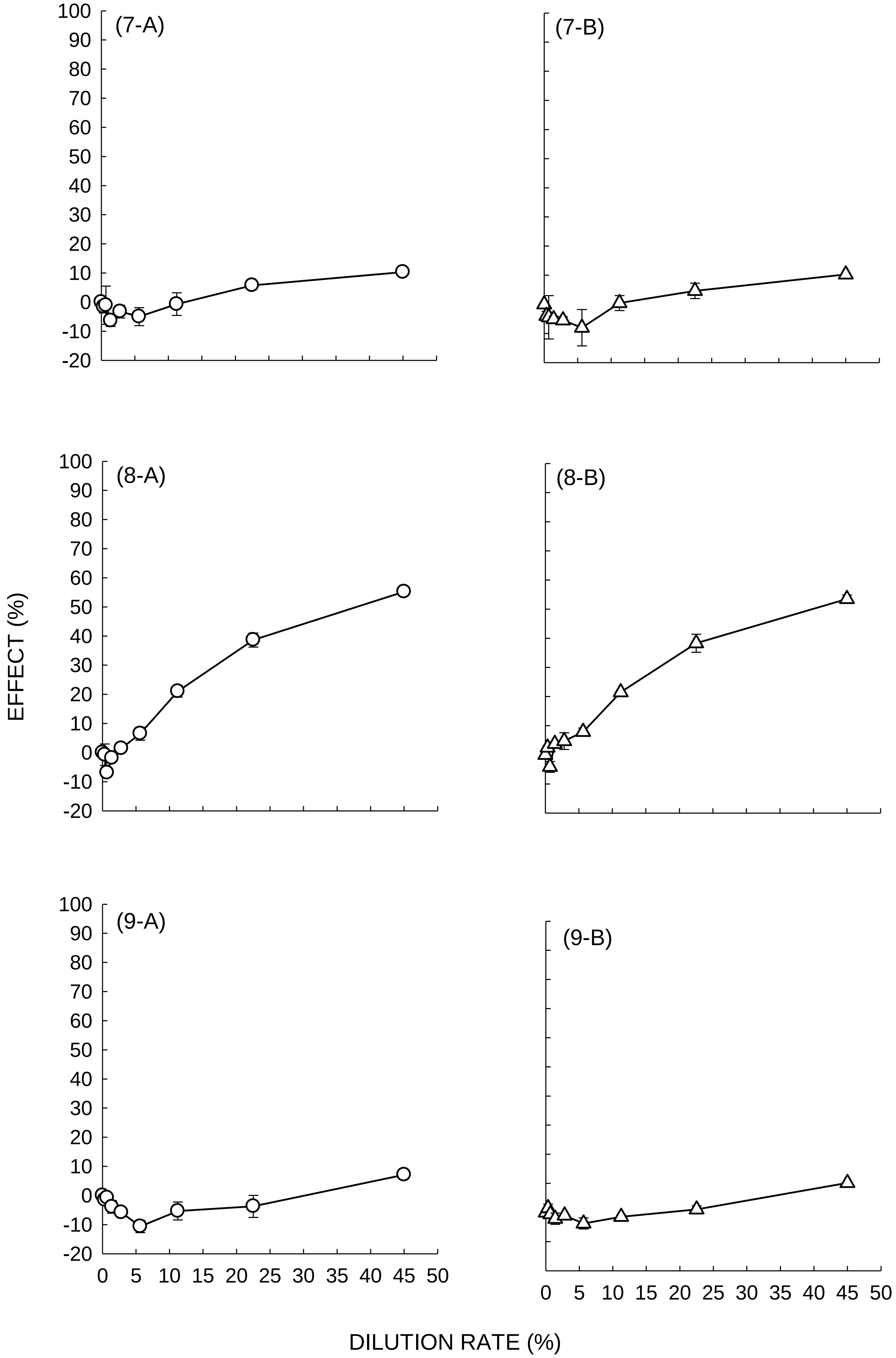
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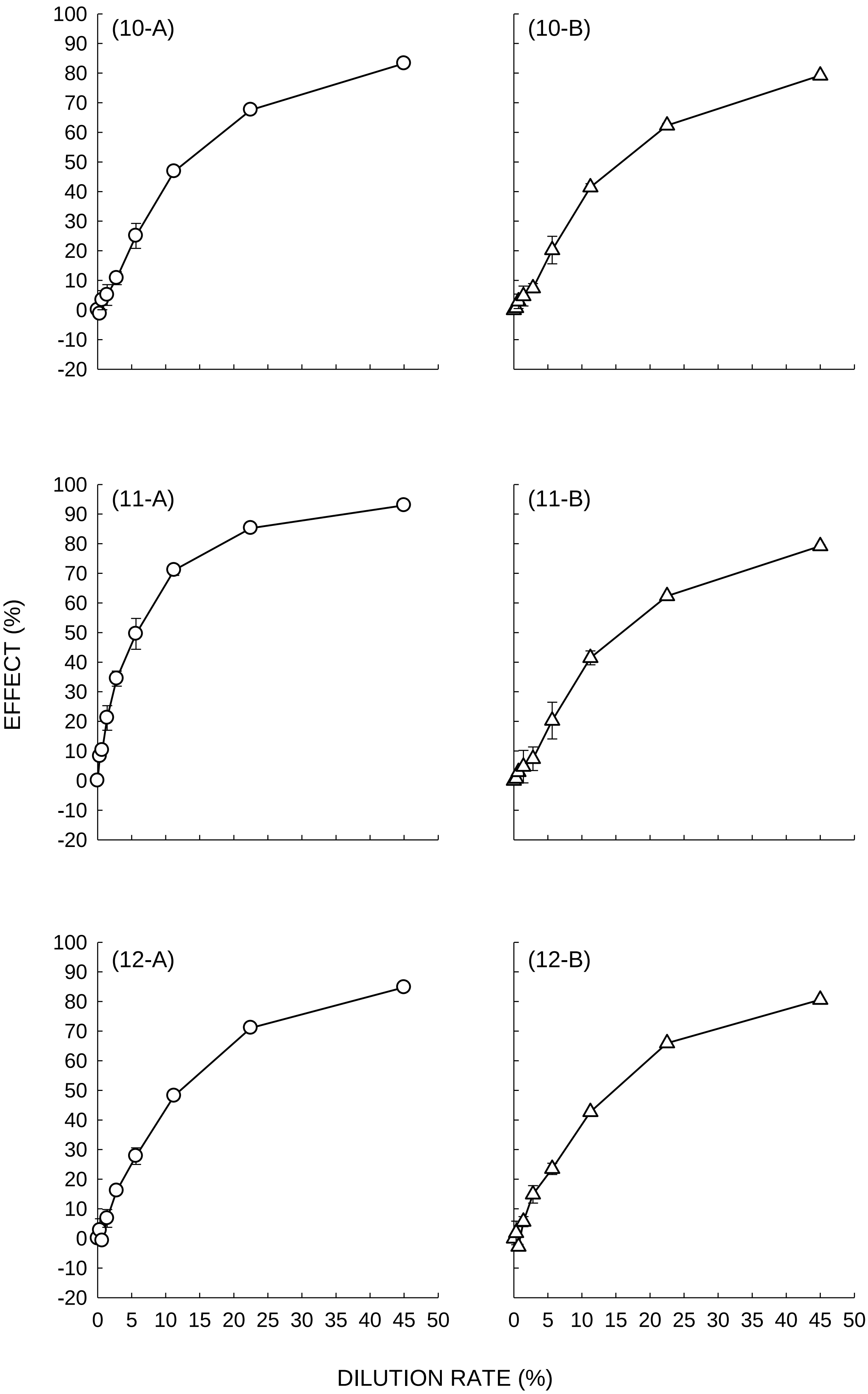
EFFECT (%)
DILUTION RATE (%)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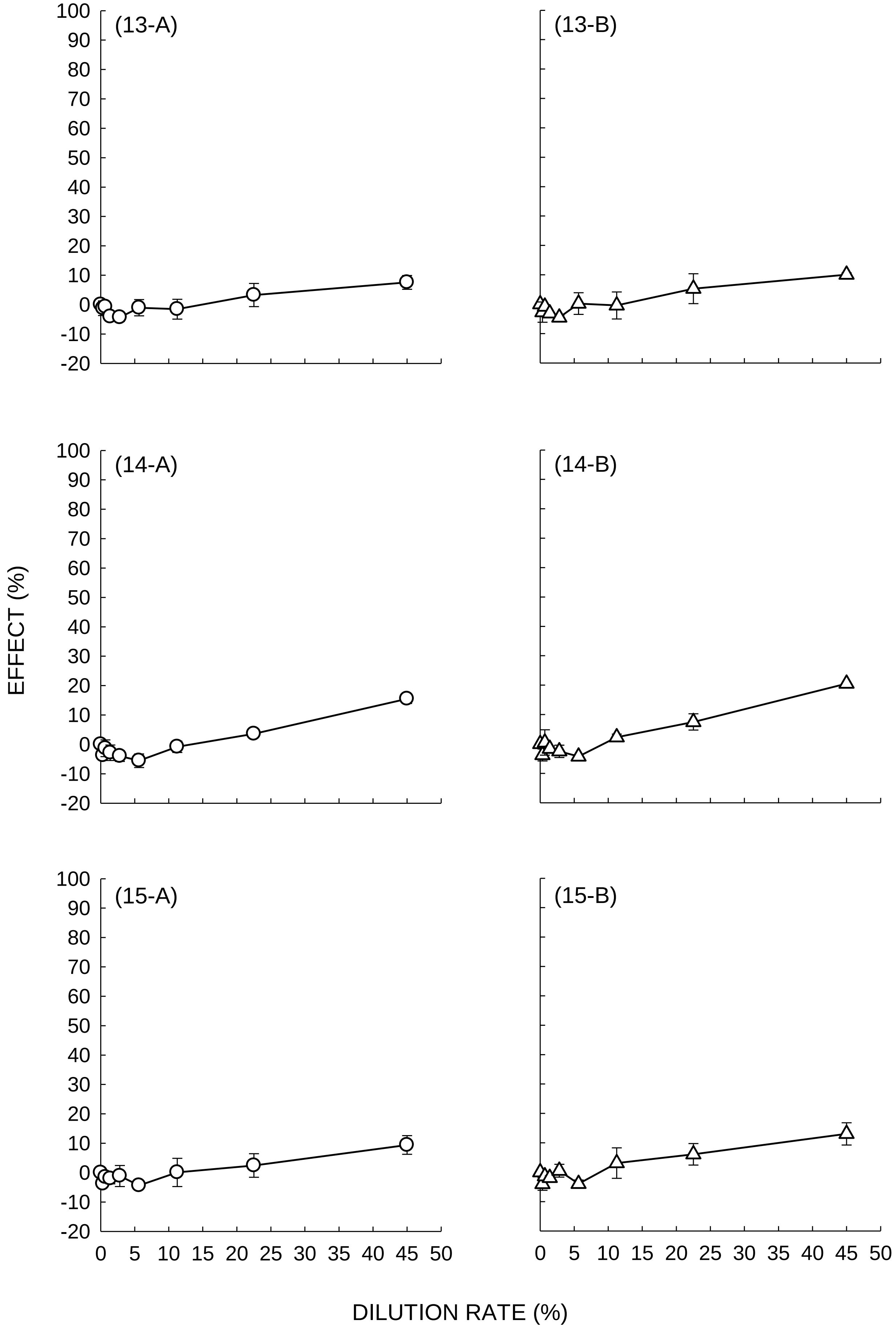
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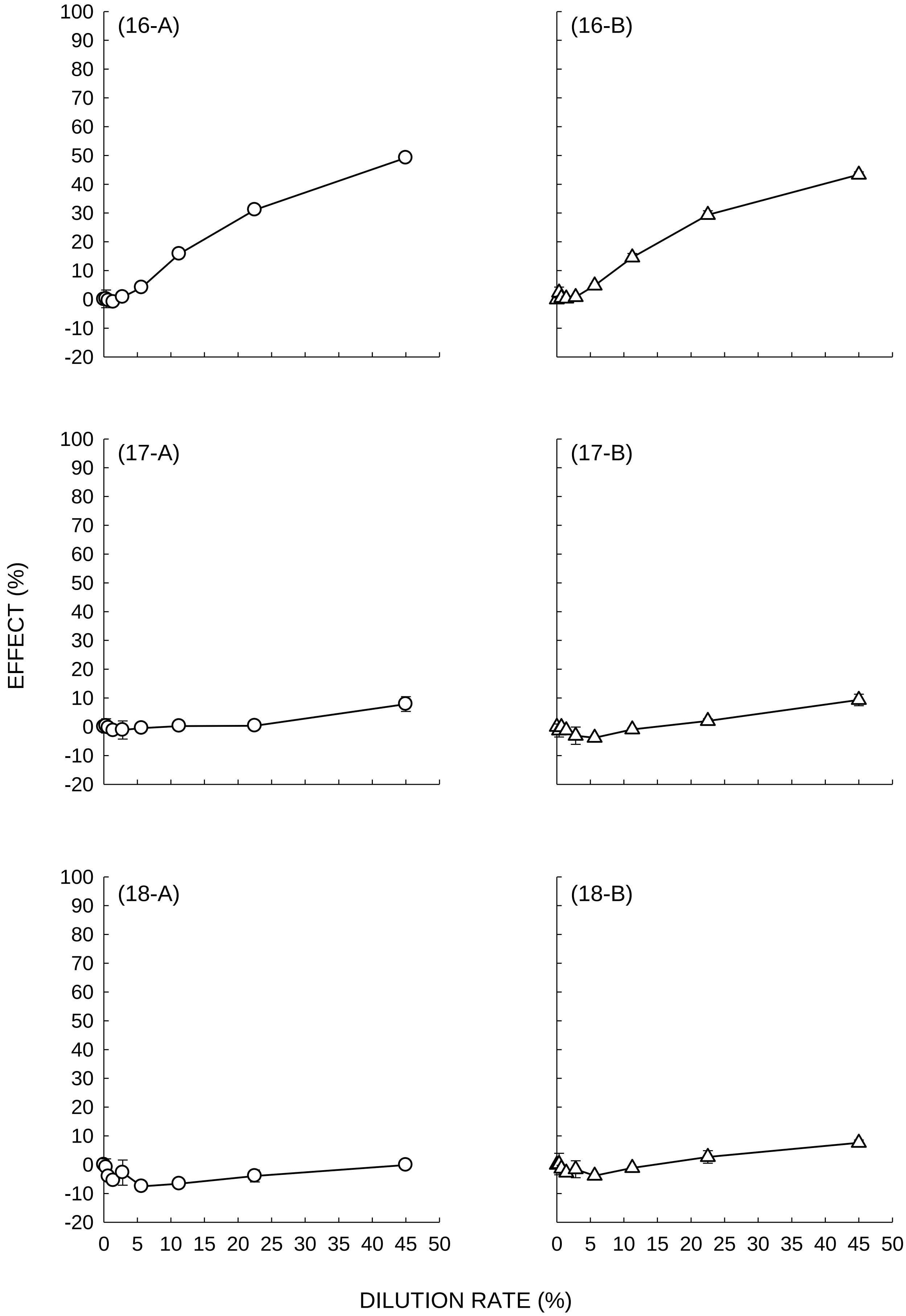
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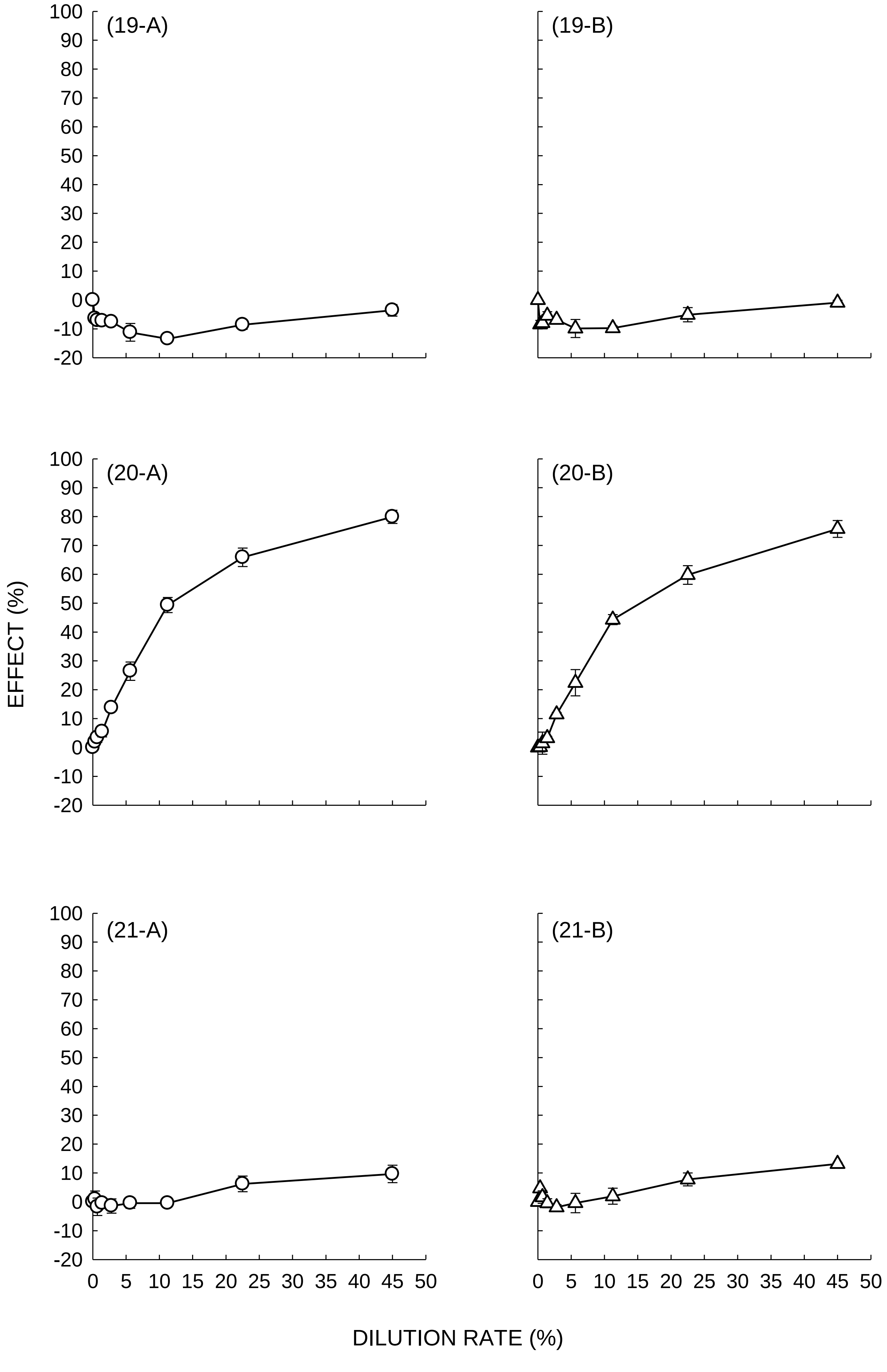
DILUTION RATE (%)



