APPENDIX C

Assessment of the Effectiveness of Secondary Wastewater Treatment Technologies to Remove Chemicals of Emerging Concern: A Review

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Summary

Pesticides, pharmaceuticals, personal care products, hormones, surfactants, synthetic musks, and other trace organics are commonly present at part-per-trillion levels in surface waters of the United States. There is a growing body of data suggesting that secondary wastewater treatment (i) is an effective barrier to release of many trace organics, and (ii) can be tuned to a degree to increase through-plant removals of these compounds. Evidence is present in the monitoring records at a great many wastewater treatment plants and in the results of pilot and laboratory-scale studies. Despite significant differences in experimental design and operational conditions, rigorous analysis of that body of data can establish the potential efficacy and limits of conventional treatment for management of trace organics. As a minimum, such an analysis will identify areas in which existing data do not support rational selection of treatment processes for protection of human and environmental health. Here we present the results of a literature review and statistical analysis of removals of chemicals of emerging concern (CECs) during conventional wastewater treatment. Process-dependent attenuations are examined for the 42 CECs most frequently measured and reported. Biological treatment processes contributing to the review include conventional activated sludge, membrane bioreactors, trickling filters, sequencing batch reactors and lagoons. Also summarized are compound-specific physical characteristics and biodegradability data that are potential determinants of removal, so that the efficiencies of conventional treatment for elimination of a great many compounds that have not been widely studied can be anticipated.

Keywords: chemicals of emerging concern; trace organics; microconstituents; wastewater treatment; activated sludge; membrane bioreactor.

1. Introduction

Trace organic chemicals present in effluents from conventional wastewater treatment plants include pharmaceuticals, personal care products, endocrine disrupting compounds, and other household and personal use organics (Kolpin et al. 2002). When discharged to surface waters, residual trace organics in treated municipal wastewater can affect aquatic health. Endocrine disrupting compounds are particularly well studied in this regard (Kidd et al. 2007, and references therein). There is a well developed body of knowledge regarding methods for measuring trace organics at part-per-trillion concentrations, leading to a rapidly expanding database regarding the presence of these compounds in surface waters and, to a lesser degree, their respective fates during wastewater treatment. Trace organics that are unregulated and which have an uncertain impact on ecosystem or human health due to chronic exposures are herein collectively called "chemicals of emerging concern" (CECs).

Relatively little is known regarding the attenuation of CECs following their release into the environment. However, several noteworthy ecological effects have been linked to aqueous-phase CECs, particularly among continuously exposed fish. Environmental and especially human health effects of CEC exposures are particularly difficult to study, due in part to the simultaneous presence of multiple CECs in waters affected by municipal effluent discharge. Uncertainties regarding chemical toxicity encourage precautionary strategies relative to wastewater treatment and water reuse. The informational and regulatory void in this area interferes with water supply planning, particularly in water-short areas such as the American Southwest, where water reuse is frequently requisite to water supply sustainability objectives.

Although wastewater treatment plants (WWTPs) were not specifically designed to remove CECs, physicochemical and biological processes that are part of current technologies contribute, with various degrees of success, to CEC removal during wastewater treatment. In a general sense, it is important to attribute the removal of CECs from wastewater to physical partitioning among liquid, gas and solid phases vis-a-vis biochemical transformation. Volatile CECs might be stripped into a gas phase contacting the wastewater in aerobic reactors. Similarly, hydrophobic CECs might partition to the sludge phase and leave the plant with biosolids. Alternatively, biochemical transformation might destroy CECs or produce potentially deleterious reaction by-products.

Here we summarize data for removal of CECs during conventional municipal wastewater treatment. We have arbitrarily confined our search to peer reviewed publications and agency reports from the last ten years. Older data appear if included in recent literature reviews. CECs selected for review include pharmaceuticals, personal care products, natural and synthetic hormones, alkylphenols and alkylphenol ethoxylates, pesticides, synthetic musks, perfluorinated surfactants and plastic-manufacture additives (e.g. plasticizers). The study includes information from full-scale plants, pilot-scale studies and laboratory experiments on removal efficiencies for CECs. For user convenience, available data were organized and classified in a Microsoft Access database. A total of 658 references that include reports from professional organizations and government agencies, peer-reviewed publications and literature reviews form the basis of this work. Forty-two compounds provided an adequate data set for statistical analysis of removal efficiency.

2. Previous work

Over the last ten years, interest has increased substantially in the occurrence, fate and transport of CECs in the environment, as reflected by numerous surveys of natural water bodies, drinking water sources and wastewater treatment facilities. A subset of these works addresses aqueous-phase removal efficiencies of CECs in WWTPs. In this section, we will summarize recent attempts to review and analyze the effectiveness of WWTPs for CEC management and generalize, if possible, regarding removals of specific families of compounds. A more extensive list of sources is provided in the Microsoft Access database derived from this work.

The US EPA and the Water Environment Research Foundation (WERF) have reviewed CEC occurrence in wastewater and WWTP removal efficiencies. The EPA measured CECs throughout nine WWTPs (US EPA 2009). CECs sampled included pharmaceuticals and personal care products, steroids and hormones, alkylphenols and alkylphenol ethoxylates, bisphenol A (BPA), polybrominated diphenyl ethers (PBDEs) and pesticides. A large fraction of the compounds were present at multiple WWTPs. However, the objective of the study was not to assess compound-specific removal efficiencies, and the authors cautioned that the data gathered were insufficient for that purpose. More recently, EPA (2010) summarized influent-to-

effluent removals for the same classes of CECs plus polynuclear aromatic hydrocarbons, plasticizers and flame retardants other than PBDEs. A total of 246 compounds were surveyed using 88 references spanning the period 2003-2008, and a database with removal efficiencies was compiled. A detailed analysis was presented for a subset of 16 compounds. The objective of that work was similar to our own, but we considered additional sources of information, expanded the reporting period and included a greater number of compounds in our survey. The EPA included tertiary treatment methods such as advanced oxidation and activated carbon treatment processes, which are not considered in the present work.

Stephenson and Oppenheimer (2007) (WERF report) surveyed WWTP removal efficiencies for 20 pharmaceuticals and personal care products (PPCPs) to assess the effect of solids retention time (SRT) on removal efficiencies. SRT ranged from 0.5 to 30 days at the six WWTPs studied. Although data on removal and occurrence were widely distributed, specific conclusions could be reached regarding relative, compound-specific removal efficiencies. For example, galaxolide was widely distributed, and its removal efficiency was generally low. In yet another survey, PPCPs were included in the more general category of household chemicals (Drewes et al. 2009). Twenty-six compounds were selected, of which twenty were present in all wastewater samples analyzed. These included all the PPCPs surveyed. Compound-specific removals during conventional activated sludge and MBR processes varied significantly.

The reviews of Halling-Sorensen et al. (1998) and Heberer et al. (2002) covered the occurrence, fate and effects of pharmaceuticals in the environment, illustrating the limited ability of conventional treatment methods to destroy pharmaceuticals and the widespread presence of these compounds in both natural and drinking waters. Following those publications, monitoring studies throughout the world have shown that PPCPs are universally present in secondary effluents from WWTPs (Clara et al. 2005, Lindqvist et al. 2005, Tauxe-Wuersch et al. 2005, Yu et al. 2009, Lishman et al. 2006, Santos et al. 2009, Jones et al. 2007, Miege et al. 2009, Ying et al. 2008, Sui et al. 2010, Sim et al. 2010, among others).

Recently, Miege et al. (2009) summarized data from 117 publications covering the occurrence and removal of 184 PPCPs at WWTPs. The frequency of quantification of PPCPs in influent and effluent was above 90% for the majority of the compounds considered. Hormones exhibited the highest removal efficiencies (70-99 %). Certain drugs such as carbamazepine (<10%), clofibric

acid diclofenac (<25%) were considerably more persistent. The authors also explored the relative efficiencies of alternative secondary treatment processes. Nitrifying activated sludge and membrane bioreactors were identified as promising technologies for PPCP removal.

The most commonly cited ecological impacts from wastewater CECs result from disruption of endocrine system function among continuously exposed aquatic life (e.g. Taylor et al. 2005, Kidd et al. 2007). For that reason, WWTP removal of estrogens and estrogen mimics has been a common research focus (Teske and Arnold 2008, and references therein.) The compounds most frequently identified as endocrine disrupting compounds (EDCs) in wastewater include natural hormones (17β-estradiol) and related metabolites (estrone and estriol). Estrogen mimics include 17α-ethinylestradiol (EE2, an oral contraceptive) and the alkylphenol polyethoxylates (APEs; a class of surfactants) and their derivatives, of which nonylphenol and octylphenol are the most important. These compounds are either measured individually, or bioassays are used to assess whole-sample estrogenic activity. Drewes et al. (2006) combined direct chemical analysis for EDCs and bioassays to determine the effectiveness of WWTP treatment. They concluded that secondary treatment with nitrification/denitrification was more effective than conventional secondary treatment alone for destruction of estrogens and reduction of estrogenic activity.

The widespread presence of APEs in United States surface waters (Kolpin et al. 2002) suggests that they may contribute to intersex characteristics (mild hermaphrodism) that are now frequently observed in natural waters affected by the discharge of treated municipal wastewater. The estrogenic potencies of APEs are several orders of magnitude below those of natural estrogens and birth control agents like EE2 (Teske and Arnold 2008). Nevertheless, the concentration of these compounds in the environment can be orders of magnitude greater than those of the hormones. Petrovic et al. (2002) studied the occurrence of APEs and both natural and synthetic steroids in wastewater treatment facilities, sludge samples, river water and sediments in Spain, concluding that "NP, estriol, and estrone, detected in water, could be responsible for the increased VTG [vitellogenin] observed in male carps" in two rivers studied, thereby providing a link between wastewater effluent and endocrine disrupter effects in fish. Cespedes et al. (2008) found that relatively short chain APEs partition readily on organic-rich particulate matter such as sludges produced during wastewater treatment, while longer chain nonylphenol ethoxylates were relatively stable in the aqueous phase and therefore present at higher concentrations in treated

wastewater. Removal efficiencies for APEs varied from 37 to 90%, depending on the treatment process employed. The *Alkylphenol Ethoxylates Research Council* has reviewed APE removals during full-scale wastewater treatment and bench-scale simulations (Melcer et al. 2007). Their scope included removal by both biological treatment (activated sludge, membrane bioreactor) and physical-chemical processes such as nanofiltration, microfiltration and advanced oxidation processes.

Despite their importance in agricultural settings and their potential health effects (Müller et al. 2007) data regarding the removal of pesticides in conventional WWTPs are surprisingly sparse. Use of lagoons and constructed wetlands for management of pesticides is relatively common, however. In this context, Braskerud and Haarstad (2003) reviewed the relationship between retention time and pesticide removal in constructed wetlands. Factors contributing to pesticide removal efficiency included compound hydrophobicity (adsorption on organic matter) and biodegradability (for the nitrogen-rich pesticides).

Synthetic musk fragrances are commonly used in the cosmetic, detergent and perfume industries. They reach μg/L-level concentrations in municipal wastewater (Lee and Lee 2010). These chemicals are usually classified as nitro-aromatics (NMs) or polycyclic musks (PCMs). The use of NMs is declining due to recent concerns regarding their toxicity in humans. However, PCM use has increased. NMs such as musk ketone and musk xylene and PCMs such as galaxolide (HHCB) and tonalide® (AHTN) represent more than 12% and 85% (respectively) of the total global consumption of synthetic musks (Heberer 2002, Lee et al. 2010).

Perfluorinated compounds (PFCs) such as perfluorooctanesulfonate (PFOS) and perfluorooctanoic acid (PFOA) are recalcitrant in the environment. Their main sources are WWTP effluents and urban runoff (Murakami et al. 2009). PFOS and PFOA are ubiquitous in United States municipal wastewaters. Reported concentrations in WWTP effluents range from 5.3-130 ng/L (PFOS) and 2.5-58 ng/L, (PFOA; Schultz et al. 2006a). It has been suggested that biodegradation of precursor compounds such as fluorotelomer sulfonates or fluorotelomer alcohols produce PFOS and PFOA during wastewater treatment (Schultz et al. 2006a,b). There is no evidence that PFOS and PFOA transformations can be encouraged by selection of specific conventional wastewater treatment processes or manipulation of operational conditions. PFOS

in particular can be removed from water via adsorption on activated carbon (personal communication, DuPont 2011).

The manufacture, use and disposal of plastics inevitably release a great variety of chemicals into the environment. Among the chemicals used to produce plastics, plasticizers such as di-(2-ethylhexyl) phthalate (DEHP) and di-(2-ethylhexyl) adipate (DEHA) are among the most common in natural waters and municipal wastewaters (Roslev et al. 2007). Plasticizers are added to plastics to provide flexibility. They are also used in the production of paints, glues, lubricants, pharmaceuticals, cosmetics, and pesticides. Most plasticizers are not chemically bound within the cross-linked polymer product, allowing them to escape into the environment during manufacture, product use, and following product disposal. WWTP effluent and urban runoff are major environmental sources of phthalates.