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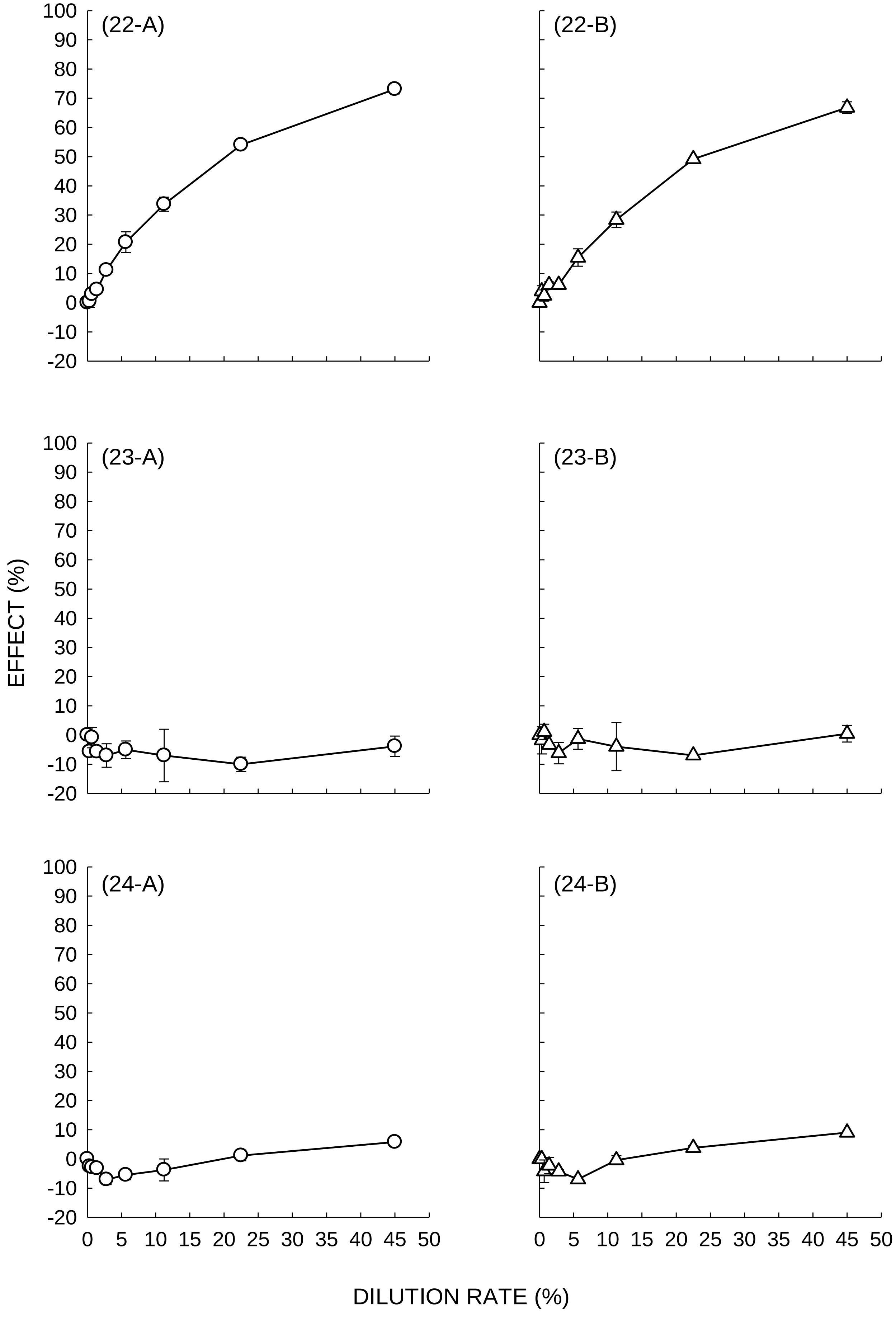
DILUTION RATE (%)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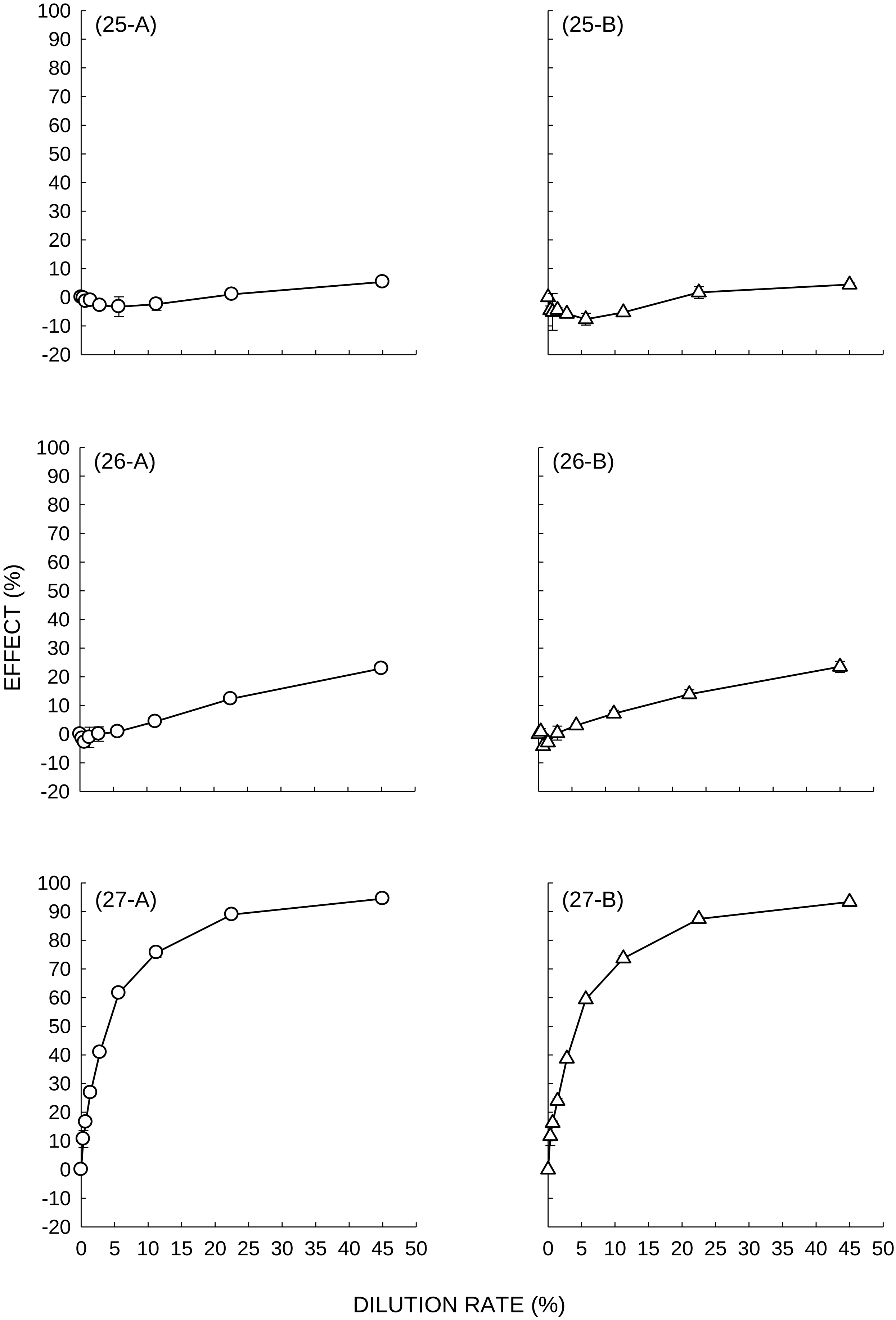
DILUTION RATE (%)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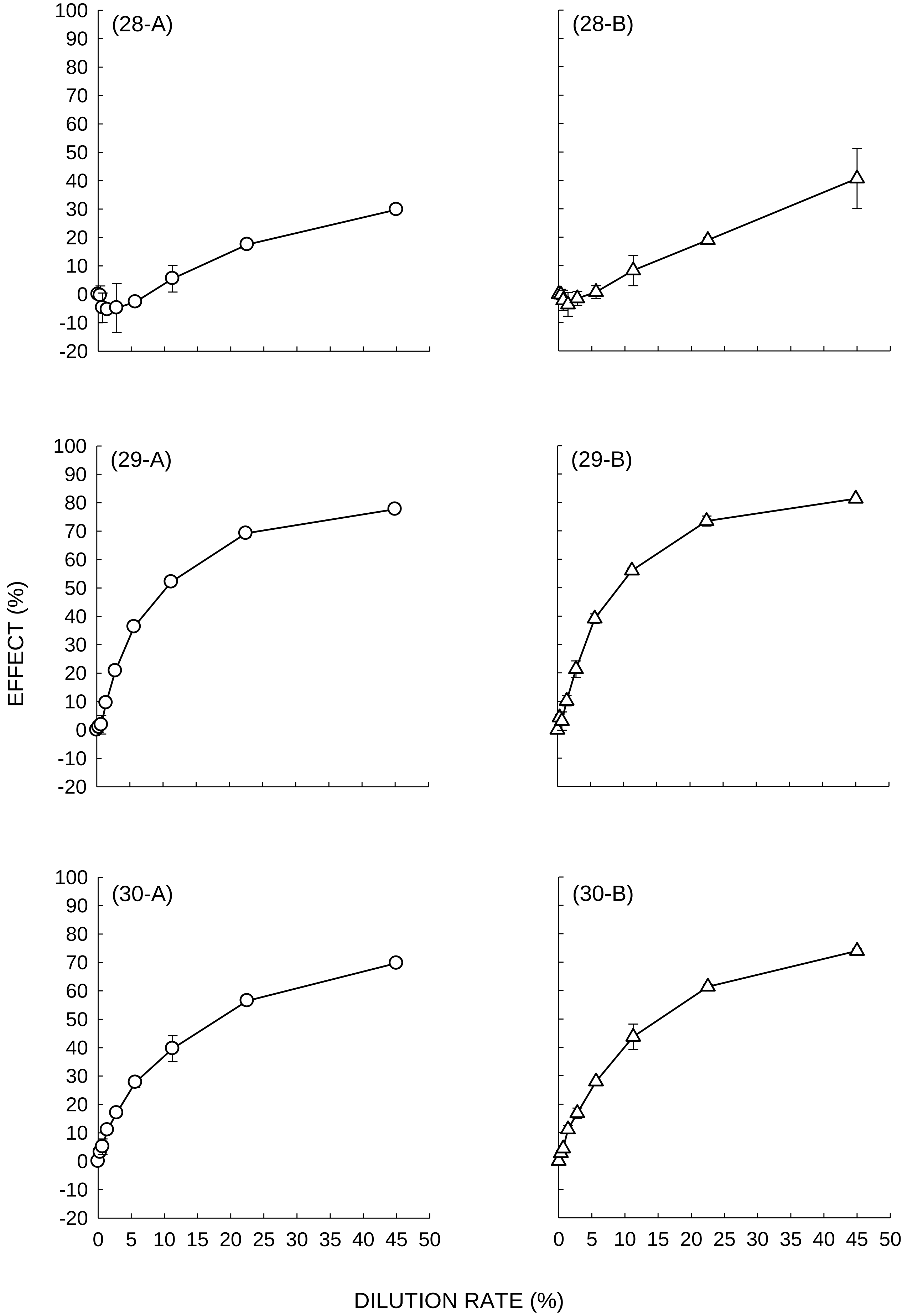
DILUTION RATE (%)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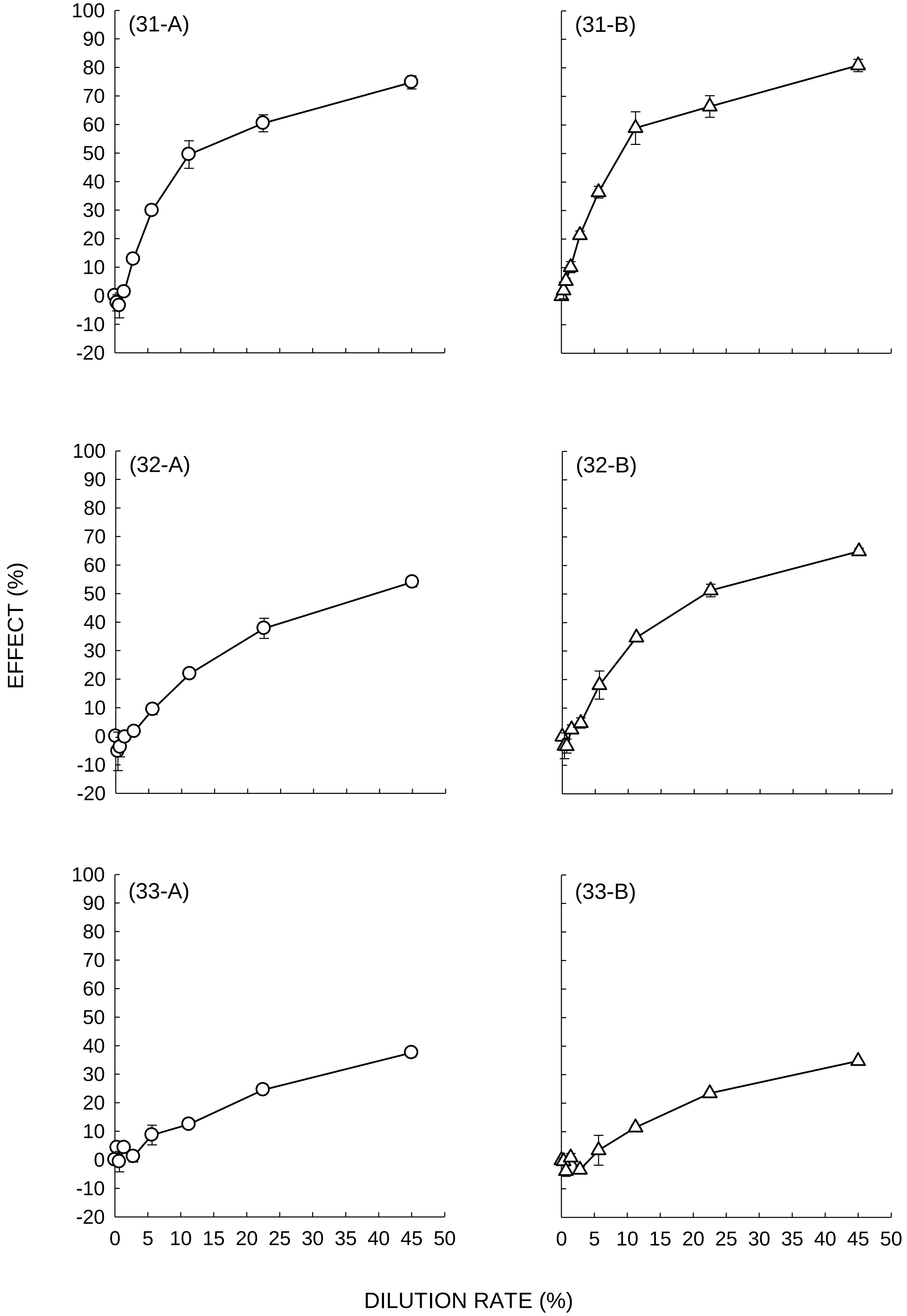
DILUTION RATE (%)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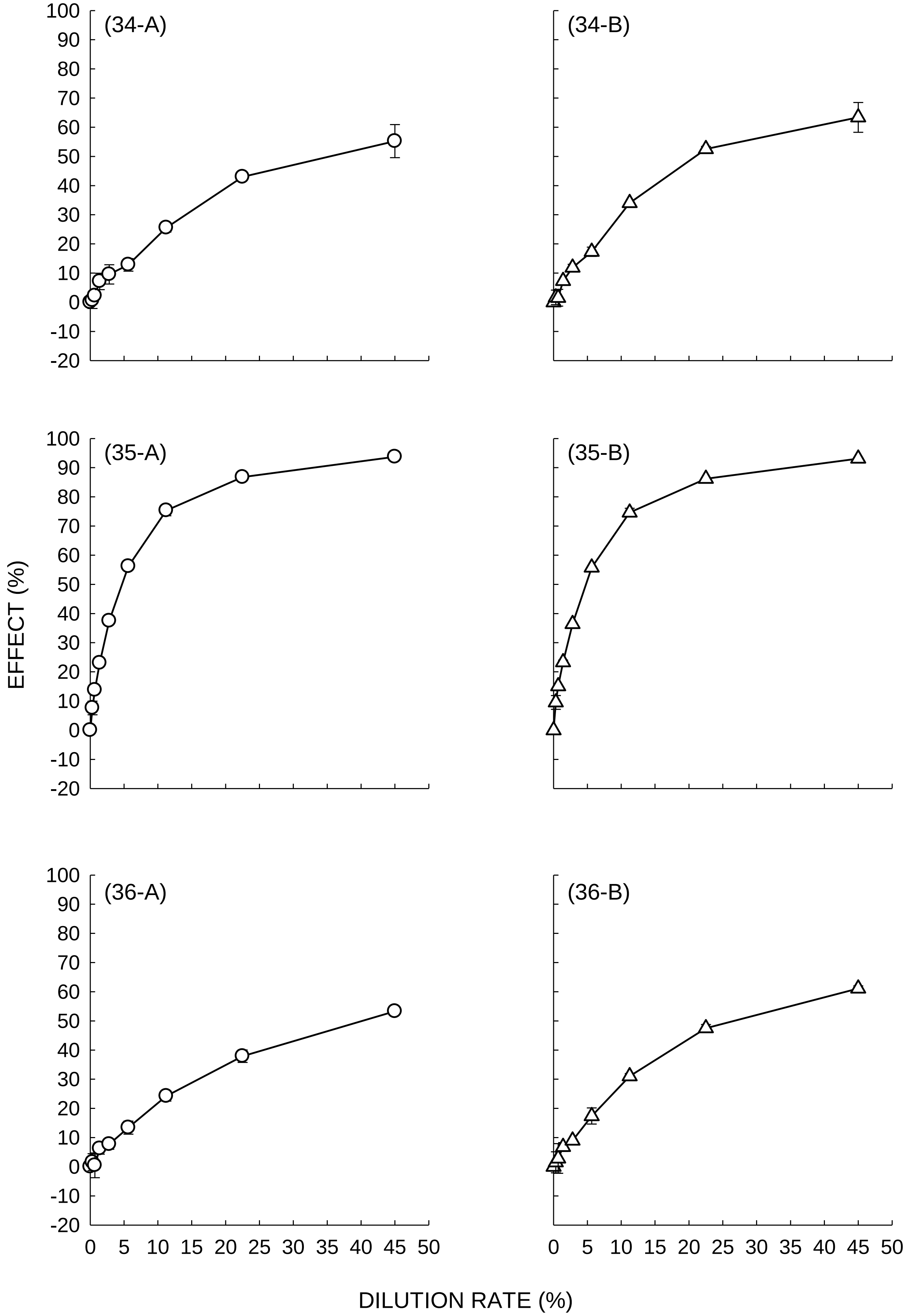
EFFECT (%)
DILUTION RATE (%)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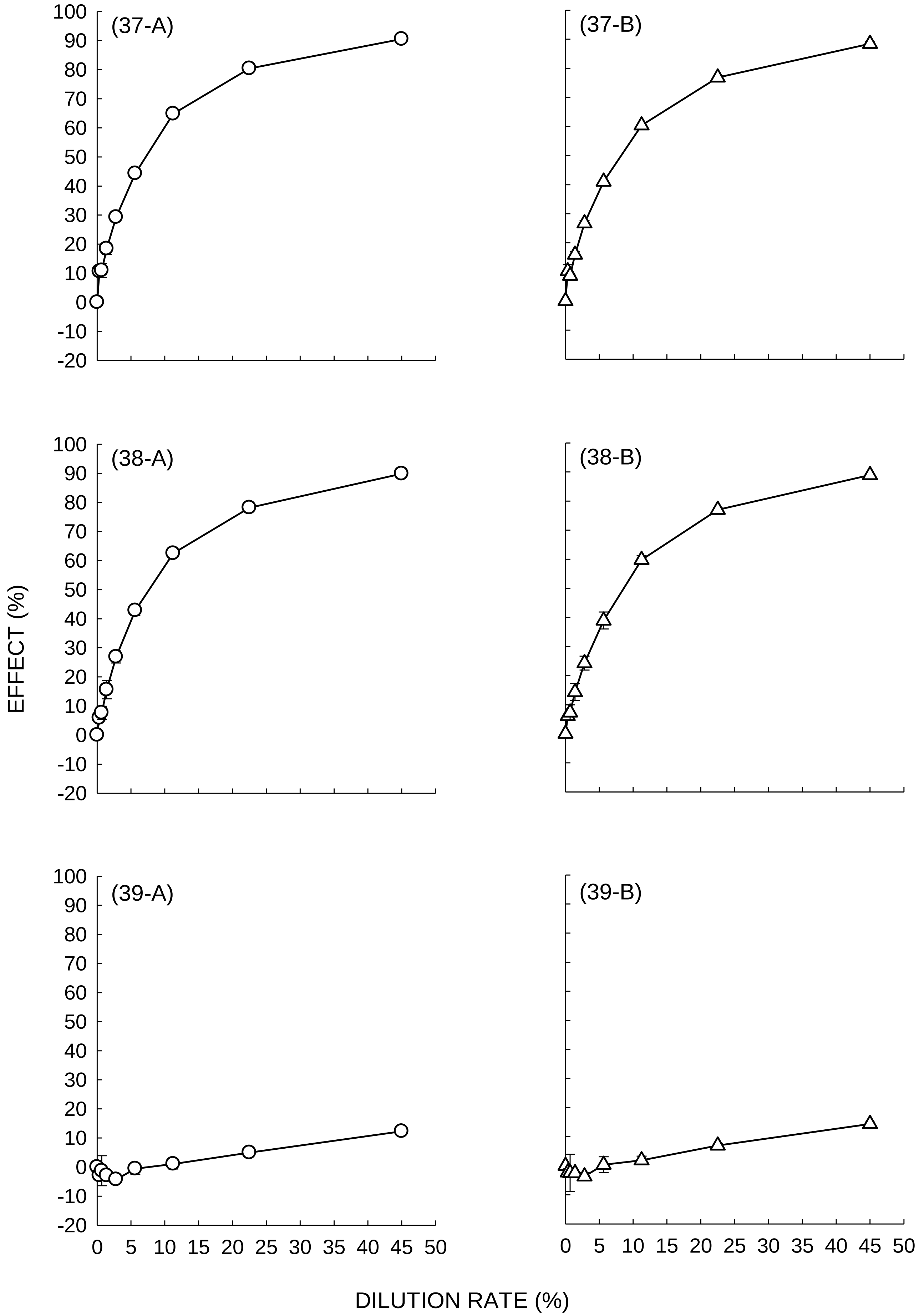
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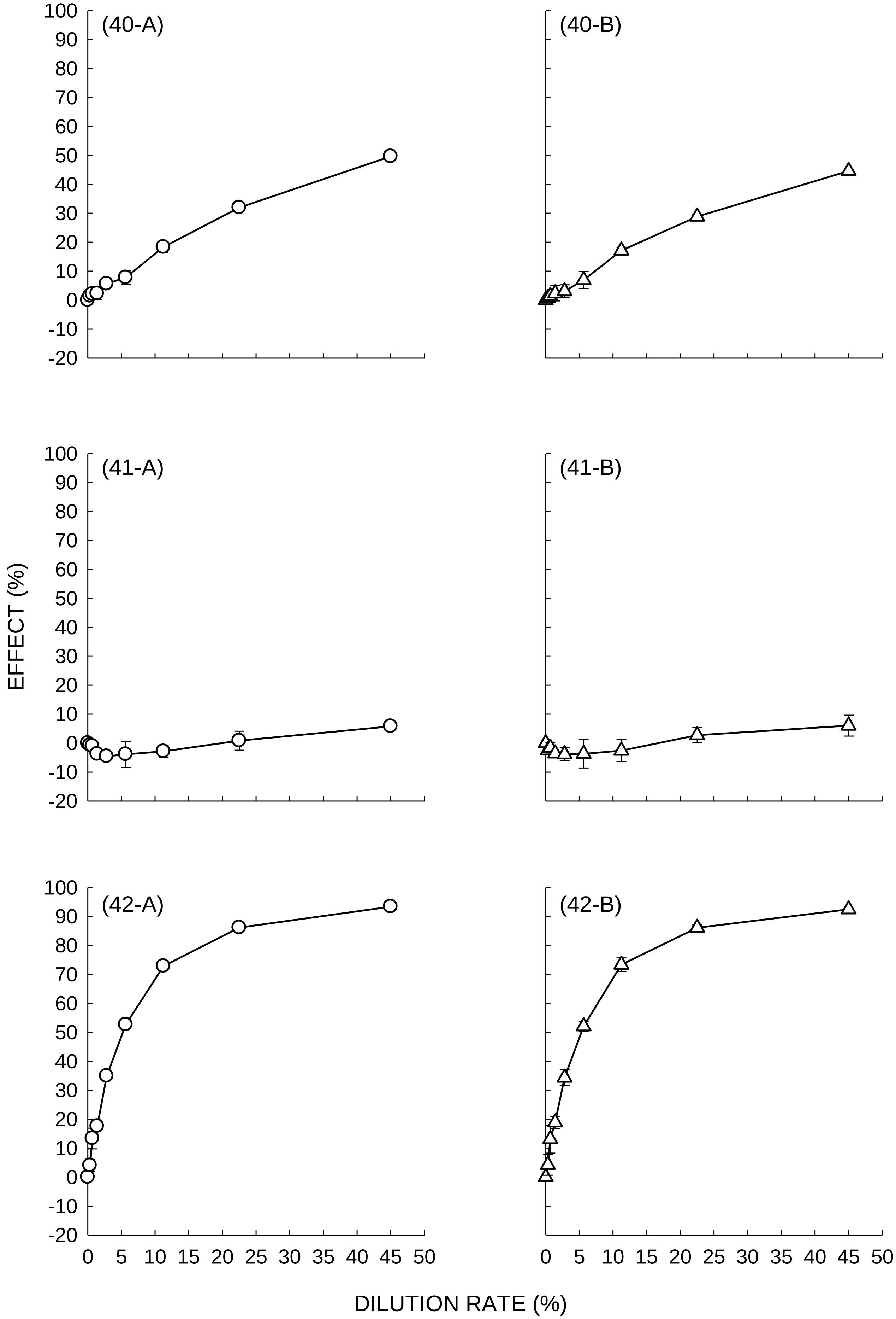
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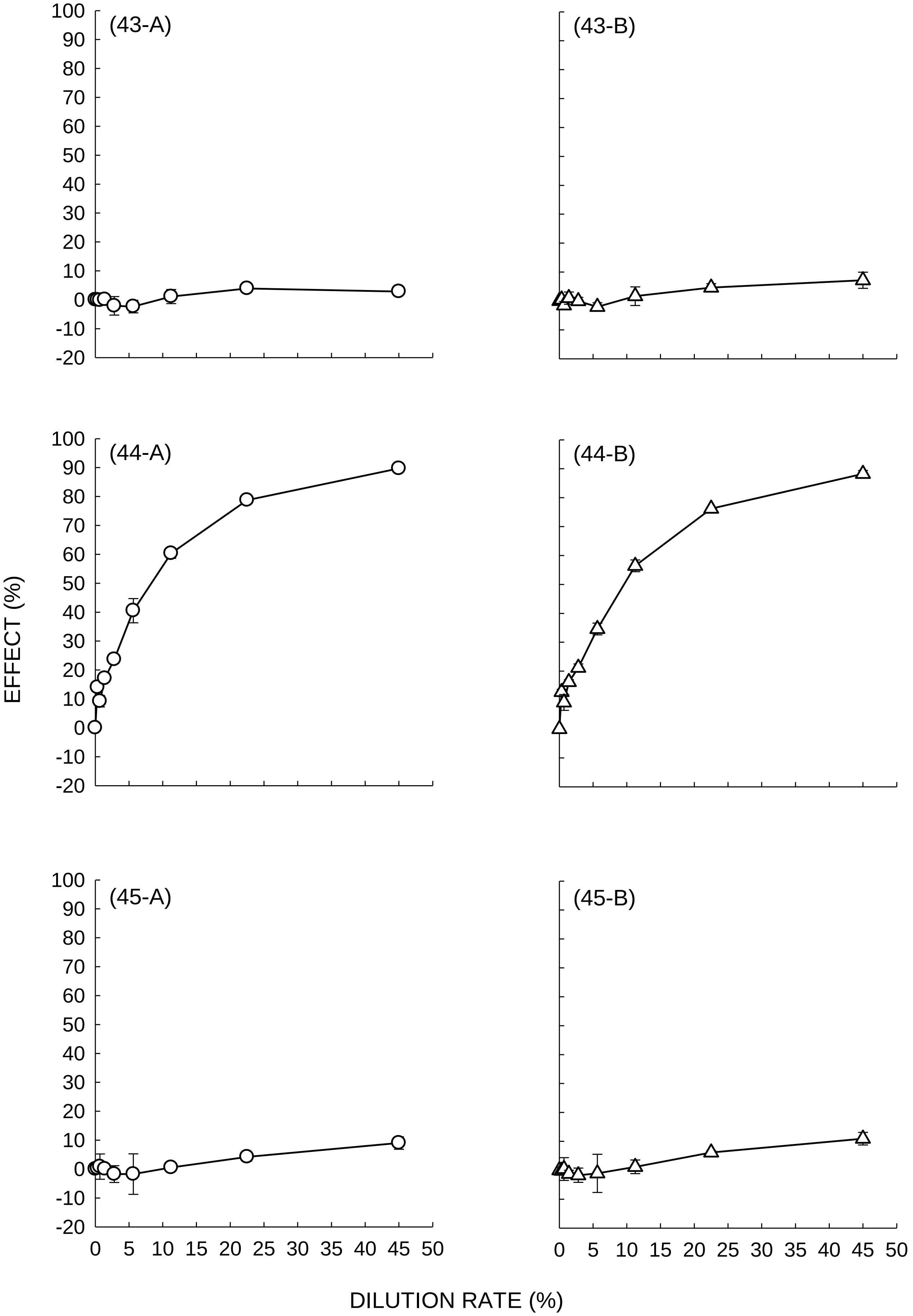
DILUTION RATE (%)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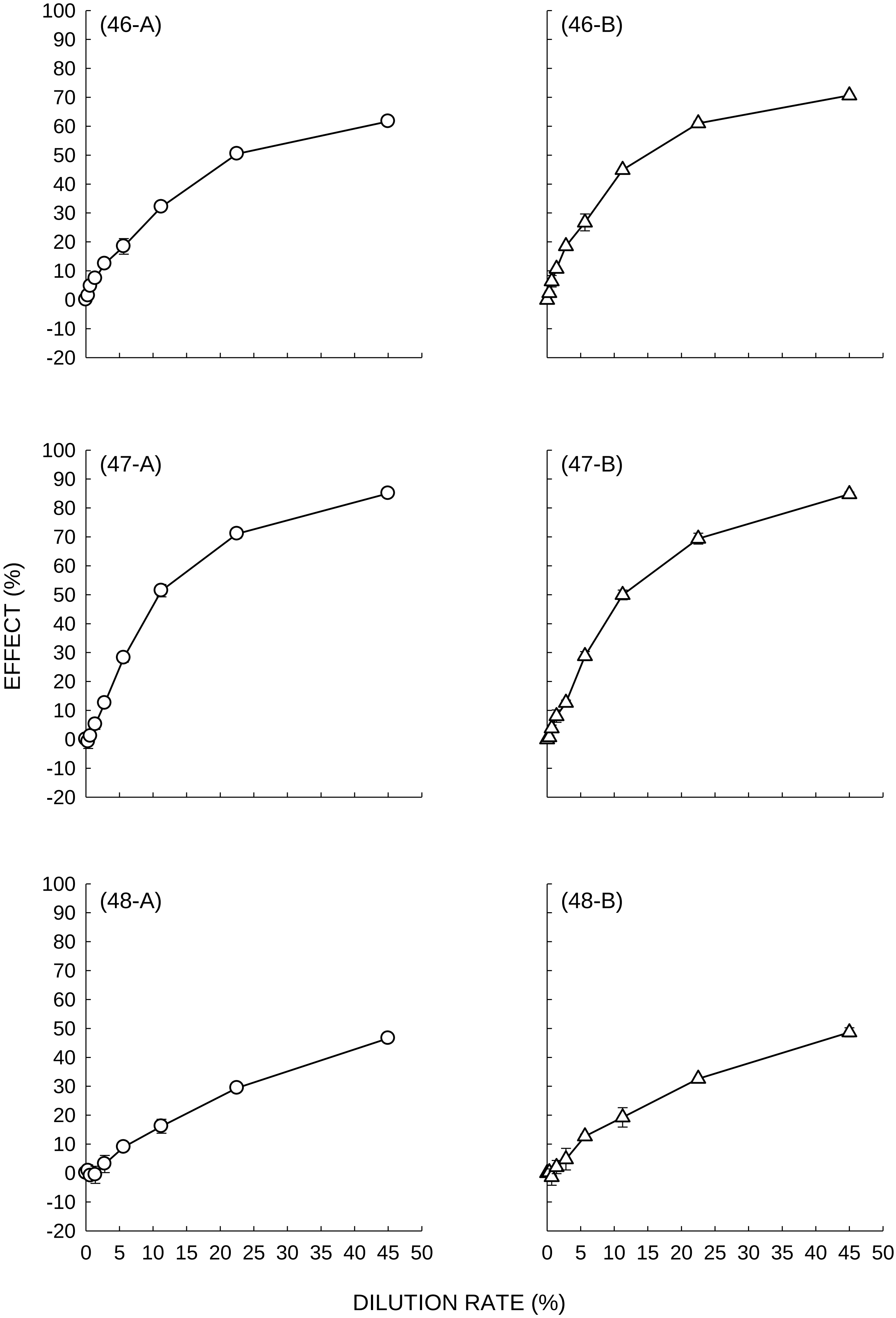
EFFECT (%)
DILUTION RATE (%)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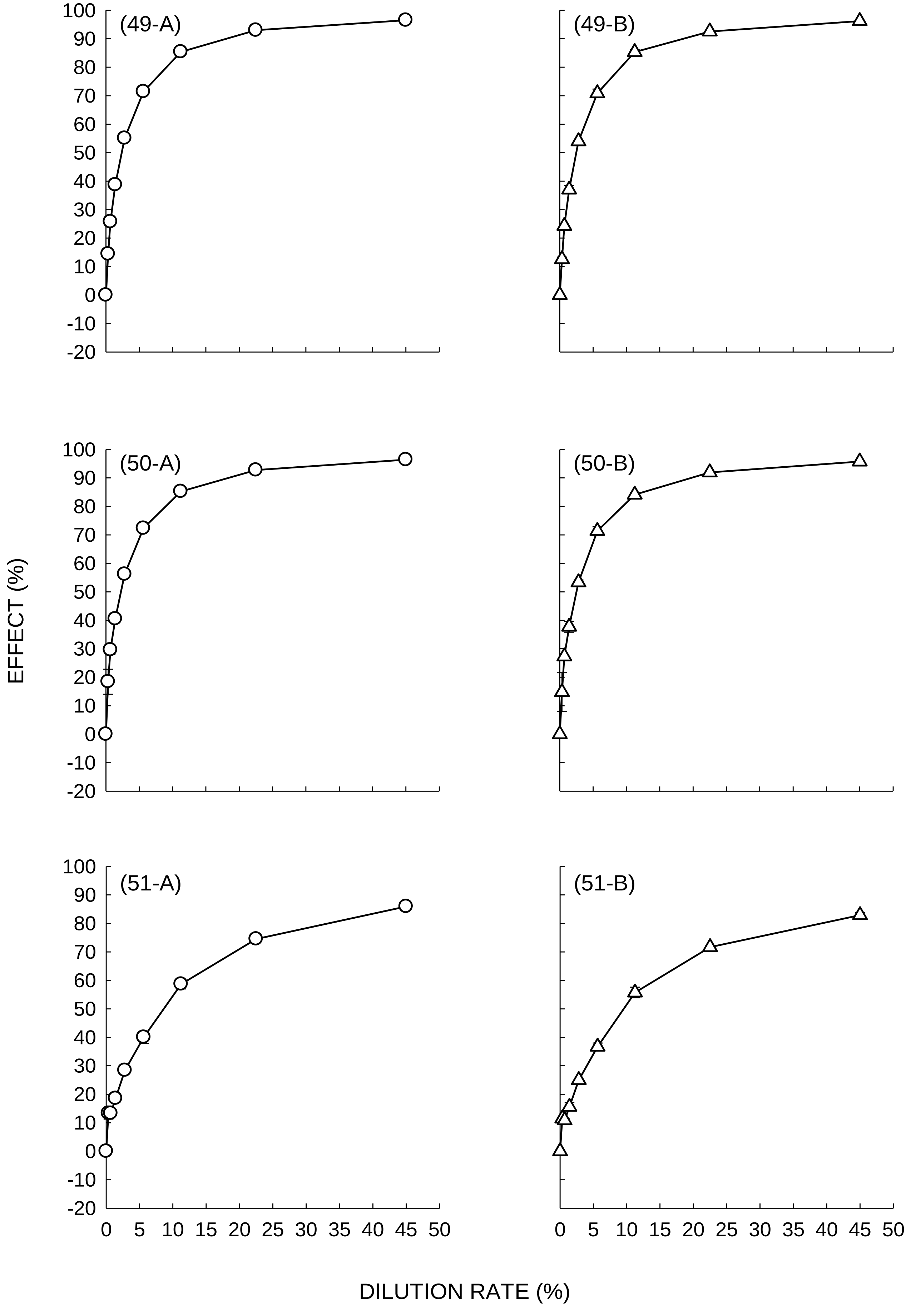