2. Methodology

CECs were selected for review base on the *Review of Chemicals of Emerging Concern and Analysis of Environmental Exposures in the Great Lakes Basin*, submitted to the International Joint Commission (Klečka et al. 2010). This list, which includes more than 300 compounds, was the starting point in our search for removal data regarding the performances of conventional wastewater treatment processes.

Our survey of CEC removal information was arbitrarily constrained by publication date (2000-2010) and treatment process selection—activated sludge, membrane bioreactors, sequencing batch reactors and lagoons. The Science Citation Index was the primary source for peer-reviewed articles. References from and citations to the articles discovered initially were also surveyed. Additionally, reports from national and international agencies were scrutinized for data or general information about removal of CECs. These agencies or institutes include: United States Environmental Protection Agency (USEPA), Water Environmental Federation (WEF), Water Environmental Research Foundation (WERF), United States Geological Services (USGS), National Water Research Institute (NWRI), Minnesota Pollution Control Agency (MPCA), American Water Works Association (AWWA), Cooperative Research Centres (CRC Australia), European Commission Environment and Environment Canada. About 800 documents dealing

with removal of organics in WWTPs and related processes were obtained and screened for information. Screening criteria included: (i) the document should provide liquid removal (influent-to-effluent) of the compounds of interest, and (ii) a description of the process or processes applied to treat the wastewater and the operating conditions should be provided. Sources that survive an initial screening step contained both (i) influent-to-effluent removal data for one or more CEC and (ii) descriptions of treatment processes and operating conditions. Documents based only in the occurrence of CECs were not further considered.

Aqueous phase removals were calculated from:

$$R = \frac{C_{influent} - C_{effluent}}{C_{influent}} x100\% \quad (1)$$

A Microsoft Access database was developed to compile and organize CEC removal data. The database was organized by compound, type of treatment and scale (laboratory, pilot or full). When sufficient information was available, database entries included (i) contemporary treatment performance data such as removal efficiencies for TOC, BOD or COD and (ii) both influent-to-effluent and overall removals compound removals. The latter accounted for contaminant mass fluxes in biosolids as well as effluent. The database also contains compound-specific (READY) biodegradability data, when available, and physical properties such as Henry's law (H) and octanol-water K_{ow} partitioning constants. Experimental values were obtained from the EPI Suites™ 4.1 software and database (EPA). When empirically determined constants were not available, EPI Suites was employed to predict values using KOWIN™ and HENRYWIN™ (Bond Contribution model). Biodegradability information was obtained using BIOWIN™ 2 and 6. BIOWIN 2 is a non-linear model that predicts the probability of "fast" biodegradation based on the fragments of the molecule and their molecular weight contribution, whereas BIOWIN 6 predicts biodegradation rate probabilities based on the OECD301C test, using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

To assist in data analysis, box-plots and cumulative probability curves were developed using OriginLab™ 8.0 software to represent distributions of compound-specific removal data. Only compounds for which sufficient activated sludge performance data are available ($n > 8$) were analyzed in this way. When sources reported more than one observation from a single facility, the average of these values was taken as a singular data point. When documents reported a range

of removals, end values of the range were taken as data points to represent worst-case performance variability. In all, 42 compounds satisfied criteria for statistical analysis. Chemical structures for these compounds are provided (Table 1), and relevant compound-specific properties are as summarized (Table 2). When possible, the removals during activated sludge, membrane bioreactor, trickling filter, sequencing batch reactor and lagoon treatments are compared. When insufficient data were available to support comparisons, results were summarized in tables instead of graphs. Compound-specific references are summarized in Appendix B.

3. Results and Discussion

3.1. Conventional Activated Sludge (CAS)

About half of the articles and reports reviewed here contain data regarding WWTP removal efficiencies of pharmaceuticals, making them the most thoroughly studied class of CECs. Twenty of the 42 compounds judged to provide an adequate database for statistical summary are pharmaceuticals. Box plot summaries of influent-to-effluent removals of prescription and non-prescription drugs during full- and pilot-scale activated sludge treatment of municipal wastewater are provided (Figures 1 and 2). Although the data are frequently scattered, the weight of evidence in the summary leads to clear conclusions in some areas and serves as a source of speculation in others. Caffeine and acetaminophen (Figure 1) are effectively removed in most conventional wastewater treatment plants. Both are removed with near 100% efficiency in well over half the treatment plants in the survey. Influent-to-effluent removals of carbamazepine and diclofenac, on the other hand, are generally poor. Roughly half the plants in the survey indicated that more than half the influent concentration of diclofenac in their influent remains in the plant effluent. Half the plants removed less than 20% of the influent concentrations of carbamazepine. Both caffeine and acetaminophen are highly biodegradable (Table 2), perhaps accounting for the efficient removal of these compounds. Removal efficiencies of diclofenac, clofibric acid and indomethacin, among others, were highly variable, suggesting that design or operating conditions can be important determinants of CEC transformation efficiencies. Coefficients of variation (the ratio of the standard deviation to the mean) for these compounds all exceed 0.5.

Reported efficiencies for removal of antibiotics during activated sludge treatment of wastewater are also highly plant specific, or at least sensitive to plant operating conditions (Figure 2). The only antibiotic with a mean removal value higher than 70% is tetracycline. Sulfamethoxazole, roxythromycin, norfloxacin and ciprofloxacin exhibit mean removal values between 50 and 70%, while sulfamerazine and trimethroprim have values below 50%. The highest coefficients of variation were obtained for sulfamerazine and erythromycin (0.75 and 0.62, respectively), while norfloxacin and tetracycline data produced values lower than 0.4. A more detailed analysis is warranted to establish operating conditions that promote CEC removal.

Removals of estrogens and estrogen mimics were generally high. Median removals efficiencies were uniformly greater than 75% (Figure 3). The greatest degree of scattering was exhibited by estrone—coefficient of variation equal to 0.37. Nevertheless, estrogen-dependent ecological effects are frequently observed among fish populations that are continuously exposed to treated wastewater. Despite relatively high removal efficiencies, human hormones probably contribute significantly to estrogenic activity in wastewater effluent. Estrone is approximately 30% as potent an estrogen as EE2, which produces measurable effects on fish populations at exposure levels of a few ng/L (Kidd et al. 2007).

The box-plots representing removal efficiencies of selected synthetic musks, triclosan, PCP, benzophenone, (a UV blocker in plastics), and DEHP (a plasticizer) indicate that polycyclic musks such as AHTN and HHCB are removed with medium to high efficiencies—mean values above 65% (Figure 4). Musk ketone, a nitro-musk, was readily removed (>90%). All the musks are classified as non biodegradable (Table 2, Balk and Ford 1999, Tas et al. 1997). However, they are relatively hydrophobic, so that observed removals could result from adsorption to sludge organics. Similarly, triclosan, which is also categorized as not (READY)-biodegradable, shows relatively high removals (median removal > 80% and 90% removal in more than 25% of plants). Triclosan remains a potential concern, however, since it is frequently present at μg/L levels in raw sewage. In addition, triclosan is hydrophobic (log K_{ow} = 4.76) and may be concentrated in sludges produced during wastewater treatment, providing another avenue for introduction into the environment when biosolids are disposed of via land application.

The plastics additives benzophenone and DEHP exhibit relatively high removal efficiencies, although based on limited sampling. Removal efficiencies of bisphenol A (BPA), a precursor

monomer of polycarbonate plastic and epoxy resins; alkylphenols and alkylphenol ethoxylates follow similar patterns (Figure 4). All have median removals from 80-85%, and near total removal is achieved in a few treatment plants. However, only the n = 1, 2 ethoxylates were included in this summary, and the simultaneous production of APs and short-chain APEs from longer-chain precursors during wastewater treatment makes data interpretation difficult. Here, negative removals, which were sometimes observed, are shown as zero-efficiencies, which may slightly distort the summaries for these compounds. The perfluorinated compounds PFOS and PFOA were poorly removed during conventional wastewater treatment. The median removal of PFOA, for example was near zero. This was to be expected since the compounds are non-biodegradable and somewhat hydrophilic (Table 2; note that, even though log K_{ow} for PFOA is relatively high, its pKa is 1, which means that it will be ionized at circumneutral pH conditions, which is different from the pH 0 condition used to determine log K_{ow}.)

A subset of the CEC data was used to produce cumulative probability distribution functions (Figures 5 and 6). In these plots, cumulative counts represent the percent of data with aqueous-phase removal efficiencies lower than the influent-to-effluent removal specified. Using caffeine as an example (Figure 5a), removal efficiencies were < 75% for only 10% of the WWTPs in the survey. Compounds that are readily removed via activated sludge processes such as caffeine, acetaminophen and ibuprofen exhibit cumulative removal patterns with upward concavity. Those that are poorly removed such as carbamazepine and clofibric acid show a downward concavity. Results can be interpreted also in terms of removal probability: the probability of removing 75% or more of the influent caffeine during conventional secondary treatment was > 90%, whereas the probability of removing 75% of the influent carbamazepine using the same processes was < 10%. When removals of specific CECs among the plants in the survey were widely and more or less uniformly distributed across the entire range of efficiencies, e.g. diclofenac and many of the antibiotics, resultant cumulative probability functions tended toward a straight line, from lower left to upper right. In a sense, these are the most interesting compounds included in the summary, since the data indicate that removals during conventional wastewater treatment may be highly sensitive to operational conditions. Examples of compounds in this category are ketoprofen (Figure 5a), diclofenac (Figure 5b), and all compounds in Figure 5c, gemfibrozil and, to some extent, clofibric acid (Figure 5d).

3.2. Membrane Bioreactors

As the large-scale deployment of MBR technology is relatively limited, there are fewer data with which to analyze CEC removal efficiencies. Data summaries (Figures 7 to 9) suggest that median CEC removals in MBRs are in general comparable to removal efficiencies in other activated sludge applications. While MBR efficiencies are modestly higher for clofibric acid and naproxen, slightly lower median removals were slightly lower for acetaminophen, diclofenac, ibuprofen and ketoprofen (Figures 1 and 7). MBR removal of carbamazepine (Figure 8) was lower but less erratic than in the comparative data set (Figure 1). For the antibiotics and bezafibrate, median performances in the MBR were slightly better than those obtained in other activated sludge reactors (Figures 8, 1 and 2). Again, MBR data are noticeably less scattered. The estrogenic compounds analyzed—BPA, *p*-nonylphenol, and the natural and metabolized hormones—were all efficiently removed in both reactor types (median removals > 80%, Figures 3, 4 and 9).

MBR removals among compounds for which the database did not support statistical analysis are also provided (Table 3). The similarity between activated sludge and MBR removals of CECs was unexpected since the performance of MBRs for removal of bulk organics and nitrogen is generally held to be superior to that of conventional activated sludge processes (Radjenovic et al. 2007). It is relatively easy to generate very long sludge ages in MBRs, allowing populations of niche microorganisms with relatively slow growth rates to be maintained.

3.3. Factors that Affect Removal Efficiencies

It is frequently held that equilibrium partitioning of organic chemicals between liquid and solid phases is governed by proportionality between the aqueous-phase concentration and concentration in organic material that contributes to the solid phase. The constant of proportionality is determined by compound-specific relative affinities for the aqueous and solid phases and is frequently represented by the octanol/water partition coefficient (K_{ow}). Using these relationships, it is possible to rationalize the sorptive removal of CECs during conventional wastewater treatment. Even when this model breaks down, it is likely that compound hydrophobicity is directly related to abiotic removal efficiency. For persistent and recalcitrant compounds, it is possible that partitioning into organic solids is the primary determinant of

through-plant removal efficiency. To test these ideas, the compound-specific cumulative probability of observing > 75% removal in facilities represented in this survey was plotted as a function of log K_{ow} (Figure 10). When the 42 compounds represented statistically in the survey were included (Figure 10a), it was difficult to find a pattern between log K_{ow} and removal efficiency. However, when the biodegradable compounds according to BIOWIN 2 (e.g. acetaminophen, estriol, caffeine nonylphenol, etc) are excluded, a better correlation between hydrophobicity and removal efficiency is apparent (Figure 10b). Compounds excluded from Figure 10b correspond to ready biodegradable and inherently biodegradable from the BIOWIN 2 calculations.

A similar analysis was carried out to investigate the importance of the quantification method used to assess compound biodegradability. Quantification of biodegradability is not an easy task due to the lack of a comprehensive literature database in the area. A comparison was performed between BIOWIN 2 and BIOWIN 6 predictions. Results are shown in Figure 11, eliminating compounds with log K_{ow} > 3.5. BIOWIN 2 gives a poor correlation with the probabilities obtained in this work. On the other hand, the dependence of removal efficiency on probability calculated with BIOWIN 6 biodegradation is evident, although data remain scattered. To refine the analysis, we selected a group of compounds for which first-order rate constants of laboratory-scale biodegradation with activated sludge have been reported (Urase and Kikuta 2005, Dickenson et al. 2010) (Figure 12). Correlation between removal efficiency and the biodegradation rate constant in the latter analysis is clear.

3.4. Comparison of Biological Treatment Alternatives

The limited number of studies available did not support extensive statistical analyses of other biological processes. Removal efficiencies for a subset of eight CECs are used to compare CEC removals observed in WWTPs using membrane bioreactors (MBR), trickling filters (TF), sequenced batch reactors (SBR) and lagoons with results from conventional activated sludge (Figure 13). Compound-specific removal efficiencies tend to be similar in all processes. For example, ibuprofen exhibits high removal efficiencies in all five processes, whereas the removal of diclofenac was modest in four of the five processes compared and low in trickling filters. The degree of variation in the data makes such comparisons less reliable.

3.5. Effects of Operating Conditions

Solids retention time (SRT) and hydraulic retention time (HRT) were used as representative parameters of the activated sludge process in order to assess the effects of operational conditions in the removal efficiency of the different chemicals. From the 42 compounds studied, only 10 chemicals (all of them pharmaceuticals), presented more than 10 data-points linking these two parameters with the removal reported. Figure 14 present an example of the dependence of removal with SRT and HRT for diclofenac and ketoprofen. No real trends can be inferred from these graphical representations. To better quantify the correlation between SRT, HRT and removal, Spearman correlation coefficients were calculated for all the available data. A correlation coefficient is a numerical measure of the strength of the relationship between two random variables. The value of correlation coefficient varies from −1 to 1. Positive value means the two variables are positive correlated, that is, the two variables vary in the same direction; while negative value indicates negative correlated. Values close to +1 or −1 reveals the two variables are highly related. Spearman correlation coefficient is a non-parametric measure that works better than other statistical correlations in detecting a non-linear relationship and for data not normally distributed. The Spearman correlation coefficients for diclofenac and ketoprofen are shown in table 4. For diclofenac, there is a slight correlation between removal and HRT and low correlation with SRT. For ketoprofen the situation is backwards, poor correlation with HRT and slight correlation with SRT. The rest of the chemicals studied (not shown) presented really poor correlation coefficients for both SRT and HRT, and some compounds present negative correlation values, which mean that the removal is more likely to decrease than to increase with increments of SRT or HRT, respectively.

4. Summary and Conclusions

Overall, the analysis indicates that biodegradability is the most important contributor to CEC removal during conventional secondary treatment processes. Perhaps this should have been anticipated. The role of hydrophobicity and physical partitioning becomes apparent only for compounds that are poorly degraded during biological processes. Compound- and process-specific data are generally scattered. Factors contributing to the scatter may include variation in operating conditions or analytical inaccuracies. At this point, statistical confidence in the results

is only assessed in terms of number of studies and degree of variation in compound-specific data. Table 2 presents the results of such an assessment, along with the probability of 75%+ removal efficiency for selected CECs. A summary of removal efficiency vs. confidence level is presented in Table 3. The classification of compounds by removal efficiency at high confidence levels (bottom row of Table 3) yields a reasonable expectancy of performance of activated sludge processes: compounds with high removal efficiency (acetaminophen, caffeine and estriol) are removed to a great extent in these processes; compounds with low removal efficiencies (e.g. carbamazepine, ciprofloxacin) should not be expected to be removed by conventional processes and, as such, are candidates for tertiary removal technologies, such as advanced oxidation, activated or membrane treatment; compounds with medium removal efficiencies (e.g. bezafibrate, BPA) could be susceptible of better removal efficiencies under specific operating conditions.

Data limitations do not allow us to reach firm conclusions regarding comparative effectiveness of alternative treatment technologies, although results indicate that compound-specific removal efficiencies amongst the various processes analyzed are similar (Figure 13). This might be expected if biodegradability and solid phase partitioning are the primary determinants of CEC removal.

5. Recommendations

This work has not attempted to correlate removal efficiencies with WWTP operating conditions. The data collected in the MS Access database include, when available, operating conditions, such as hydraulic and sludge retention times in activated sludge processes, as well as quantitative parameters related to plant performance (nitrogen and/or phosphorus removal, organic carbon removal). Analysis of the effect of operating conditions on removal efficiencies can be potentially important for those compounds classified as having medium removal efficiencies in Table 3. As further information on these compounds appears in the literature, such analysis can establish WWTP operational characteristics that would be favorable for the optimization of removal of these compounds.

One aspect that has limited our data analysis has been the scarcity of quantitative studies on biodegradability of CECs under typical WWTP conditions. An expanded database of information on laboratory studies on biodegradability and correlation between these studies and WWTP performance would provide tools for better assessment of CEC removal efficiency.

Despite the amount of information available, knowledge gaps for specific CECs are evident, and statistically based conclusions can be reached with confidence for only a handful of the CECs of potential interest. Low-confidence-level compounds (Table 3) plus compounds included in the database that lacked sufficient data for meaningful statistical analysis should be object of further data collection. Higher priority should be placed on the development of data among mass produced, toxic chemicals for which physical and biochemical data suggest that removal during conventional wastewater treatment will be low.

References

Balk F, Ford RA (1999) Environmental Risk assessment for the polycyclic musk AHTN and HHCB in the EU: Fate and exposure assessment. Toxicol Letters 111: 57-79.

Beach SA, Newsted JL, Coady K, Giesy JP (2006) Ecotoxicological evaluation of perfluorooctanesulfonate (PFOS). Rev Environ Contam Toxicol 186: 133–174.

Braskerud BC, Haarstad K (2003) Screening the retention of thirteen pesticides in a small constructed wetland. Water Sci Technol 48(5): 267–274.

Cespedes R, Lacorte S, Ginebreda A, Barcelo D (2008) Occurrence and fate of alkylphenols and alkylphenol ethoxylates in sewage treatment plants and impact on receiving waters along the Ter River (Catalonia, NE Spain). Environ Pollution 153: 384-392.

Clara M, Strenn B, Gans O, Martinez E, Kreuzinger N, Kroiss H (2005) Removal of selected pharmaceuticals, fragrances and endocrine disrupting compounds in a membrane bioreactor and conventional wastewater treatment plants. Water Res 39: 4797–4807.

Dickenson ERV, Drewes JE, Stevens-Garmon J, Khan S, McDonald J (2010) *Evaluation of QSPR techniques for wastewater treatment processes*. WERF – U2R07. IWA Publishing, London, UK.

Drewes JE, Hemming JDC, Schauer J, Sonzogni WC (2006) *Removal of endocrine disrupting compounds in water reclamation processes.* WERF–01-HHE-20T. IWA Publishing, London, UK.

Drewes JE, Dickenson ERV, Snyder S (2009) *Contributions of household chemicals to sewage and their relevance to municipal wastewater systems and the environment*. WERF–03-CTS-21UR. IWA Publishing, London, UK.

Halling-Sorensen B, Nielsen N, Lanzky PF, Ingerslev F, Holten Lützheft HC, Jergensen SE (1998) Ocurrence, fate and effects of pharmaceutical substances in the environment - A review. Chemosphere 36: 357-393.

Heberer Th, Reddersen K, Mechlinski A (2002) From municipal sewage to drinking water: fate and removal of pharmaceutical residues in the aquatic environment in urban areas, Water Sci Technol 46: 81–88.

Heberer T (2002) Occurrence, fate and assessment of polycyclic musk residues in the aquatic environment of urban areas – a review. Acta Hydrochim Hydrobiol 30: 227–243.

Jones OAH, Voulvoulis N, Lester JN (2007) The occurrence and removal of selected pharmaceutical compounds in a sewage treatment works utilising activated sludge treatment. Environ Pollution 145: 738-744.

Kidd KA, Planchfield PJ, Mils KH, Palace VP, Evans RE, Lazorchak JM, Flick RW (2007) Collapse of a fish population after exposure to a synthetic estrogen. Proc Nat Acad Sci 104: 8897–8901.

Klečka G, Persoon C, Currie R. (2010) Chemicals of emerging concern in the Great Lakes Basin: An analysis of environmental exposures. Rev Environ Contam Toxicol 207: 1-93.

Kolpin DW, Furlong ET, Meyer MT, Thurman EM, Zaugg SD, Barber LB, Buxton, HT (2002) Pharmaceuticals, hormones, and other organic wastewater contaminants in U.S. streams, 1999–2000: A national reconnaissance. Environ Sci Technol 36: 1202–1211.

Lee IS, Lee SH (2010) Occurrence and fate of synthetic musk compounds in water environment. Water Res 44: 214-222.

Lindqvist N, Tuhkanen T, Kronberg L (2005) Occurrence of acidic pharmaceuticals in raw and treated sewages and in receiving waters. Water Res 39: 2219–2228.

Lishman L, Smyth SA, Sarafin K, Kleywegt S, Toito J, Peart T, Lee B, Servos M, Beland M, Seto P (2006) Occurrence and reductions of pharmaceuticals and personal care products and estrogens by municipal wastewater treatment plants in Ontario, Canada. Sci Total Environ 367: 544-558.

Melcer H, Klečka G, Monteith H, Staples C (2007) *Wastewater treatment of alkylphenols and their ethoxylates: a state of the science review.* Alkylphenols & Ethoxylates Research Council, Water Environment Federation, Alexandria, VA.

Miege C, Choubert JM, Ribeiro L, Eusebe M, Coquery M (2009) Fate of pharmaceuticals and personal care products in wastewater treatment plants – Conception of a database and first results. Environ Pollution 157: 1721–1726.

Müller K, Magesan GN, Bolan NS (2007) A critical review of the influence of effluent irrigation on the fate of pesticides in soil. Agriculture Ecosys Environ 120: 93–116.

Murakami M, Shinohara H, Takada H (2009) Evaluation of wastewater and street runoff as sources of Perfluorinated surfactants (PFSs) over water. Chemosphere 74: 487–493.

Petrovic M, Sole M, Lopez De Alda MA, Barcelo D (2002) Endocrine disruptors in sewage treatment plants, receiving waters, and sediments: integration of chemical analysis and biological effects on feral carp. Environ Toxicol Chem 21: 2146–2156.

Radjenovic J, Petrovic M, Barcelo D (2007) Analysis of pharmaceuticals in wastewater and removal using a membrane bioreactor. Anal Bioanal Chem 387: 1365–1377.

Roslev P, Vorkamp K, Aarup J, Frederiksen K, Nielsen PH (2007) Degradation of phthalate esters in an activated sludge wastewater treatment plant. Water Res 41: 969–976.

Santos JL, Aparicio I, Callejón M, Alonso E (2009) Occurrence of pharmaceutically active compounds during 1-year period in wastewaters from four wastewater treatment plants in Seville (Spain). J Hazardous Mat 164: 1509–1516.

Schultz MM, Barofsky DF, Field JA (2006a) Quantitative determination of fluorinated alkyl substances by large-volume-injection liquid chromatography tandem mass spectrometry – Characterization of municipal wastewaters. Environ Sci Technol 40: 289–295.

Schultz MM, Higgins CP, Huset CA, Luthy RG, Barofsky DF, Field JA (2006b) Fluorochemical mass flows in a municipal wastewater treatment facility. Environ Sci Technol 40: 7350–7357.

Sim W, Lee J, Oh J (2010) Occurrence and fate of pharmaceuticals in wastewater treatment plants and rivers in Korea. Environ Pollution 158: 1938–1947.

Stephenson R, Opppenheimer J (2007) *Fate of pharmaceutical and personal care products through municipal wastewater treatment processes*. WERF-03-CTS-22UR. IWA Publishing, London, UK.

Sui Q, Huang J, Deng S, Yu G, Fan Q (2010) Occurrence and removal of pharmaceuticals, caffeine and DEET in wastewater treatment plants of Beijing, China. Water Res 44: 417-426.

Tas JW, Balk F, Ford RA, Van de Plassche EJ (1997) Environmental risk assessment of musk ketone and musk xylene in the Netherlands in accordance with the EU-TGD. Chemosphere 35: 2973-3002.

Tauxe-Wuersch A, De Alencastro LF, Grandjean D, Tarradellas J (2005) Occurrence of several acidic drugs in sewage treatment plants in Switzerland and risk assessment. Water Res 39: 1761–1772.

Taylor AAL, Jobling S, Nolan M, Tyler CR, van Aerle R, Brighty G (2005) Spatial survey of the extent of sexual disruption in wild roach in English and Welsh rivers. Science Report P6-018/SR Environment Agency.

Teske SS, Arnold RG (2008) Removal of natural and xeno-estrogens during conventional wastewater treatment. Rev Environ Sci Biotechnol 7: 107-124.

Urase T, Kikuta T (2005) Separate estimation of adsorption and degradation of pharmaceutical substances and estrogens in the activated sludge process. Water Res 39: 1289-1300.