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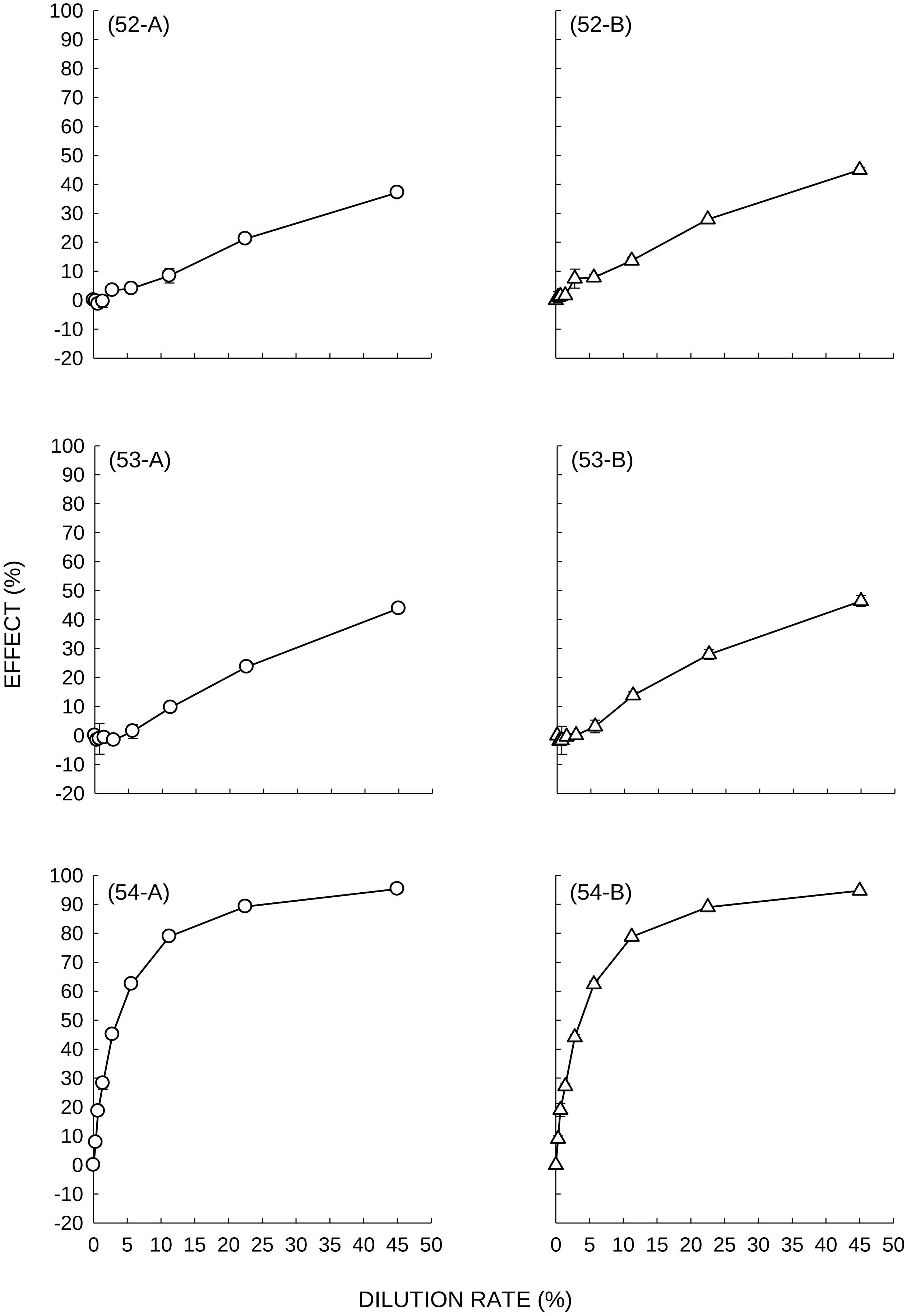
EFFECT (%)
DILUTION RATE (%)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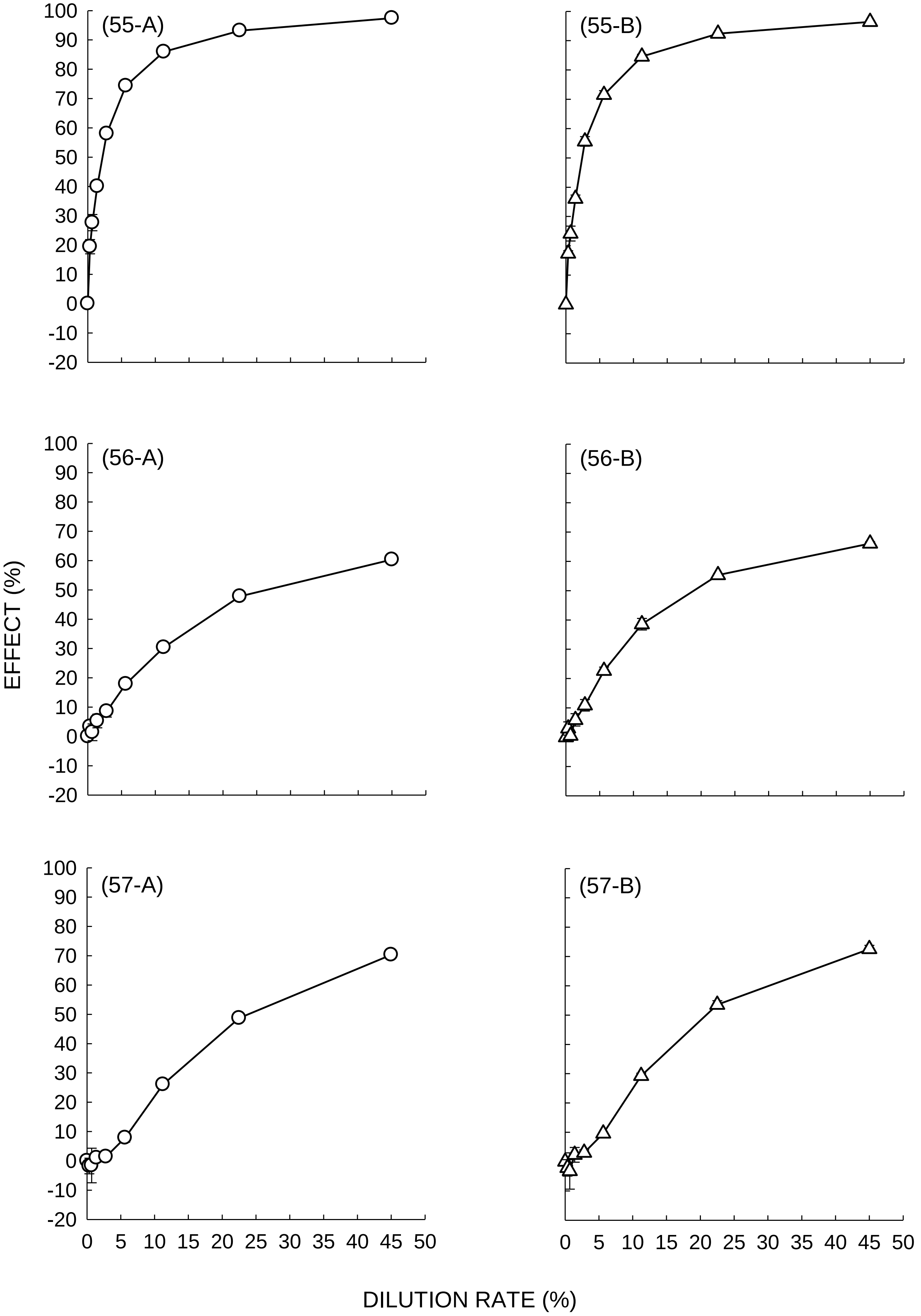
EFFECT (%)
DILUTION RATE (%)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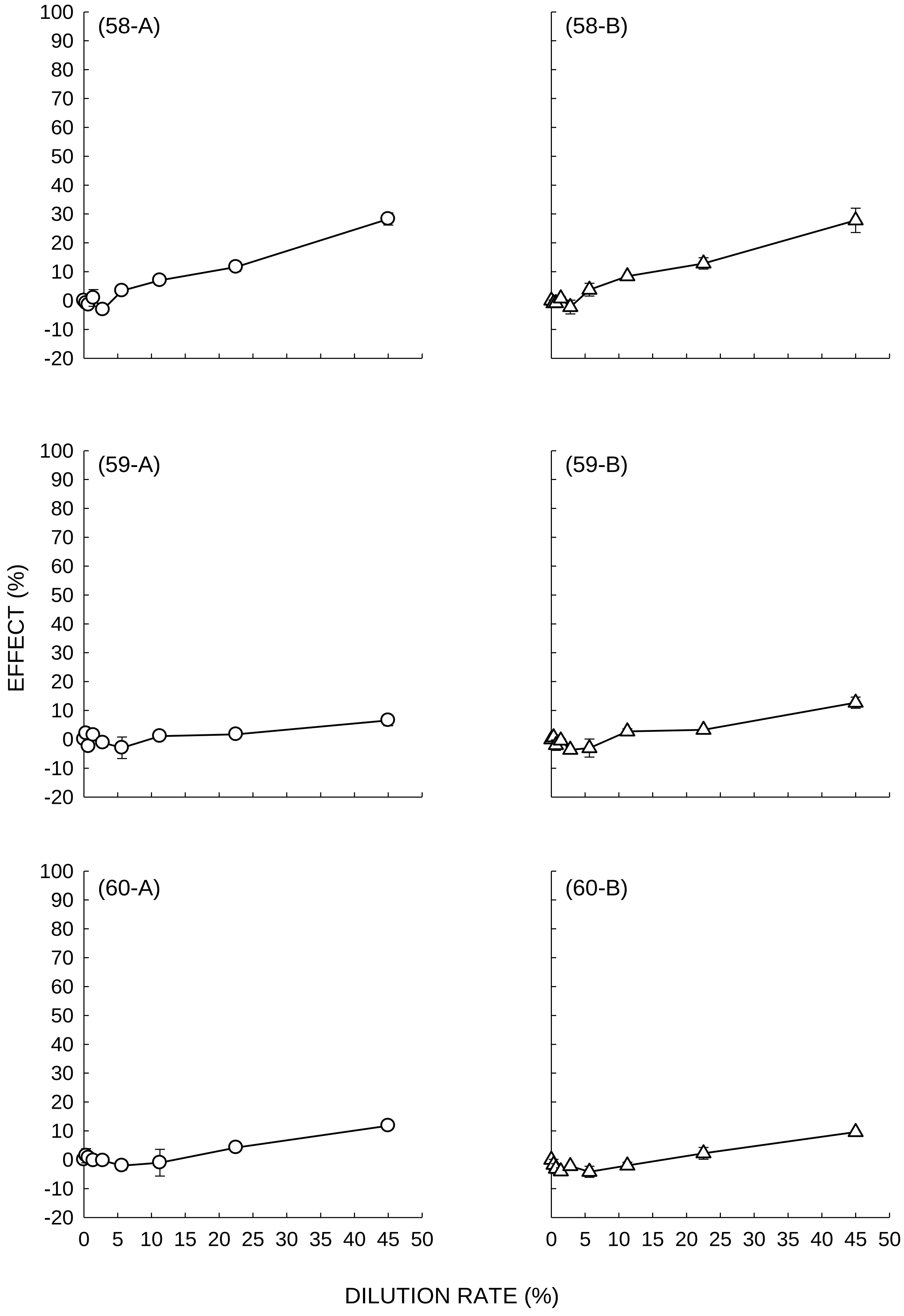
DILUTION RATE (%)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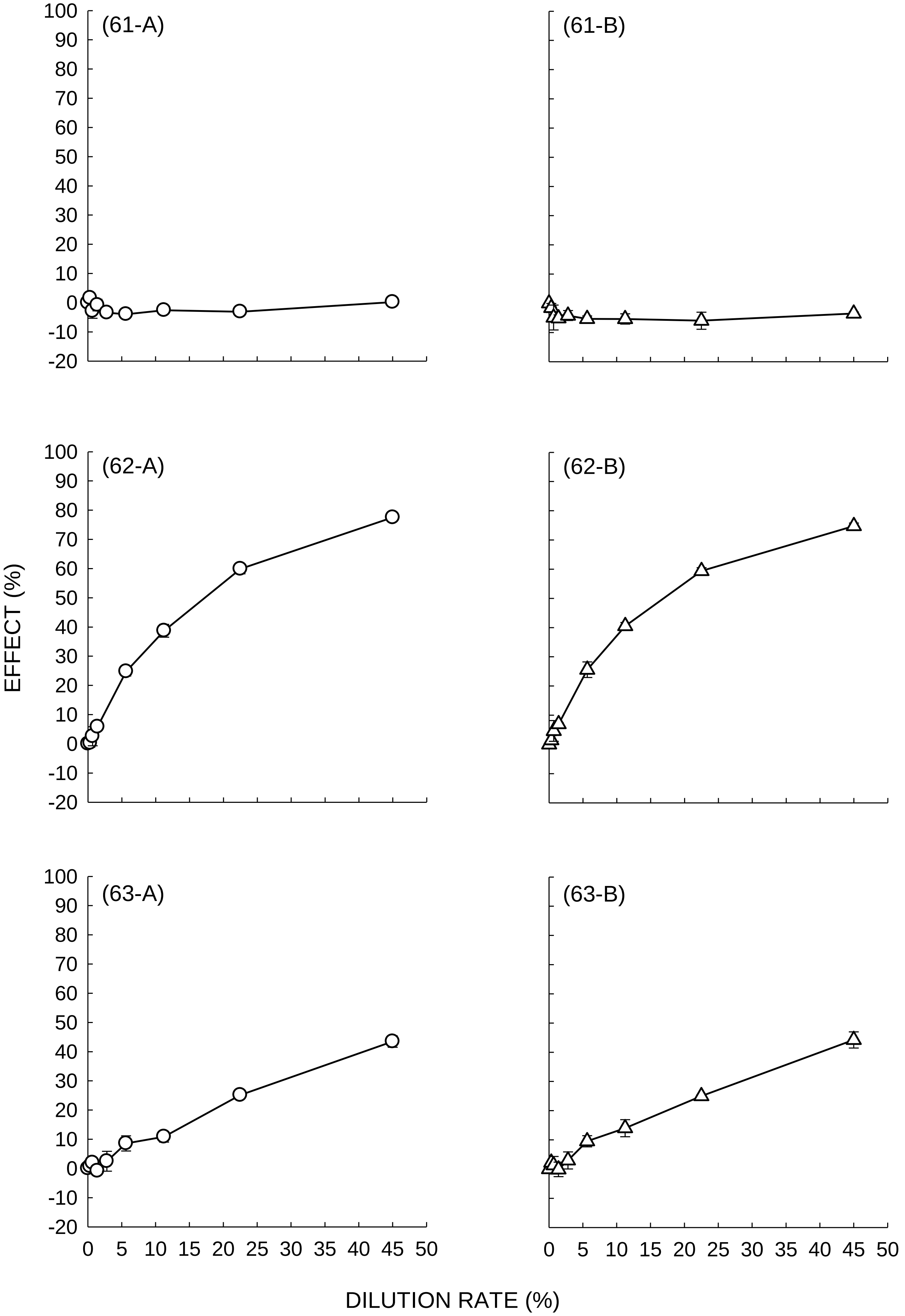
DILUTION RATE (%)