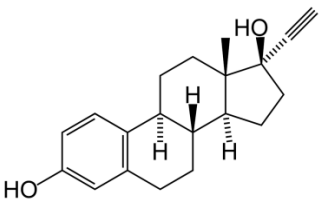
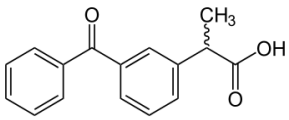
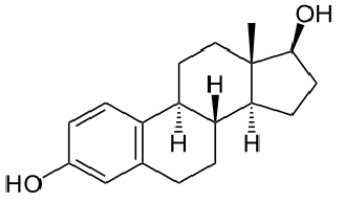
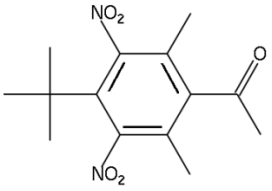
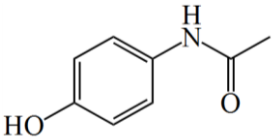
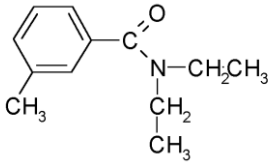
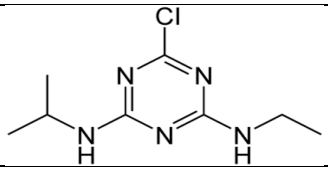
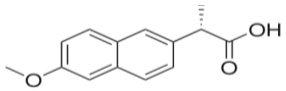
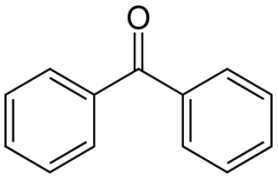
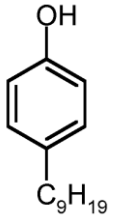
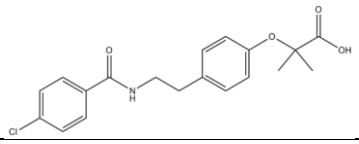
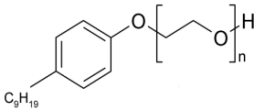
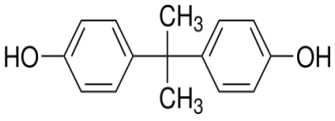
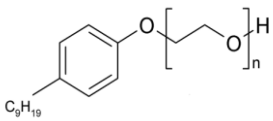
US EPA (2009) *Occurrence of contaminants of emerging concern in wastewater from nine publicly owned treatment works.* EPA-821-R-09-009. Environmental Protection Agency, Washington DC.

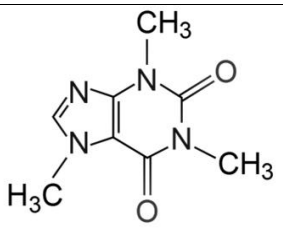
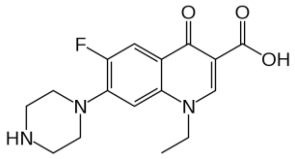
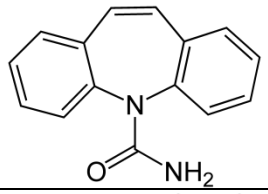
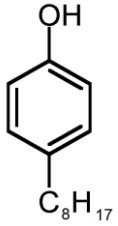
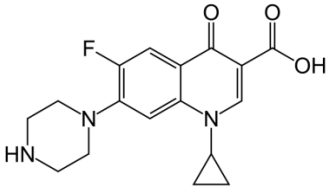
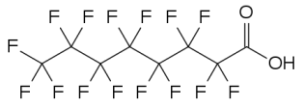
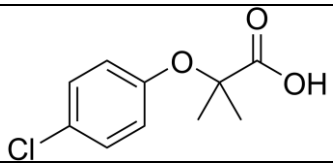
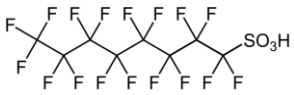
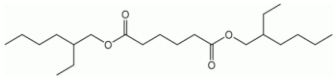
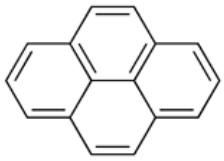
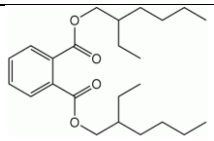
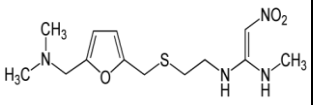
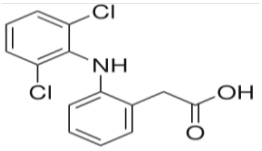
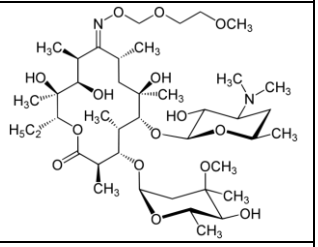
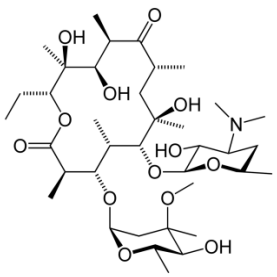
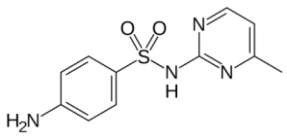
US EPA (2010) *Treating contaminants of emerging concern: a literature review database*. EPA-820-R-10-002. Environmental Protection Agency, Washington DC.

Ying GG, Kookana R, Kumar A (2008) Fate of estrogens and xenoestrogens in four sewage treatment plants with different technologies. Environ Toxicol Chem 27: 87-94.

Yu T, Lin AY, Lateef SK, Lin C, Yang P (2009) Removal of antibiotics and non-steroidal anti-inflammatory drugs by extended sludge age biological process. Chemosphere 77: 175–181.

Table 1. Chemicals of emerging concern studied and their structures.

CEC General Class	**Structure**	**CEC**	**Structure**
17α-Ethynyl estradiol (EE2) Hormone		**Ketoprofen** Pharmaceutical	
17β-Estradiol (E2) Hormone		**Musk ketone** Synthetic Musk	
Acetaminophen Pharmaceutical		**N,N-diethyl-toluamide (DEET)** Insect repellant	
Atrazine Pesticide		**Naproxen** Pharmaceutical	
Benzophenone Plasticizer		**Nonylphenol** Alkylphenol	
Bezafibrate Pharmaceutical		**Nonylphenol diethoxylate (NP2EO)** (n=2)	
Bisphenol A Plastic manufacture		**Nonylphenol monoethoxylate (NP1EO)** (n=1) Alkylphenol Ethoxylates	

Caffeine Pharmaceutical		**Norfloxacin** Pharmaceutical	
Carbamazepine Pharmaceutical		**Octylphenol** Alkylphenol	
Ciprofloxacin Pharmaceutical		**Perfluorooctanoic acid (PFOA)** Perfluorinated Surfactant	
Clofibric acid Pharmaceutical		**Perfluorooctyl sulfonate (PFOS)** Perfluorinated Surfactant	
Di (2-ethylhexyl) adipate (DEHA) Plasticizer		**Pyrene** Polycyclic Aromatic	
Di (2-ethylhexyl) phthalate (DEHP) Plasticizer		**Ranitidine** Pharmaceutical	
Diclofenac Pharmaceutical		**Roxithromycin** Pharmaceutical	
Erythromycin Pharmaceutical		**Sulfamerazine** Pharmaceutical	

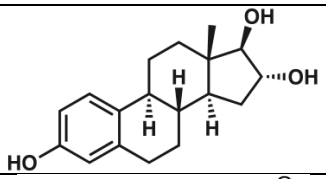
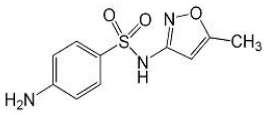
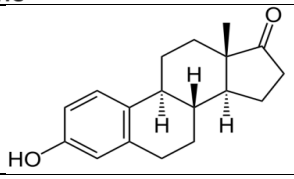
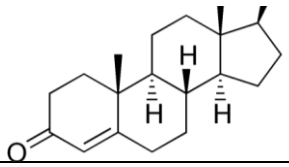
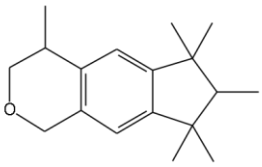
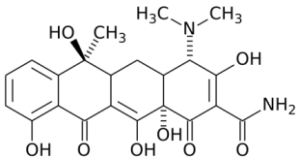
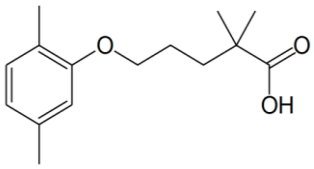
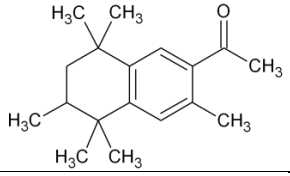
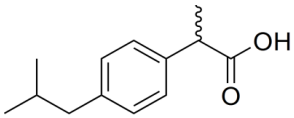
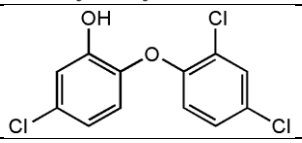
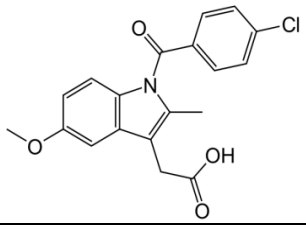
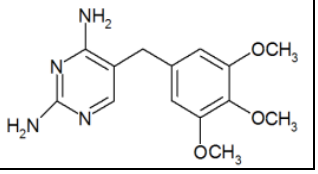
Estriol (E3) Hormone		**Sulfamethoxazole** Pharmaceutical	
Estrone (E1) Hormone		**Testosterone** Hormone	
Galaxolide (HHCB) Synthetic Musk		**Tetracycline** Pharmaceutical	
Gemfibrozil Pharmaceutical		**Tonalide (AHTN)** Synthetic Musk	
Ibuprofen Pharmaceutical		**Triclosan** Personal Care Product	
Indomethacin Pharmaceutical		**Trimethoprim** Pharmaceutical	

Table 2. Physical properties, biodegradability data and assessment of removal in CAS for selected CECs.

CEC	CAS #	Biodegradability BIOWIN 2	Log K_{OW}	H (atm-m^3/mole)	Lab Test Removal Range % (# studies)	Pilot Plant Removal Range % (# studies)	Full Scale Removal Range % (# studies)	Prob. of 75% removal	Removal Efficiency in CAS	Confidence in Assessment
17α-ethynyl estradiol (EE2)	57-63-6	Not Ready Biodegradable	3.67	7.94E-12[b]	39-100 (n=9)	59-100 (n=9)	47-100 (n=18)	30.0	Medium	High
17β-estradiol (E2)	50-28-2	Ready Biodegradable	4.01	3.64E-11[b]	20-100 (n=11)	36.3-100 (n=7)	10-100 (n=44)	50.0	Medium	High
Acetaminophen	103-90-2	Ready Biodegradable	0.46	6.42E-13[b]	91-100 (n=7)	20-99.9 (n=3)	98.4-100 (n=6)	91.83	High	High
Atrazine	1912-24-9	Not Ready Biodegradable	2.61	4.47E-09[b]	25 (n=1)	-	22.7-95 (n=4)	20.00	Low	Low
Benzophenone	119-61-9	Ready Biodegradable	3.18	1.94E-06[b]	95 (n=1)	-	62-99 (n=4)	57.71	Medium	Low
Bezafibrate	41859-67-0	Inherently Biodegradable	4.25[a]	2.12E-15[b]	-	80.8-99 (n=2)	15-99 (n=12)	49.71	Medium	High
Bisphenol A	80-05-7	Inherently Biodegradable	3.32	9.16E-12[b]	28-99 (n=5)	71.3 (n=1)	23-99 (n=23)	66.08	Medium	High
Caffeine	58-08-2	Inherently Biodegradable	-0.07	3.58E-11	94-100 (n=1)	68-100 (n=3)	40-99 (n=20)	89.00	High	High
Carbamazepine	298-46-4	Inherently Biodegradable	2.45	1.08E-10	0-99 (n=14)	0-99 (n=9)	0-99 (n=39)	7.89	Low	High
Ciprofloxacin	85721-33-1	Not Ready Biodegradable	0.28	5.09E-19[b]	4-100 (n=5)	-	0-100 (n=15)	22.56	Low	High
Clofibric acid	882-09-7	Not Ready Biodegradable	2.57	2.19E-08[b]	16-75 (n=5)	1-30 (n=4)	15-99.6 (n=12)	13.48	Low	High
Di (2-ethylhexyl) adipate (DEHA)	103-23-1	Ready Biodegradable	8.12[a]	4.34E-07	-	-	80-99 (n=2)	90.00	High	Low
Di (2-ethylhexyl) phthalate (DEHP)	117-81-7	Ready Biodegradable	7.6	2.70E-07	-	8.54 (n=1)	60-99 (n=8)	42.30	Medium	Medium
Diclofenac	15307-86-5	Not Ready Biodegradable	4.51	4.73E-12[b]	0-58 (n=13)	0-75 (n=11)	0-98 (n=340	24.38	Low	High
Erythromycin	114-07-8	Not Ready Biodegradable	3.06	5.42E-29[b]	2-89 (n=7)	35.4 (n=1)	0-100 (n=19)	23.00	Low	High
Estriol (E3)	50-27-1	Ready Biodegradable	2.45	1.33E-12[b]	91-99 (n=3)	0-80 (n=2)	16-100 (n=19)	85.35	High	High
Estrone (E1)	53-16-7	Not Ready Biodegradable	3.13	3.80E-10[b]	20-100 (n=8)	52-100 (n=8)	0-100 (n=43	55.59	Medium	High
Galaxolide (HHCB)	1222-05-5	Not Ready Biodegradable	5.9	1.32E-04[b]	0-92 (n=2)	0-86 (n=2)	40-99 (n=13)	51.00	Medium	High

Gemfibrozil	25812-30-0	Ready Biodegradable	4.77[a]	1.19E-08[b]	50-96 (n=4)	-	0-99 (n=15)	25.31	Low	Medium
Ibuprofen	15687-27-1	Ready Biodegradable	3.97	1.50E-07	74-100 (n=11)	41-99 (n=12)	15.5-99 (n=38)	67.78	Medium	High
Indomethacin	53-86-1	Inherently Biodegradable	4.27	3.13E-14[b]	23.4-100 (n=2)	-	0-98 (n=4)	43.54	Medium	Low
Ketoprofen	22071-15-4	Ready Biodegradable	3.12	2.12E-11[b]	30-98 (n=8)	10-97 (n=3)	11.2-100 (n=20)	35.00	Medium	High
Musk ketone	81-14-1	Not Ready Biodegradable	4.3	4.80E-10[b]	-	-	53-85 (n=5)	88.00	High	Low
N,N-diethyl-toluamide (DEET)	134-62-3	Ready Biodegradable	2.18	2.08E-08[a]	-	-	0-91 (n=5)	87.50	High	Low
Naproxen	22204-53-1	Ready Biodegradable	3.18	3.39E-10[b]	50-100 (n=10)	55-93.3 (n=8)	43-99.6 (n=28)	50.10	Medium	High
Nonylphenol	25154-52-3	Ready Biodegradable	5.76	3.40E-05	28-99 (n=6)	74-96 (n=5)	24-100 (n=39)	52.00	Medium	High
Nonylphenol diethoxylate (NP2EO)	20427-84-3	Ready Biodegradable	5.20[a]	2.56E-09[b]	3.76-99 (n=8)	46-95 (n=6)	0-99 (n=21)	57.0	Medium	High
Nonylphenol monoethoxylate (NP1EO)	104-35-8	Ready Biodegradable	5.58[a]	1.65E-07[b]						
Norfloxacin	70458-96-7	Ready Biodegradable	-1.03	8.70E-19[b]	20-98 (n=2)	-	41-97 (n=12)	27.93	Medium	Medium
Octylphenol	1806-26-4	Ready Biodegradable	5.5[a]	4.50E-06[b]	-	50-64.6 (n=2)	0-99 (n=20)	54.00	Medium	High
Perfluorooctanoic acid (PFOA)	335-67-1	Not Ready Biodegradable	4.81[a]	9.08E-02[b]	0 (n=1)	-	0-48 (n=7)	0.36	Low	Medium
Perfluorooctyl sulfonate (PFOS)	1763-23-1	Not Ready Biodegradable	-1.08[**]	1.10E-02[b]	0.93 (n=1)	-	0-42 (n=8)	0.10	Low	Medium
Pyrene	0129-00-0	Not Ready Biodegradable	4.88	1.19E-05	51-95 (n=4)	-	56-68 (n=1)	19.00	Low	Low
Ranitidine	66357-35-5	Not Ready Biodegradable	0.27	3.42E-15[b]	-	24.7 (n=1)	31.2-98 (n=8)	26.36	Medium	Medium
Roxithromycin	80214-83-1	Not Ready Biodegradable	2.75[a]	4.97E-31[b]	25-91 (n=2)	82-94 (n=2)	0-75 (n=12)	29.00	Medium	Medium
Sulfamerazine	127-79-7	Not Ready Biodegradable	0.14	1.75E-10[b]	100 (n=1)	-	0-75 (n=4)	25.59	Medium	Low
Sulfamethoxazole	723-46-6	Not Ready Biodegradable	0.89	9.56E-13[b]	30-96 (n=6)	73.8-99 (n=4)	17-96 (n=32)	43.79	Medium	High
Testosterone	58-22-0	Not Ready Biodegradable	3.32	3.53E-09[b]	-	100 (n=1)	69-100 (n=4)	77.47	High	Low

Tetracycline	60-54-8	Not Ready Biodegradable	-1.3	4.66E-24 [b]	37-89 (n=5)	79-89 (n=1)	0-100 (n=12)	33.84	Medium	Medium
Tonalide (AHTN)	1506-02-1	Not Ready Biodegradable	5.7	1.39E-04	50 (n=1)	60-85 (n=2)	6-98 (n=13)	46.00	Medium	High
Triclosan	3380-34-5	Not Ready Biodegradable	4.76	4.99E-09 [b]	10-94 (n=5)	0-97 (n=2)	0-99 (n=22)	49.00	Medium	High
Trimethoprim	738-70-5	Not Ready Biodegradable	0.91	2.39E-14 [b]	11-74 (n=3)	0-40.4 (n=2)	0-100 (n=26)	8.50	Low	High

Biodegradability predictions are estimations made with BIOWIN™ 2 (EPI Suite™); exceptions: (*) measured biodegradability taken from the literature (results that differ from BIOWIN 2 predictions); classification: ready biodegradable corresponds to >60% degradation in Ready test, inherently biodegradable corresponds to degradation between 40 and 60% and not Ready biodegradable corresponds to <40% degradation.

Experimental values of K_{ow} and Henry's law constants were taken from EPI Suite™ database, except for (a) K_{ow} values calculated by simulations with KOWWIN™, and (b) Henry's law constants calculated by simulation with HENRYWIN™ (Bond Contribution Model), both from EPI Suites™.

Removal efficiency levels in CAS were determined as follows: high corresponds to CECs with >75% probability of 75%+ removal, medium corresponds to CECs with 25-75% probability of 75%+ removal, low corresponds to CECs with <25% probability of 75%+ removal. Confidence in assessment was judged as follows: high means that more than 15 studies were available, medium corresponds to compounds for which between 9 and 15 studies were available, low corresponds to compounds for which less than 9 studies were available.

[**] K_{ow} for PFOS obtained from Beach et al. (2006)

Table 3. Summary of confidence level vs. removal efficiency for selected CECs (activated sludge processes).

Confidence level	Low removal efficiency (<25% probability of 75%+ removal)	Medium removal efficiency (25–75% probability of 75%+ removal)	High removal efficiency (>75% probability of 75%+ removal)
Low (n<9)	Atrazine, Pyrene	Indomethacin, Sulfamerazine	Musk ketone, DEET, DEHA , Testosterone,
Medium (9≤n≤15)	Gemfibrozil, PFOA, PFOS	DEHP, Norfloxacin, Ranitidine, Roxithromycin, Tetracycline	
High (n>15)	Carbamazepine, Ciprofloxacin, Clofibric acid, Diclofenac, Erythromycin, Trimethoprim	Bezafibrate, Bisphenol A, E1, EE2, E2, Galaxolide, Ibuprofen, Ketoprofen, Naproxen, Nonylphenol, NP1EO, NP2EO, Octylphenol, Sulfamethoxazole, Tonalide, Triclosan	Acetaminophen, Caffeine, E3

Table 4. Spearman Correlation Coefficient for the removal efficiencies of diclofenac and ketoprofen in activated sludge processes.

Compound	***Spearman Correlation Coefficient***	
	SRT	***HRT***
Diclofenac	*0.13649*	*0.51163*
Ketoprofen	*0.54624*	*0.02951*

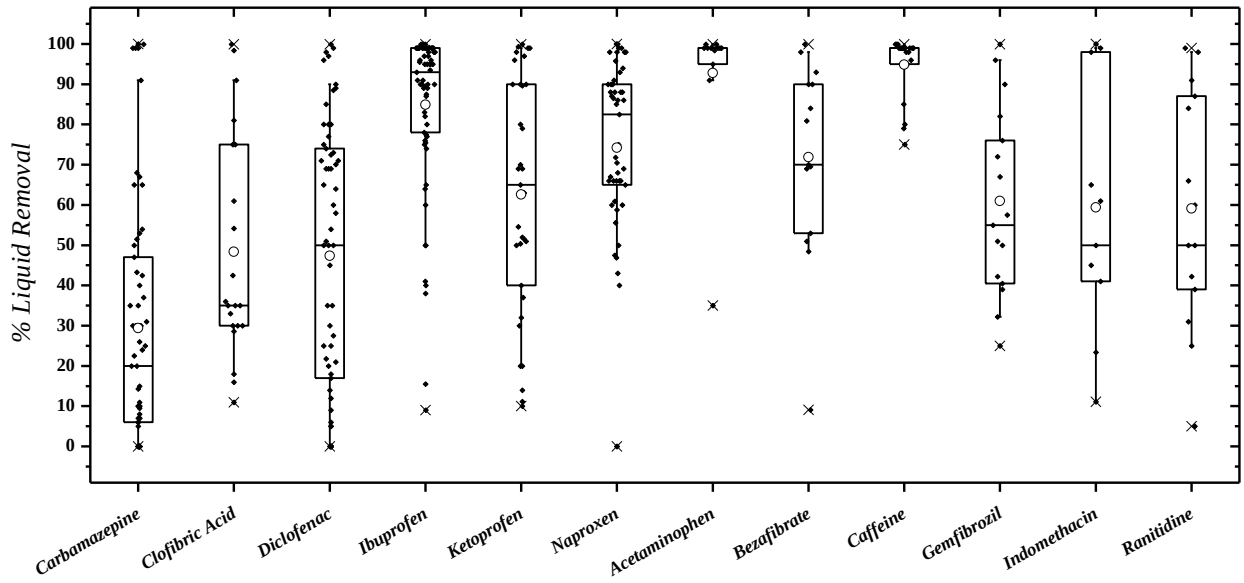


Figure 1. Box plots of liquid removal in activated sludge processes for selected prescription and non-prescription pharmaceuticals.

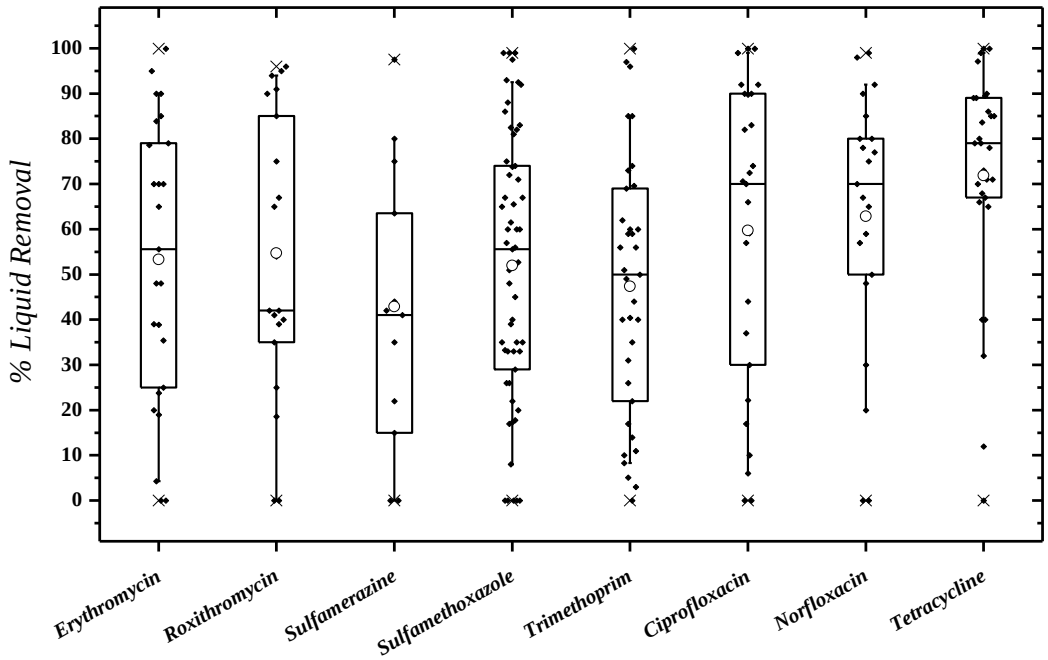


Figure 2. Box plots of liquid removal in activated sludge processes for selected antibiotics.

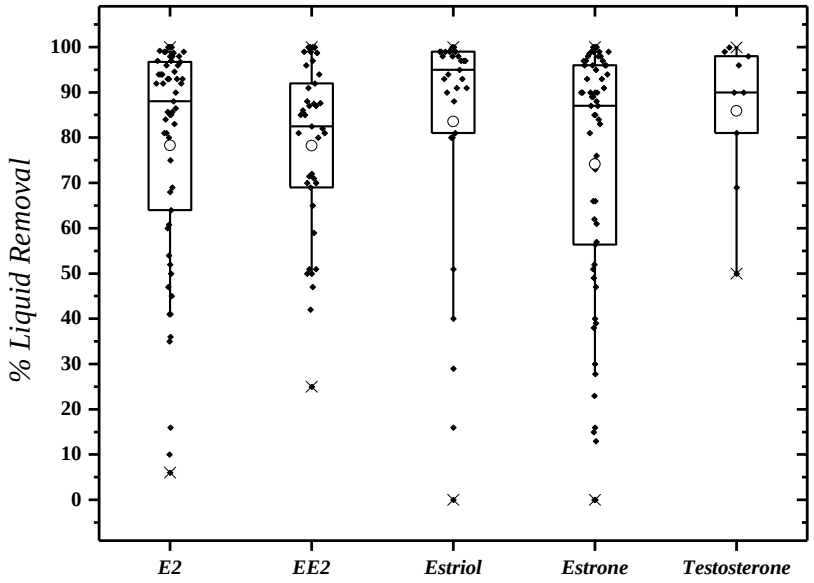


Figure 3. Box plots of liquid removal in activated sludge processes for selected natural and synthetic hormones.