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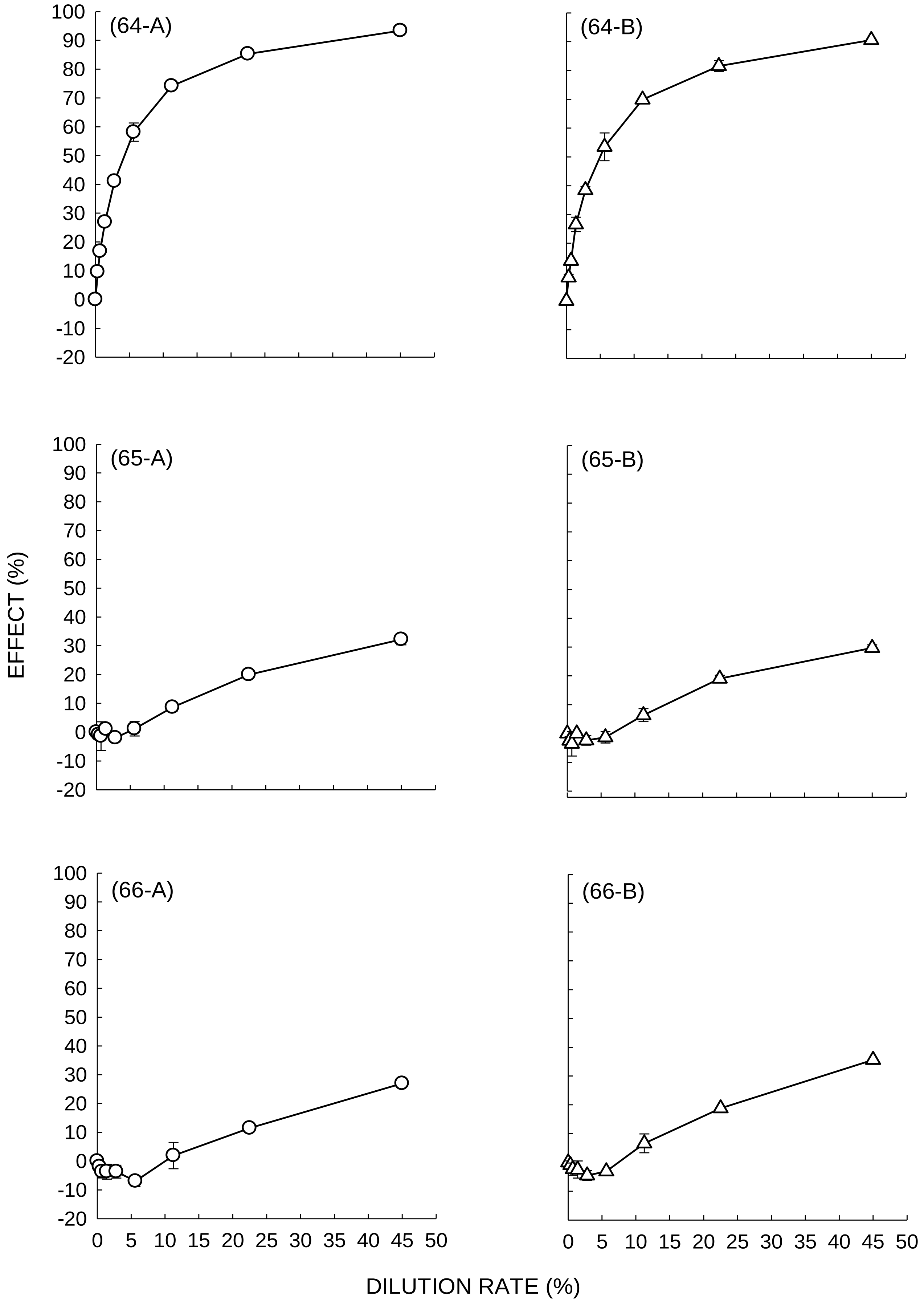

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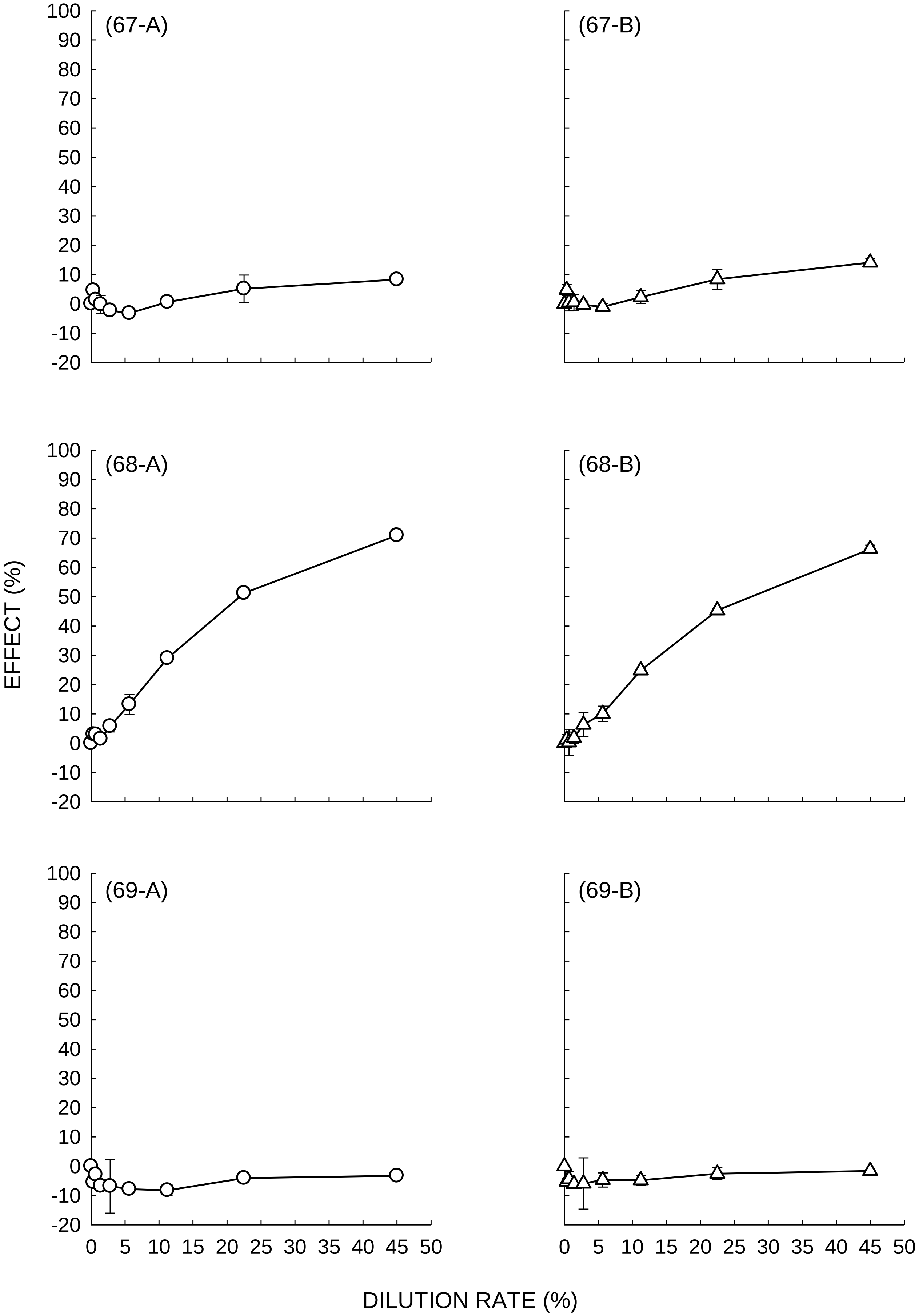
DILUTION RATE (%)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EFFECT (%)
DILUTION RATE (%)
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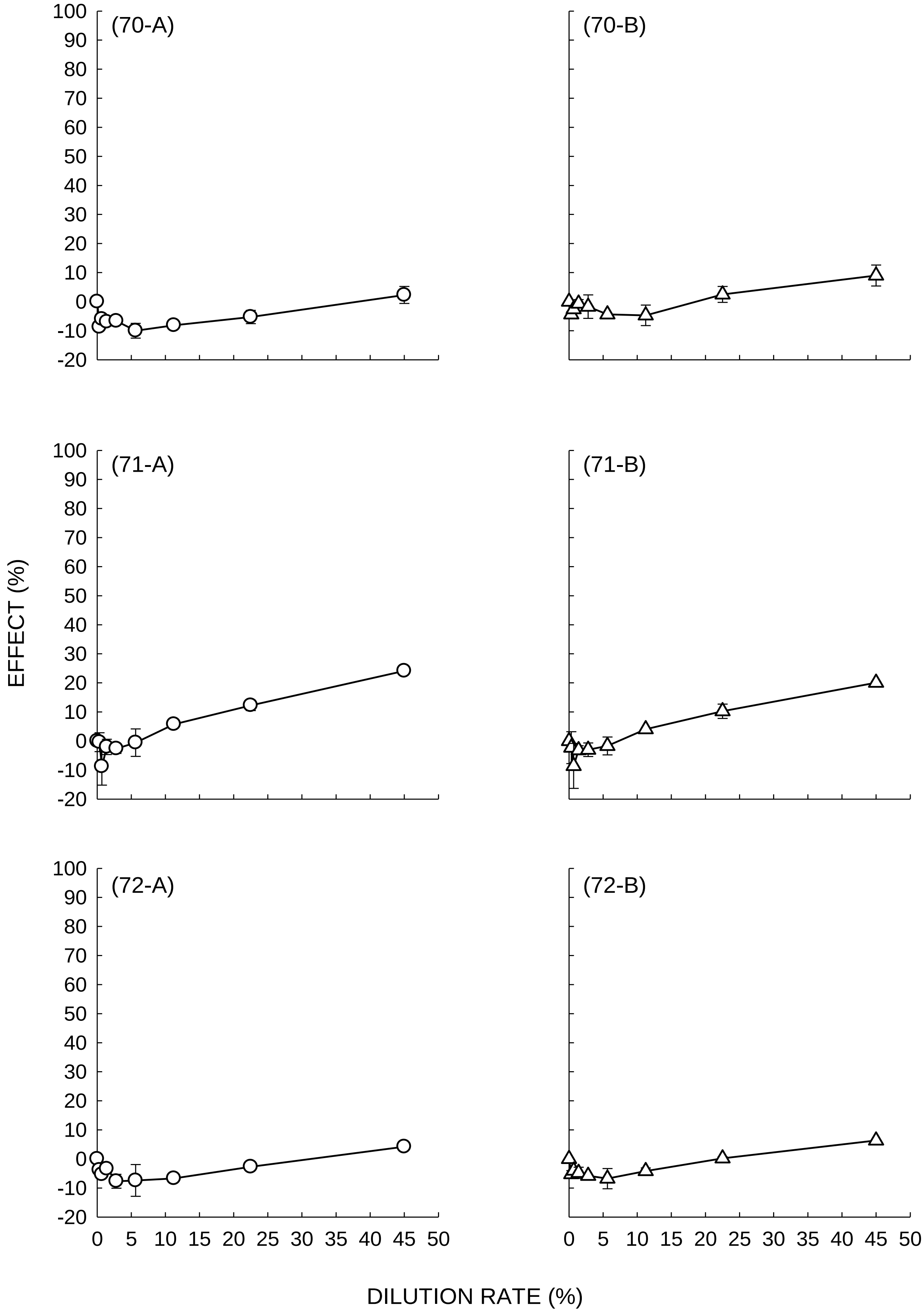
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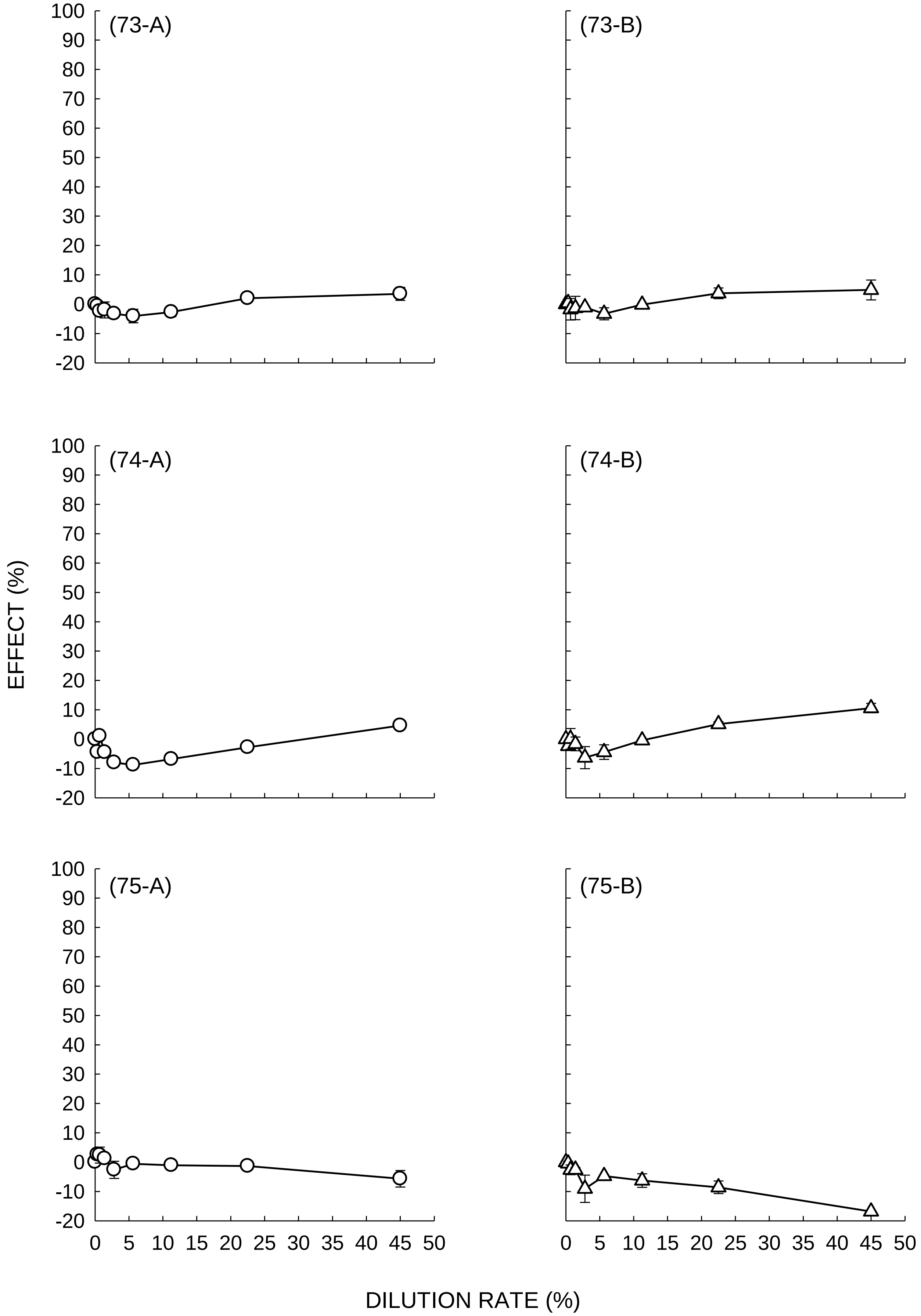
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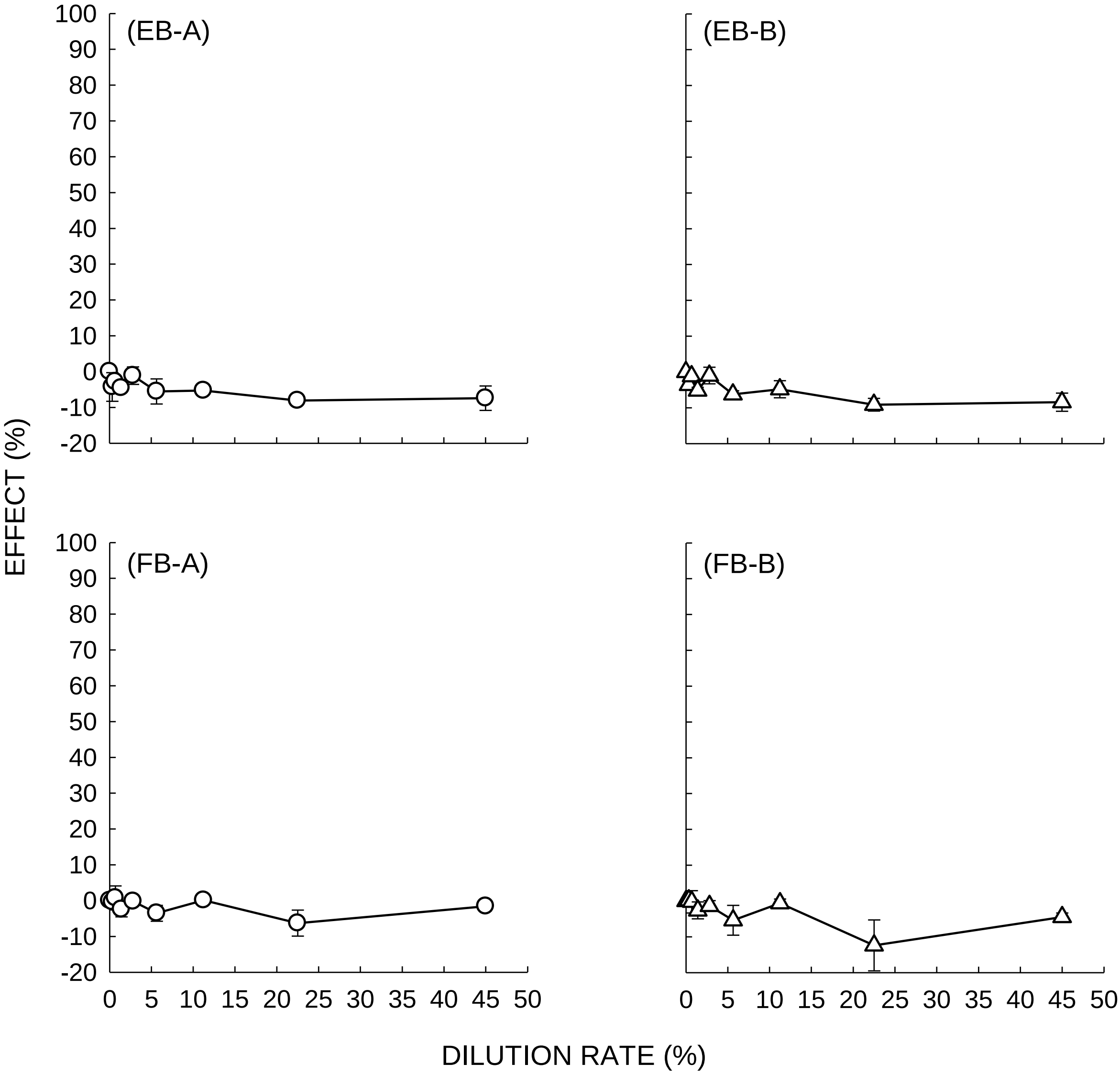
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0
-10
-20
0 5 10 15 20 25 30 35 40 45 50
DILUTION RATE (%)