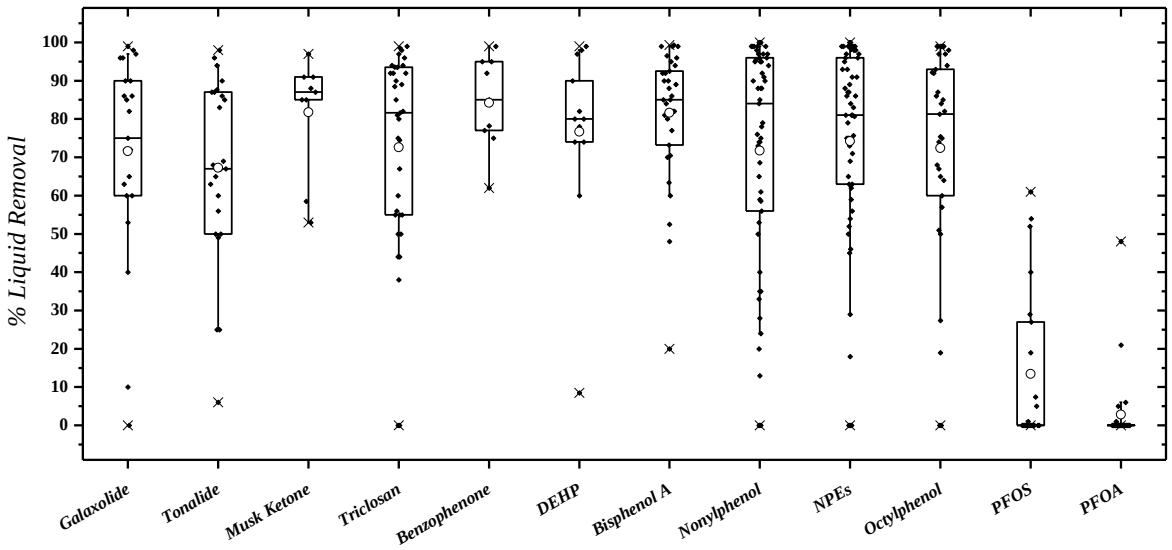


Figure 4. Box plots of liquid removal in activated sludge processes for selected organic wastewater contaminants.

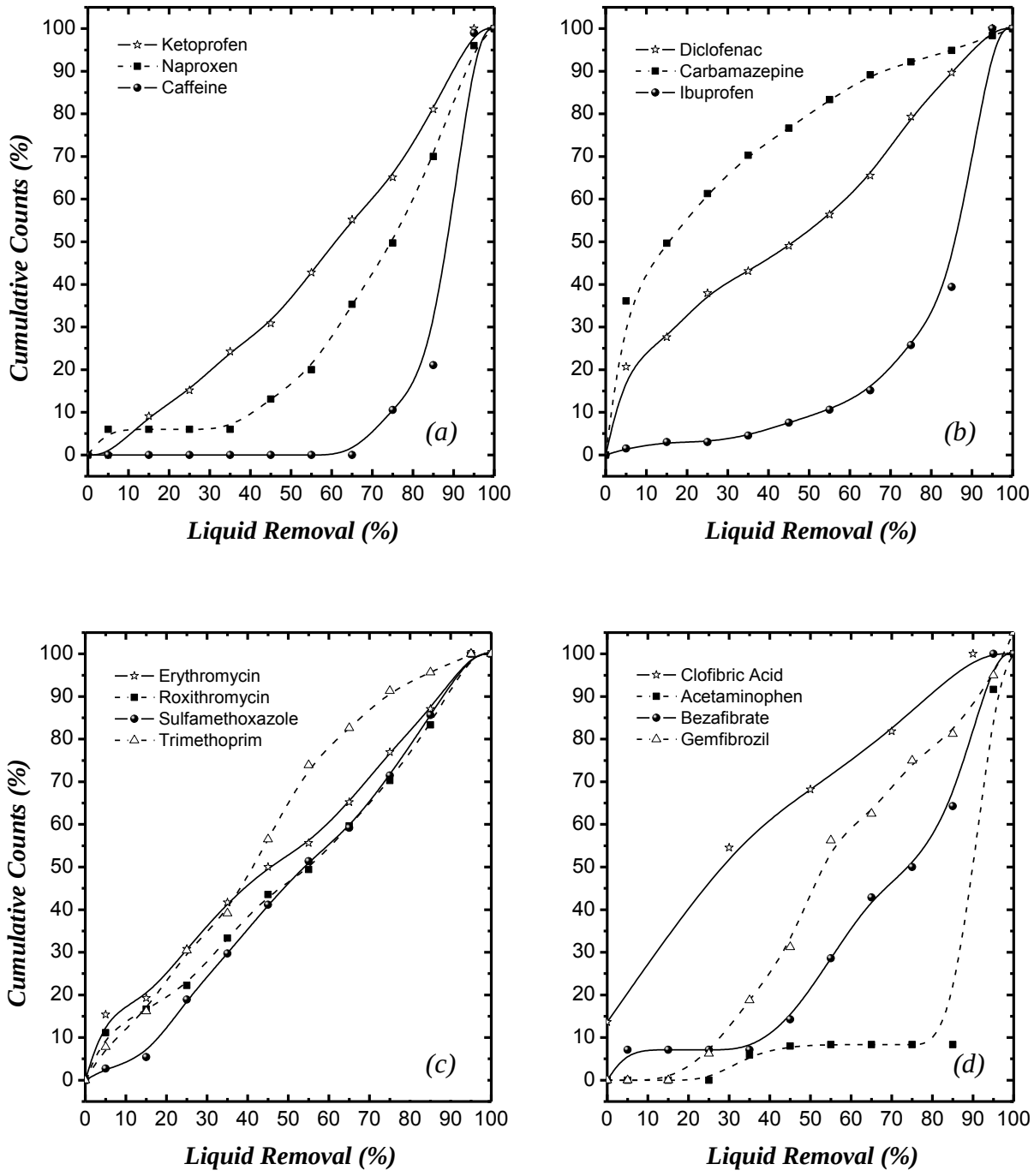


Figure 5. Cumulative Probability for selected pharmaceuticals in CAS.

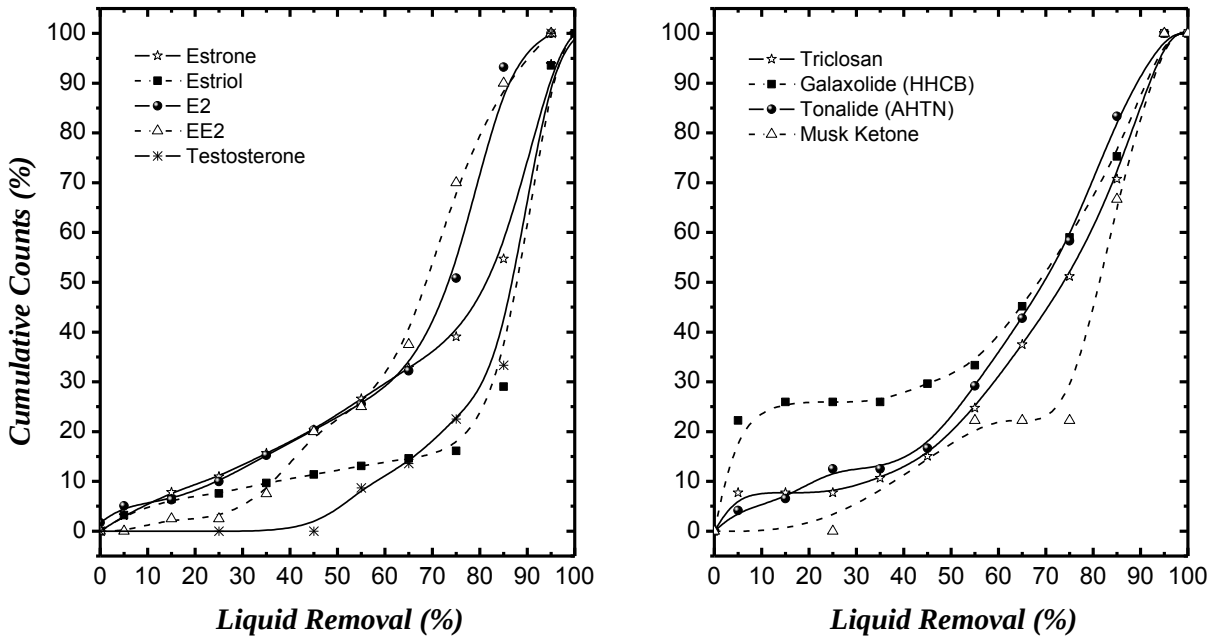


Figure 6. Cumulative Probability for selected hormones and synthetic musks in CAS.

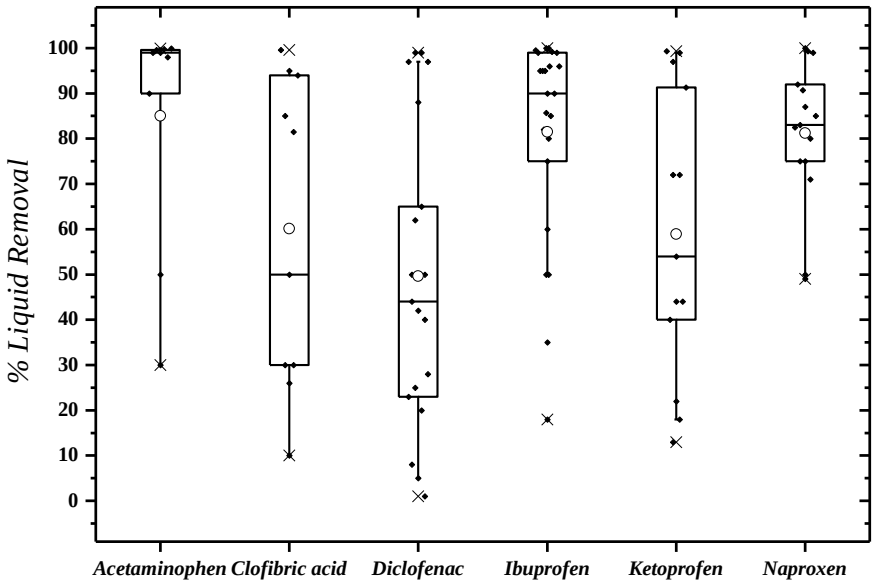


Figure 7. Box plots of liquid removal for selected pharmaceuticals in MBR process.

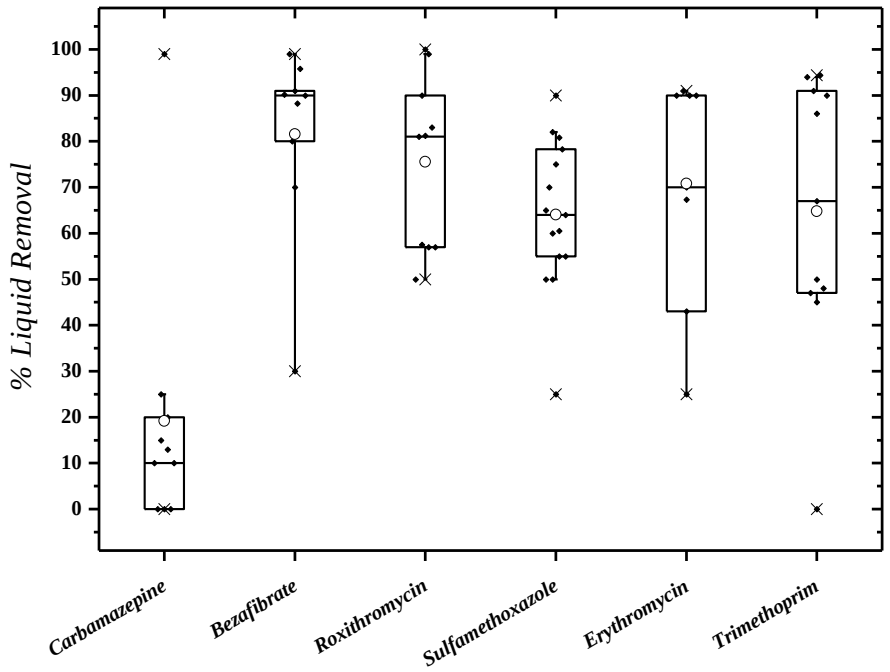


Figure 8. Box plots of liquid removal for selected antibiotics in MBR process.

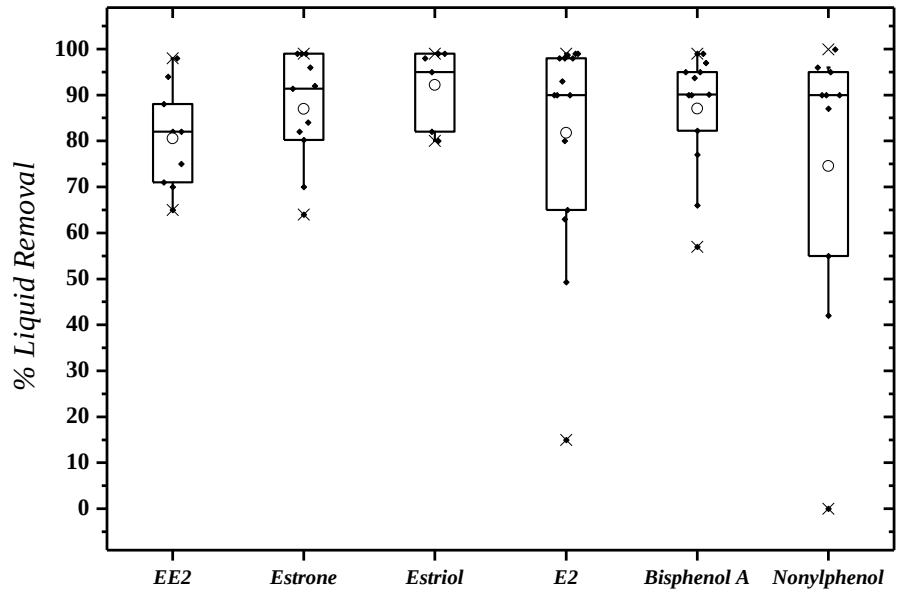
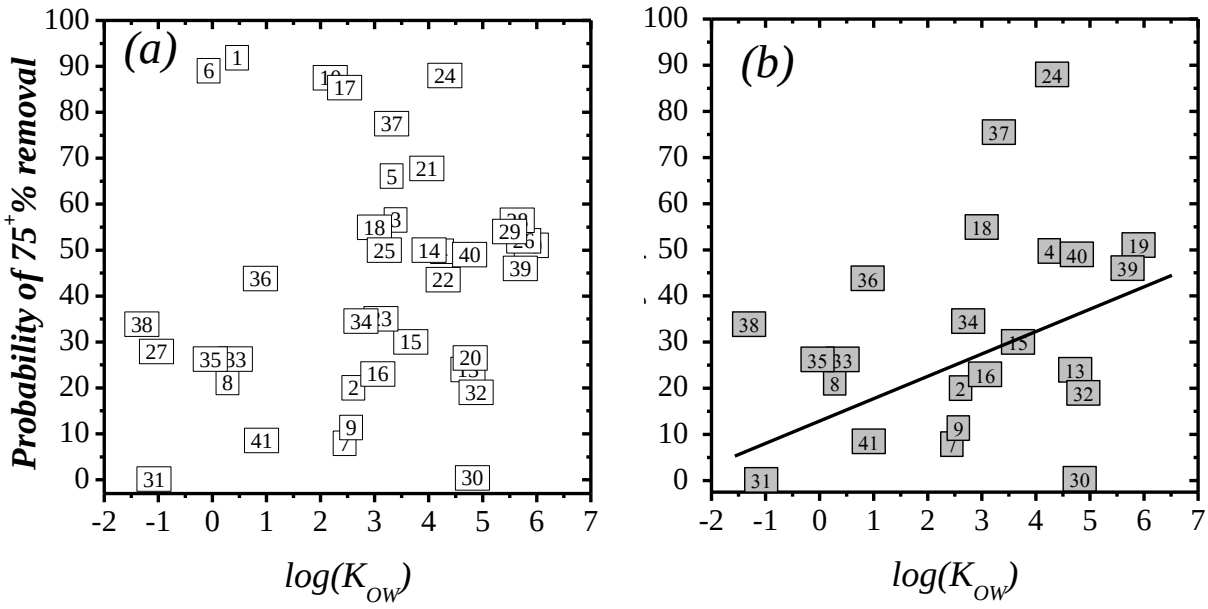


Figure 9. Box plots of liquid removal for selected natural and synthetic hormones, bisphenol A and nonylphenol in MBR process.



1	Acetaminophen	10	DEET	19	Galaxolide	28	NPEs	37	Testosterone
2	Atrazine	11	DEHA	20	Gemfibrozil	29	Octylphenol	38	Tetracycline
3	Benzophenone	12	DEHP	21	Ibuprofen	30	PFOA	39	Tonalide
4	Bezafibrate	13	Diclofenac	22	Indomethacin	31	PFOS	40	Triclosan
5	Bisphenol A	14	E2	23	Ketoprofen	32	Pyrene	41	Trimethropim
6	Caffeine	15	EE2	24	Musk ketone	33	Ranitidine		
7	Carbamazepine	16	Erythromycin	25	Naproxen	34	Roxythomycin		
8	Ciprofloxacin	17	Estriol	26	Nonylphenol	35	Sulfamethoxazole		
9	Clorofibric acid	18	Estrone	27	Norfoflaxacin	36	Sulfamezarine		

Figure 10. (a) Probability of achieving 75%+ removal efficiency for selected CECs as a function of octanol-water partition coefficient; (b) same as (a) but biodegradable (Ready and inherent biodegradable compounds from Table 2) compounds have been eliminated. Solid line in (b) is a visual guide.

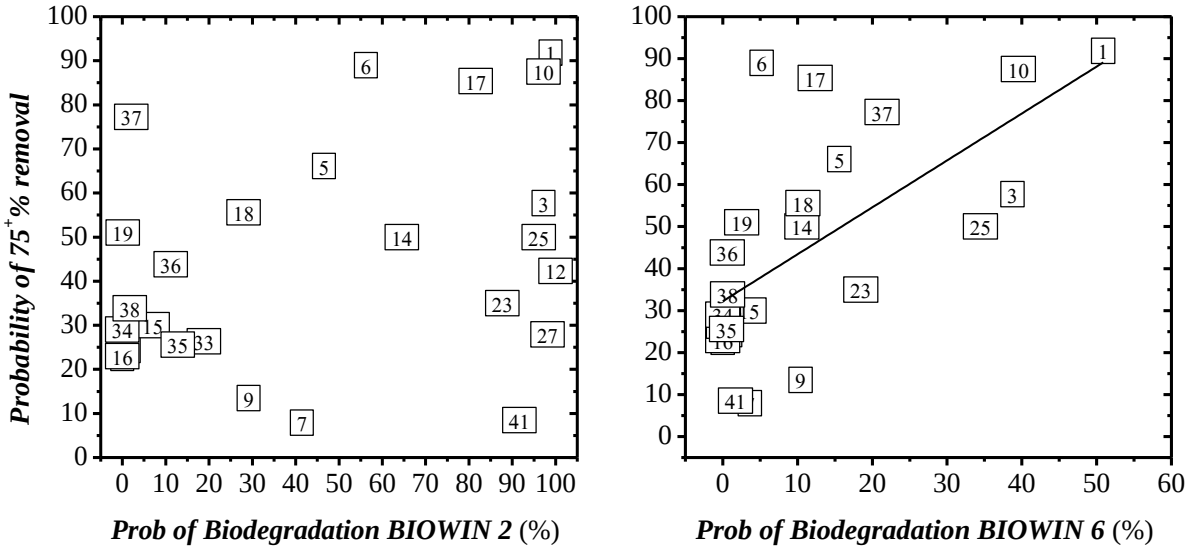


Figure 11. Probability of achieving 75%$^{+}$ removal efficiency in CAS vs. BIOWIN 2 (left) and BIOWIN 6 (right) estimation of biodegradation probabilities. Numbers correspond to legend in Figure 10. Solid line represents a linear fitting.

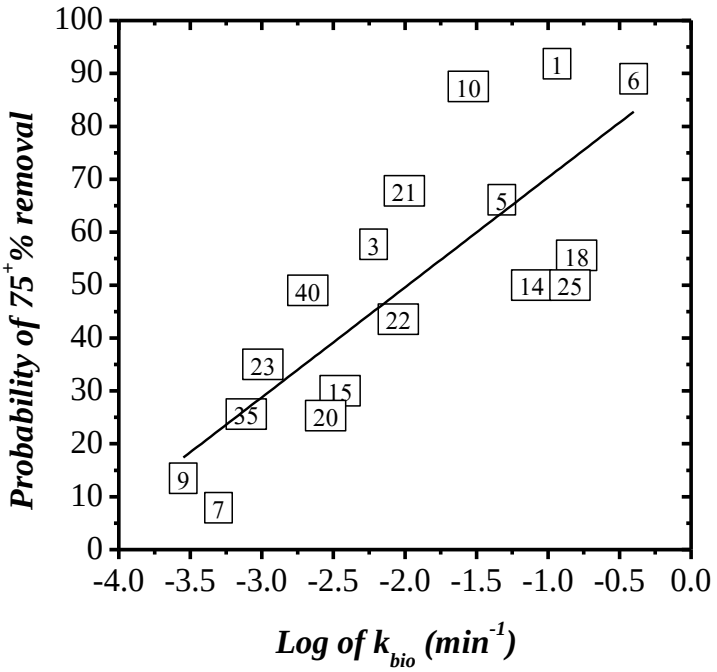


Figure 12. Probability of achieving 75%$^{+}$ removal efficiency as a function of biodegradation rate constants (as reported by Urase and Kikuta 2005, and Dickenson et al. 2010) in activated sludge for selected compounds. Numbers correspond to legend in Figure 10. Solid line is a visual guide.

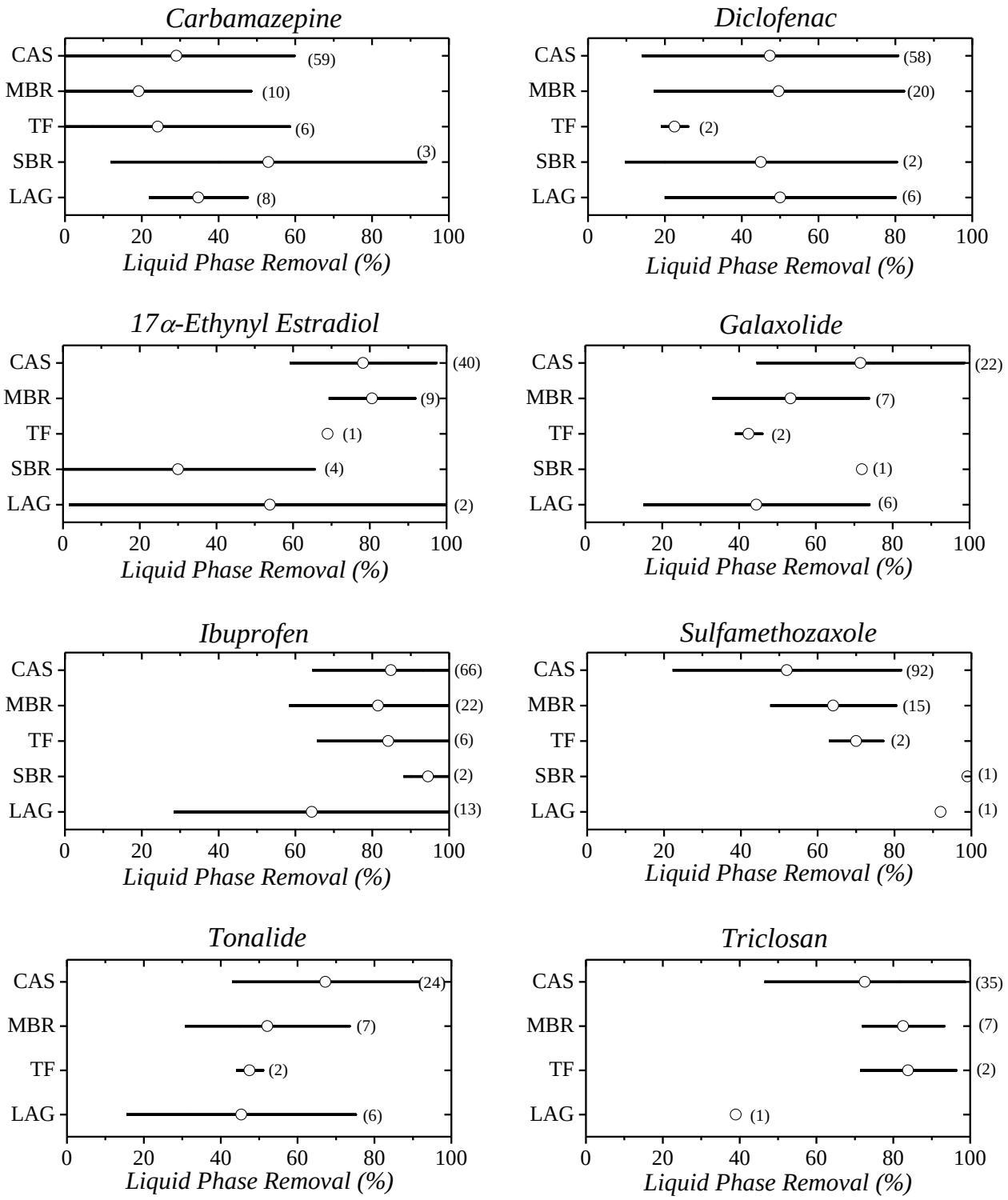


Figure 13. Removal efficiency comparison for conventional activated sludge (CAS), membrane bioreactor (MBR), tricking filters (TF), sequenced batch reactors (SBR) and lagooning (LAG) for selected CECs. Open circles represent the mean and the horizontal bars represent plus and minus one standard deviation. The number of data points is indicated for each case.