APPENDIX C: ALGAE TOXICITY VALUES OF EACH CHEMICAL COLLECTED FROM ECOSAR

Table C.1. EC_{50} (algae) values of each compounds taken from ECOSAR.

Compound	Organism	Duration	End Point	Concentration (mg/L)	Reference
1,2,3-Benzotriazole	Green Algae	96h	EC_{50}	15.4000	Nabholz, 1987
1,2,5,6,9,10-Hexabromocyclododecane	Green Algae	96h	EC_{50}	0.0236	Organic Module Result
1,3-Dinitropyrene	Green Algae	96h	EC_{50}	0.1433	Organic Module Result
1,6-Dinitropyrene	Green Algae	96h	EC_{50}	1.6936	Organic Module Result
1,8-Dinitropyrene	Green Algae	96h	EC_{50}	1.6936	Organic Module Result
17-alpha-Estradiol	Green Algae	96h	EC_{50}	0.1623	Organic Module Result
17-alpha-Ethinylestradiol	Green Algae	96h	EC_{50}	0.1351	Organic Module Result
17-beta-Estradiol	Green Algae	96h	EC_{50}	0.1623	Organic Module Result
1-Hydroxyibuprofen	Green Algae	96h	EC_{50}	156.7380	Organic Module Result
2-(2-Naphthalenyl) benzothiophene	Green Algae	96h	EC_{50}	0.1725	Organic Module Result
2,2',3,3',4,4',5,5',6,6'-Decabromodiphenyl ether	Green Algae	96h	EC_{50}	0.0000	Organic Module Result
2,2',3,3',4,4',5,5',6-Nonabromodiphenyl ether	Green Algae	96h	EC_{50}	0.0001	Organic Module Result
2,2',3,4,4',5,5',6-Octabromodiphenyl ether	Green Algae	96h	EC_{50}	0.0005	Organic Module Result
2,2',3,4,4',5',6-Heptabromodiphenyl ether	Green Algae	96h	EC_{50}	0.0018	Organic Module Result
2,2',4,4',5,5'-Hexabromodiphenyl ether	Green Algae	96h	EC_{50}	0.0065	Organic Module Result
2,2',4,4',5,6'-Hexabromodiphenyl ether	Green Algae	96h	EC_{50}	0.0065	Organic Module Result
2,2',4,4'-Tetrabromodiphenyl ether	Green Algae	96h	EC_{50}	0.0843	Organic Module Result
2,3,3',4,4',5,5',6-Octabromodiphenyl ether	Green Algae	96h	EC_{50}	0.0005	Organic Module Result
2,4,4'-tribromodiphenylether	Green Algae	96h	EC_{50}	0.2916	Organic Module Result
2,4,6-Tribromophenol	Green Algae	96h	EC_{50}	0.1360	Organic Module Result
2,4-Dibromophenol	Green Algae	96h	EC_{50}	0.4098	Organic Module Result
2,4-Dihydroxybenzophenone	Green Algae	96h	EC_{50}	2.1195	Organic Module Result
2,4-Dinitrophenol	Green Algae	96h	EC_{50}	3.3740	Organic Module Result
2-Hydroxyibuprofen	Green Algae	96h	EC_{50}	485.9485	Organic Module Result
2-Mercapto-benzothiazole	Green Algae	96h	EC_{50}	0.2501	Organic Module Result
2-Methylanthraquinone	Green Algae	96h	EC_{50}	3.7870	Organic Module Result
3-Chloroaniline	Green Algae	96h	EC_{50}	4.2744	Organic Module Result
3-Nitrobenzanthrone	Green Algae	96h	EC_{50}	1.6574	Organic Module Result
4,4'-Dichlorobenzophenone	Green Algae	96h	EC_{50}	1.7968	Organic Module Result
4-Aminomethyl-benzenesulfonamide	Green Algae	96h	EC_{50}	223.9088	Organic Module Result
4-Chloroaniline	Green Algae	96h	EC_{50}	4.2744	Organic Module Result
4-Methyl-1H-benzotriazole	Green Algae	96h	EC_{50}	4.8247	Organic Module Result
4-Methylbenzylidenecamphor	Green Algae	96h	EC_{50}	0.0668	Organic Module Result
4-Nonylphenoxy acetic acid	Green Algae	96h	EC_{50}	2.2502	Organic Module Result
4-tert-Octylphenol diethoxylate	Green Algae	96h	EC_{50}	1.6522	Organic Module Result

Table C.1. EC_{50} (algae) values of each compounds taken from ECOSAR (continued).

Compound	Organism	Duration	End Point	Concentration (mg/L)	Reference
4-tert-Octylphenol monoethoxylate	Green Algae	96h	EC_{50}	0.7600	Organic Module Result
5,6-Dimethyl-1H-benzotriazole	Green Algae	96h	EC_{50}	2.8111	Organic Module Result
5-Methyl-1H-benzotriazole	Green Algae	96h	EC_{50}	4.8247	Organic Module Result
7H-Benzo(de)anthracen-7-one	Green Algae	96h	EC_{50}	1.0368	Organic Module Result
8-Hydroxyquinoline	Green Algae	96h	EC_{50}	2.9346	Organic Module Result
Acetaminophen (Paracetamol)	Green Algae	96h	EC_{50}	2.2170	Organic Module Result
Acetamiprid	Green Algae	96h	EC_{50}	1.7287	Organic Module Result
Acetochlor	Green Algae	96h	EC_{50}	0.0033	Organic Module Result
Aclonifen	Green Algae	96h	EC_{50}	1.7045	Organic Module Result
ADBI (Celestolide)	Green Algae	96h	EC_{50}	0.1623	Organic Module Result
AHDI (Phantolide)	Green Algae	96h	EC_{50}	0.1825	Organic Module Result
Alachlor	Green Algae	96h	EC_{50}	0.0016	OPP Pesticide Ecotoxicity DB
alpha-Terpineol	Green Algae	96h	EC_{50}	6.4160	Organic Module Result
Amoxicillin	Green Algae	96h	EC_{50}	366.5435	Organic Module Result
Anthracene	Green Algae	96h	EC_{50}	1.4746	Organic Module Result
ATII (Traseolide)	Green Algae	96h	EC_{50}	0.0934	Organic Module Result
Atrazine	Green Algae	96h	EC_{50}	0.1054	Organic Module Result
Atrazine-desethyl	Green Algae	96h	EC_{50}	0.3371	Organic Module Result
Azinphos-methyl	Green Algae	96h	EC_{50}	5.0269	Organic Module Result
Azithromycin	Green Algae	96h	EC_{50}	1.8738	Organic Module Result
Azoxystrobin	Green Algae	96h	EC_{50}	94.5422	Organic Module Result
Bayrepel	Green Algae	96h	EC_{50}	0.3086	Organic Module Result
Banzaldehyde,(phenylmethylene)hydrazone	Green Algae	96h	EC_{50}	0.1746	Organic Module Result
Benzenesulfonamide	Green Algae	96h	EC_{50}	55.0165	Organic Module Result
Benzo[a]anthracene	Green Algae	96h	EC_{50}	0.2898	Organic Module Result
Benzo[a]pyrene	Green Algae	96h	EC_{50}	0.1255	Organic Module Result
Benzo[b]fluoranthene	Green Algae	96h	EC_{50}	0.1255	Organic Module Result
Benzo[ghi]perylene	Green Algae	96h	EC_{50}	0.0538	Organic Module Result
Benzo[k]fluoranthene	Green Algae	96h	EC_{50}	0.1255	Organic Module Result
Benzothiazole	Green Algae	96h	EC_{50}	35.8794	Organic Module Result
Benzylamine	Green Algae	96h	EC_{50}	9.1995	Organic Module Result
Benzyldimethyldodecylammonium	Green Algae	96h	EC_{50}	1.1104	Organic Module Result
Benzyldimethylhexadecylammonium	Green Algae	96h	EC_{50}	0.0515	Organic Module Result
Benzyldimethyltetradecylammonium	Green Algae	96h	EC_{50}	0.2270	Organic Module Result
Benzyltrimethylammonium	Green Algae	96h	EC_{50}	2692.8047	Organic Module Result
Bifenox	Green Algae	96h	EC_{50}	1.2662	Organic Module Result
Bisphenol-A	Green Algae	96h	EC_{50}	2.7000	Alexander et al., 1988
Boisvelone / Iso-Esuper	Green Algae	96h	EC_{50}	0.5091	Organic Module Result
Boscalid	Green Algae	96h	EC_{50}	0.6627	Organic Module Result
Buprofezin	Green Algae	96h	EC_{50}	2.7297	Organic Module Result
Butylmethoxydibenzoylmethane	Green Algae	96h	EC_{50}	0.2619	Organic Module Result
Cadusafos	Green Algae	96h	EC_{50}	1.3287	Organic Module Result

Table C.1. EC_{50} (algae) values of each compounds taken from ECOSAR (continued).

Compound	Organism	Duration	End Point	Concentration (mg/L)	Reference
Carbazole	Green Algae	96h	EC_{50}	8.1697	Organic Module Result
Carbendazim	Green Algae	96h	EC_{50}	0.3515	Organic Module Result
Carbofuran	Green Algae	96h	EC_{50}	2.5888	Organic Module Result
Chloramphenicol	Green Algae	96h	EC_{50}	185.3083	Organic Module Result
Chlorfenvinphos	Green Algae	96h	EC_{50}	1.3432	Organic Module Result
Chloridazon	Green Algae	96h	EC_{50}	1.4080	Organic Module Result
Chlorpyrifos	Green Algae	96h	EC_{50}	0.2607	Organic Module Result
Chlorsulfuron	Green Algae	96h	EC_{50}	0.1291	Organic Module Result
Ciprofloxacin	Green Algae	96h	EC_{50}	1621.6285	Organic Module Result
Clarithromycin	Green Algae	96h	EC_{50}	2.0813	Organic Module Result
Clofentezine	Green Algae	96h	EC_{50}	34.2748	Organic Module Result
Clothianidin	Green Algae	96h	EC_{50}	64.0000	OPP Pesticide Ecotoxicity DB
Cybutryne	Green Algae	96h	EC_{50}	0.0013	OPP Pesticide Ecotoxicity DB
Cyclopentadecanolide	Green Algae	96h	EC_{50}	0.0354	Organic Module Result
Cypermethrin	Green Algae	96h	EC_{50}	0.0429	Organic Module Result
Cyprodinil	Green Algae	96h	EC_{50}	3.3033	Organic Module Result
Cyromazine	Green Algae	96h	EC_{50}	1.2768	Organic Module Result
Damascone	Green Algae	96h	EC_{50}	0.8281	Organic Module Result
Di(2- ethylhexyl)phthalate	Green Algae	96h	EC_{50}	0.0016	Organic Module Result
Diazinon	Green Algae	96h	EC_{50}	1.3725	Organic Module Result
Dichlorvos	Green Algae	96h	EC_{50}	200734.9500	Organic Module Result
Dicloxacillin	Green Algae	96h	EC_{50}	11.0730	Organic Module Result
Dicyclohexylamine	Green Algae	96h	EC_{50}	0.0729	Organic Module Result
Difenoconazole	Green Algae	96h	EC_{50}	0.3000	OPP Pesticide Ecotoxicity DB
Dimethoate	Green Algae	96h	EC_{50}	48.7586	Organic Module Result
Dimethomorph	Green Algae	96h	EC_{50}	0.3803	Organic Module Result
Diphenylamine	Green Algae	96h	EC_{50}	7.5082	Organic Module Result
Diuron	Green Algae	96h	EC_{50}	0.0024	OPP Pesticide Ecotoxicity DB
Dodecyl sulfate	Green Algae	96h	EC_{50}	47.3000	Organic Module Result
Doxycycline	Green Algae	96h	EC_{50}	1491.0856	Organic Module Result
Drometrizole	Green Algae	96h	EC_{50}	1.8175	Organic Module Result
Epoxiconazole	Green Algae	96h	EC_{50}	5.8359	Organic Module Result
Erythromycin	Green Algae	96h	EC_{50}	6.3693	Organic Module Result
Ethofumesate	Green Algae	96h	EC_{50}	8.0605	Organic Module Result
Ethoprophos	Green Algae	96h	EC_{50}	4.5698	Organic Module Result
Ethyl paraben	Green Algae	96h	EC_{50}	8.9610	Organic Module Result
Ethylhexylmethoxycinnamate	Green Algae	96h	EC_{50}	0.0754	Organic Module Result
Fenamiphos	Green Algae	96h	EC_{50}	4.4722	Organic Module Result
Fenarimol	Green Algae	96h	EC_{50}	2.7717	Organic Module Result
Fenpropimorph	Green Algae	96h	EC_{50}	0.3200	OPP Pesticide Ecotoxicity DB
Fenthion	Green Algae	96h	EC_{50}	1.1000	OPP Pesticide Ecotoxicity DB
Fluopyram	Green Algae	96h	EC_{50}	0.2493	Organic Module Result

Table C.1. EC_{50} (algae) values of each compounds taken from ECOSAR (continued).

Compound	Organism	Duration	End Point	Concentration (mg/L)	Reference
Fluoranthene	Green Algae	96h	EC_{50}	0.6555	Organic Module Result
Fluquinconazole	Green Algae	96h	EC_{50}	1.0652	Organic Module Result
Flutolanil	Green Algae	96h	EC_{50}	0.2456	Green Algae
Flutriafol	Green Algae	96h	EC_{50}	14.0859	Organic Module Result
Fosthiazate	Green Algae	96h	EC_{50}	1507.0903	Organic Module Result
Galaxolide	Green Algae	96h	EC_{50}	0.1010	Organic Module Result
g-Methylionone	Green Algae	96h	EC_{50}	0.4071	Organic Module Result
Hexa(methoxymethyl)melamine	Green Algae	96h	EC_{50}	0.8722	Organic Module Result
Hexachlorobenzene	Green Algae	96h	EC_{50}	0.2106	Organic Module Result
Hexaconazole	Green Algae	96h	EC_{50}	2.4472	Organic Module Result
Hexylcinnamaldehyde	Green Algae	96h	EC_{50}	0.8955	Organic Module Result
Hexythiazox	Green Algae	96h	EC_{50}	0.0520	Organic Module Result
Homosalate	Green Algae	96h	EC_{50}	0.0381	Organic Module Result
Imazalil	Green Algae	96h	EC_{50}	1.8177	Organic Module Result
Imazamox	Green Algae	96h	EC_{50}	263.6154	Organic Module Result
Imidacloprid	Green Algae	96h	EC_{50}	50.6581	Organic Module Result
Indeno[1,2,3-cd]pyrene	Green Algae	96h	EC_{50}	0.0538	Organic Module Result
Isobutyl paraben	Green Algae	96h	EC_{50}	2.4247	Organic Module Result
Isoproturon	Green Algae	96h	EC_{50}	0.1353	Organic Module Result
Lenacil	Green Algae	96h	EC_{50}	0.0209	Organic Module Result
Linuron	Green Algae	96h	EC_{50}	0.1539	Organic Module Result
Malathion	Green Algae	96h	EC_{50}	24.5822	Organic Module Result
Mandipropamid	Green Algae	96h	EC_{50}	6.4468	Organic Module Result
Mepiquat chloride	Green Algae	96h	EC_{50}	4662.0747	Organic Module Result
Mesotrione	Green Algae	96h	EC_{50}	1.9000	OPP Pesticide Ecotoxicity DB
Metalaxyl	Green Algae	96h	EC_{50}	14.5298	Organic Module Result
Methamidophos	Green Algae	96h	EC_{50}	1856.9369	Organic Module Result
Methidathion	Green Algae	96h	EC_{50}	1.2244	Organic Module Result
Methomyl	Green Algae	96h	EC_{50}	0.4542	Organic Module Result
Methoxyfenozide	Green Algae	96h	EC_{50}	0.5330	Organic Module Result
Methyl -iso-propylcyclohexenone	Green Algae	96h	EC_{50}	8.1704	Organic Module Result
Methyl paraben	Green Algae	96h	EC_{50}	18.0918	Organic Module Result
Methyldihydrojasmonate	Green Algae	96h	EC_{50}	5.5693	Organic Module Result
Methylsalicylate	Green Algae	96h	EC_{50}	6.8089	Organic Module Result
Metolachlor	Green Algae	96h	EC_{50}	0.0100	OPP Pesticide Ecotoxicity DB
Metrafenone	Green Algae	96h	EC_{50}	1.8520	Organic Module Result
Microcystin-LR	Green Algae	96h	EC_{50}	24.2752	Organic Module Result
Microcystin-RR	Green Algae	96h	EC_{50}	91.0022	Organic Module Result
Microcystin-YR	Green Algae	96h	EC_{50}	28.0206	Organic Module Result
Molinate	Green Algae	96h	EC_{50}	0.2200	OPP Pesticide Ecotoxicity DB
Monocrotophos	Green Algae	96h	EC_{50}	1083.2916	Organic Module Result
Musk ambrette	Green Algae	96h	EC_{50}	0.1875	Organic Module Result

Table C.1. EC_{50} (algae) values of each compounds taken from ECOSAR (continued).

Compound	Organism	Duration	End Point	Concentration (mg/L)	Reference
Musk ketone	Green Algae	96h	EC_{50}	0.1807	Organic Module Result
Musk xylene	Green Algae	96h	EC_{50}	0.1618	Organic Module Result
Myclobutanil	Green Algae	96h	EC_{50}	0.9626	Organic Module Result
N,N-Diethyl-m-toluamide	Green Algae	96h	EC_{50}	4.4838	Organic Module Result
N-Benzyldimethylamine	Green Algae	96h	EC_{50}	3.8588	Organic Module Result
N-Benzylmethylamine	Green Algae	96h	EC_{50}	4.8762	Organic Module Result
N-Ethyl-2-tolysulfonamide	Green Algae	96h	EC_{50}	8.0880	Organic Module Result
N-methyl aniline	Green Algae	96h	EC_{50}	67.8688	Organic Module Result
Nonylphenol diethoxylate	Green Algae	96h	EC_{50}	0.5553	Organic Module Result
Norfloxacin	Green Algae	96h	EC_{50}	2567.4946	Organic Module Result
N-phenyl-2-napthylamine	Green Algae	96h	EC_{50}	1.4930	Organic Module Result
Ofloxacin	Green Algae	96h	EC_{50}	2444.5432	Organic Module Result
Omethoate	Green Algae	96h	EC_{50}	2242.2551	Organic Module Result
Oxadiazon	Green Algae	96h	EC_{50}	0.2413	Organic Module Result
Oxadixyl	Green Algae	96h	EC_{50}	1.2440	Organic Module Result
Oxybenzone	Green Algae	96h	EC_{50}	0.2595	Organic Module Result
Penconazole	Green Algae	96h	EC_{50}	0.3276	Organic Module Result
Pendimethalin	Green Algae	96h	EC_{50}	0.1104	Organic Module Result
Pentachlorobenzene	Green Algae	96h	EC_{50}	0.5172	Organic Module Result
Pinoxaden	Green Algae	96h	EC_{50}	0.5434	Organic Module Result
Piperonylbutoxide	No available data				
Pirimicarb	Green Algae	96h	EC_{50}	8.0429	Organic Module Result
Polychlorinated biphenyls	Green Algae	96h	EC_{50}	0.0160	Organic Module Result
Prochloraz	Green Algae	96h	EC_{50}	0.1923	Organic Module Result
Prometryn	Green Algae	96h	EC_{50}	0.0374	Organic Module Result
Propazine	Green Algae	96h	EC_{50}	0.0665	Organic Module Result
Propetamphos	Green Algae	96h	EC_{50}	2.9397	Organic Module Result
Propiconazole	Green Algae	96h	EC_{50}	0.7369	Organic Module Result
Propyl paraben	Green Algae	96h	EC_{50}	4.4068	Organic Module Result
Prothioconazole	Green Algae	96h	EC_{50}	0.4626	Organic Module Result
Pyraclostrobin	Green Algae	96h	EC_{50}	0.2156	Organic Module Result
Pyridaben	Green Algae	96h	EC_{50}	0.1786	Organic Module Result
Pyrimethanil	Green Algae	96h	EC_{50}	10.3945	Organic Module Result
Pyriproxyfen	Green Algae	96h	EC_{50}	0.3916	Organic Module Result
Quinalphos	Green Algae	96h	EC_{50}	4.4582	Organic Module Result
Quinoxyfen	Green Algae	96h	EC_{50}	0.2996	Organic Module Result
Simazine	Green Algae	96h	EC_{50}	0.1664	Organic Module Result
Spiroxamine	Green Algae	96h	EC_{50}	0.0050	OPP Pesticide Ecotoxicity DB
Sulfamethoxazole	Green Algae	96h	EC_{50}	21.8199	Organic Module Result
Tebuconazole	Green Algae	96h	EC_{50}	0.8708	Organic Module Result
Terbuthylazine	Green Algae	96h	EC_{50}	0.0636	Organic Module Result
Terbutryn	Green Algae	96h	EC_{50}	0.0358	Organic Module Result

Table C.1. EC_{50} (algae) values of each compounds taken from ECOSAR (continued).

Compound	Organism	Duration	End Point	Concentration (mg/L)	Reference
Tetraacetylethylenediamine	Green Algae	96h	EC_{50}	40.7058	Organic Module Result
Tetrabromobisphenol A	Green Algae	96h	EC_{50}	0.1984	Organic Module Result
Tetracycline	Green Algae	96h	EC_{50}	1885.5634	Organic Module Result
Thiacloprid	Green Algae	96h	EC_{50}	2.7716	Organic Module Result
Thiophanate-methyl	Green Algae	96h	EC_{50}	0.7237	Organic Module Result
Thioridazine	Green Algae	96h	EC_{50}	1.3234	Organic Module Result
Tolfenpyrad	Green Algae	96h	EC_{50}	0.0221	Organic Module Result
Tonalide	Green Algae	96h	EC_{50}	0.0882	Organic Module Result
Triasulfuron	Green Algae	96h	EC_{50}	0.3137	Organic Module Result
Triazophos	Green Algae	96h	EC_{50}	1.5997	Organic Module Result
Triclosan	Green Algae	96h	EC_{50}	0.0567	Organic Module Result
Trifloxystrobin	Green Algae	96h	EC_{50}	0.0042	Organic Module Result
Trifluralin	Green Algae	96h	EC_{50}	0.0856	Organic Module Result
Trimethoprim	Green Algae	96h	EC_{50}	20.7447	Organic Module Result
Triphenylphosphineoxide			No available data		
Triphenyltin			No available data		
Tris(1-chloro-2-propanyl) phosphate	Green Algae	96h	EC_{50}	9.2957	Organic Module Result
Tris(2-butoxyethyl) phosphate	Green Algae	96h	EC_{50}	9.4937	Organic Module Result
Vancomycin	Green Algae	96h	EC_{50}	27863.9100	Organic Module Result