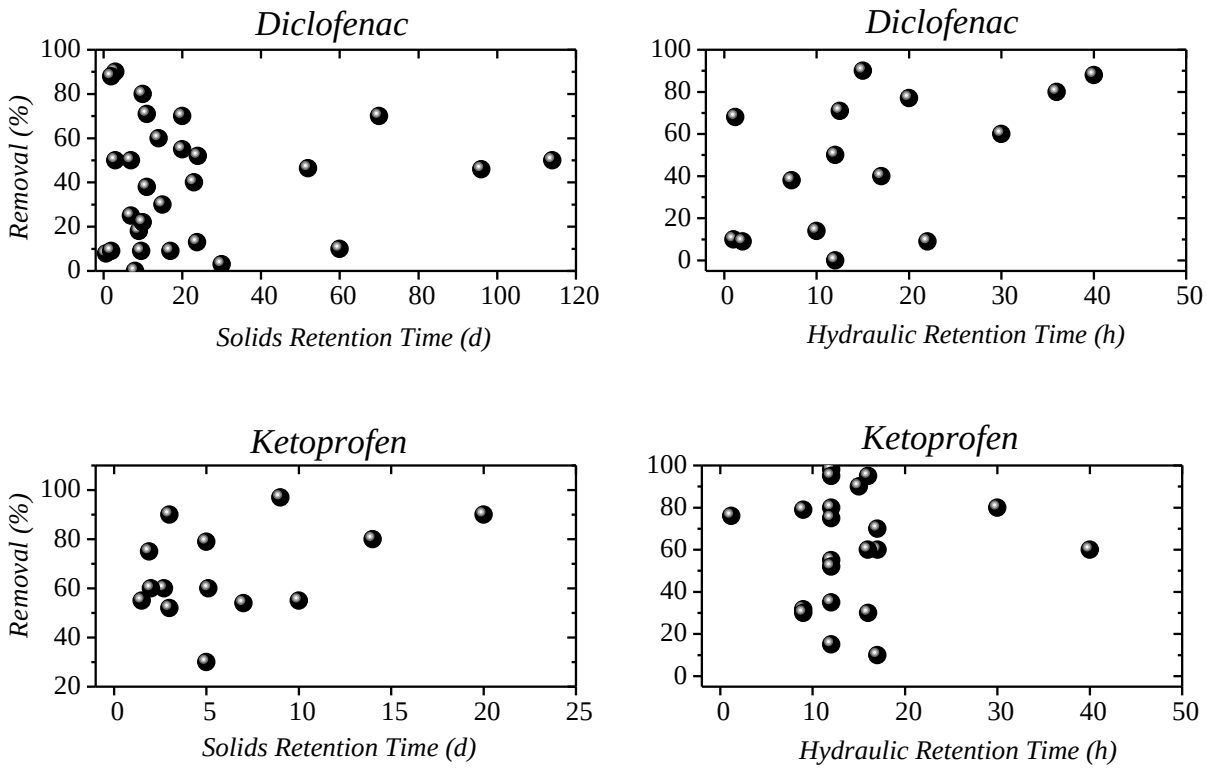


Figure 14. Removal efficiencies (%) as functions of SRT and HRT for diclofenac and ketoprofen in activated sludge process.

APPENDIX A

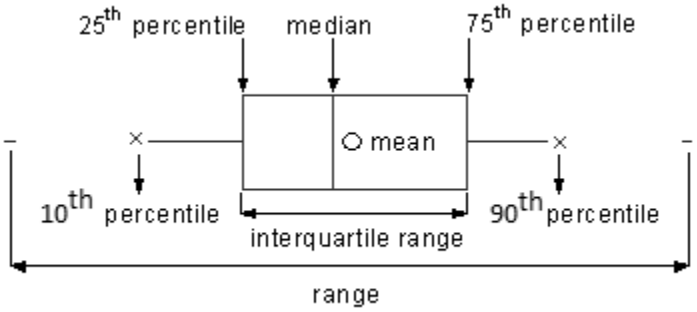


Figure A.1. Box or whisker plot characteristics.

APPENDIX B

Table B.1. References used to build the box-plot and cumulative distribution functions.

CEC	References from MS Access database
17α-Ethynyl estradiol (EE2)	1, 8, 10, 41, 107, 116, 153, 155, 165, 202, 222, 262, 309, 315, 323, 335, 341, 342, 359, 397, 416, 421, 430, 487, 492, 627, 632, 641
17β-Estradiol (E2)	8, 14, 24, 35, 41, 107, 116, 143, 146, 153, 155, 165, 172, 189, 202, 211, 212, 213, 229 , 236, 262, 273, 280, 309, 315, 323, 335, 337, 342, 359, 397, 406, 416, 421, 487, 492, 622, 623, 626, 635 , 637, 641, 644
Acetaminophen	57, 123, 193, 200, 287, 313, 377, 437, 616, 627, 480
Atrazine	101, 233, 369, 447, 640
Benzophenone	323, 437, 637, 640, 646
Bezafibrate	8, 10, 28, 29, 44, 168, 222, 313, 437, 632
Bisphenol A	14, 127, 143, 170, 210, 215, 222, 227, 317, 323, 349, 395, 409, 416, 419 , 492, 611, 640
Caffeine	44, 132, 298, 334, 377, 416, 490,637, 646
Carbamazepine	7, 8, 10, 31, 36, 44, 92, 107, 132, 133, 136, 143, 153, 154, 170, 200, 203, 222, 224, 226, 227, 233 , 248, 249, 262, 264, 289, 291, 298, 311, 313, 317, 319, 334, 341, 363, 364, 376, 377, 385, 416, 430, 437, 438, 467, 620, 627, 632, 635, 637
Ciprofloxacin	22, 102, 109, 118, 140, 177, 199, 292, 344, 368, 376, 378, 383, 417, 437 , 480, 601, 632, 637
Clofibric acid	44, 73, 145, 154, 195, 200, 224, 264, 277, 288, 291, 298, 341, 367, 378, 437, 627, 632, 635
Di (2-ethylhexyl) adipate (DEHA)	14, 21, 458
Di (2-ethylhexyl) phthalate (DEHP)	5, 14, 21, 78, 139, 355, 356, 458, 606
Diclofenac	7, 8, 10, 28, 31, 36, 41, 73, 92, 107, 133, 153, 193, 195, 200, 222, 224, 226, 235, 249, 277, 289, 298, 313, 317, 319, 323, 334, 341, 364, 367, 369, 376, 378, 385, 416, 430, 437, 447, 467, 480, 490, 603, 616, 620, 627, 628, 631, 632, 635, 636
Erythromycin	41, 118, 143, 177, 200, 222, 298, 313, 368, 416, 423, 437, 616, 632, 637
Estriol (E3)	8, 116, 143, 155, 165, 170, 189, 211, 229, 236, 269, 335, 359, 416, 451, 482, 623, 626, 630, 632, 641, 644
Estrone (E1)	8, 24, 35, 107, 116, 153, 155 , 165, 172, 189, 202, 222, 229, 236, 262, 269, 273, 280, 315, 323 , 337, 342, 349, 397, 406, 416, 421, 482, 487, 492, 622, 623, 626, 632, 637, 641, 644
Galaxolide (HHCB)	29, 43, 107, 112, 114, 133, 205, 386, 396, 416, 450, 488, 636, 637, 646
Gemfibrozil	
Ibuprofen	123, 132, 133, 138, 143, 145, 153, 154, 168, 170, 195, 222, 224, 226, 248, 249, 277, 289, 291, 298, 313, 317, 319 , 323, 334, 341, 364, 367, 369 , 378, 385, 388, 430, 437, 467, 480, 488, 490, 603, 616, 627, 628 , 631, 632, 635, 636, 646
Indomethacin	31, 200, 313, 323, 437, 603
Ketoprofen	28, 73, 123, 132, 143, 154, 170, 193, 200, 224, 226, 248, 313, 317, 319, 323, 369, 416, 437, 467, 480, 490, 616, 628, 632, 636
Musk Ketone	43, 272, 450, 627, 646
N,N-Diethyl-toluamide (DEET)	44, 416, 637, 640, 646
Naproxen	7, 28, 36, 41, 73, 121, 132, 133, 143, 153, 170, 193, 195, 200, 216, 217, 226, 248, 289, 313, 317, 319, 323, 364, 369, 378, 385, 430, 437, 467, 480, 488, 490, 603,

	616, 627 , 628, 631, 632, 635, 636
Nonylphenol	29, 38, 100, 106, 127, 143, 218, 222, 251, 267, 309, 348, 349, 355, 380, 381, 395, 409, 415, 416, 419, 431, 451, 470, 482, 483, 484, 485, 486, 492, 630, 636, 637, 638
NPEs	14, 29, 38, 100, 106, 127, 142, 218, 222, 309, 355, 380, 381, 382, 415, 419, 431, 458, 470, 482, 484, 485, 486, 492
Norfloxacin	22, 102, 140, 187, 199, 292, 344, 368, 378, 417, 437, 442, 480, 632
Octylphenol	14, 24, 29, 106, 127, 142, 143, 170, 218, 309, 395, 409, 416, 458, 486, 492, 630, 637, 646
Perfluorooctanoic acid (PFOA)	51, 125, 239, 305, 387, 418, 440
Perfluorooctyl sulfonate (PFOS)	51, 125, 228, 239, 305, 387, 418, 440
Pyrene	33, 90, 190, 267, 408
Ranitidine	200, 226, 291, 313, 317, 437, 438, 471, 480
Roxithromycin	22, 29, 41, 133, 143, 153, 417, 423, 430, 616, 627, 632
Sulfamerazine	22, 368, 371, 400, 463
Sulfamethoxazole	8, 22, 29, 31, 41, 87, 107, 109, 133, 143, 153, 177, 200, 222, 224, 225, 291, 298, 313, 368, 371, 376, 377, 383, 400, 423, 430, 437, 442, 447, 480, 488, 601, 616, 631, 632, 636, 637
Testosterone	335, 349, 451, 482, 641, 644
Tetracycline	22, 109, 118, 187, 196, 197, 199, 290, 292, 298, 344, 368, 376, 383, 480, 627, 632, 637
Tonalide (AHTN)	8, 10, 43, 107, 112, 114, 133, 341, 386, 396, 416, 450, 488, 636, 637
Triclosan	29, 43, 107, 112, 114, 133, 205, 386, 396, 416, 450, 488, 636, 637, 646
Trimethoprim	7, 22, 41, 44, 104, 109, 123, 143, 187, 222, 298, 313, 317, 367, 368, 383, 395, 416, 417, 423, 437, 616, 627, 637

APPENDIX C

Table C1. Removal efficiencies for selected CECs by MBR treatment.

CEC	Reference	Scale	Liquid % Removal	CEC	Reference	Scale	Liquid % Removal
Atrazine	233	Full, Lab	9	Musk Ketone	646	Full, Pilot	36-49
Benzophenone	646	Full, Pilot	88->99	Norfloxacin	632	Full	80
	74	Lab	60-80	Octylphenol	646	Full, Pilot	>99
	639	Full	>90		29	Full	44-99
	640	Full	98		106	Pilot	85
Caffeine	639	Full	>90	PFOA	305	Full	<0
	646	Full, Pilot	79->99.9	PFOS	305	Full	<0
	416	Full	>99	Ranitidine	200	Full	95
Ciprofloxacin	17	Pilot	98.9		313	Pilot	29.5-44.2
DEET	640	Full	40.6	Sulfamethazine	58	Lab	77
	646	Full, Pilot	>84		632	Full	35
	639	Full	50-90	Tetracycline	197	Pilot	79-89
	416	Full	90		632	Full	65
	632	Full	70	Tonalide (AHTN)	10	Pilot	80-85
DEHA	21	Pilot	3.31		416	Full	30
DEHP	21	Pilot	10.22		66	Pilot	40-45
Galaxolide (HHCB)	66	Pilot	40-45		133	Full	45-50
	133	Full	35-60	Triclosan	627	Full, Pilot	66-73
	416	Full	90		632	Full	85
	646	Full, Pilot	36-68		639	Full	>90
Indomethacin	200	Full, Lab	46.6		640	Full	90.2
	313	Pilot	39.7-41.4		646	Full, Pilot	78-96

In this and subsequent tables, reference numbers correspond to database.

Table C2. Removal efficiencies for selected CECs by tricking filters.

CEC	Reference	Scale	Liquid % Removal	CEC	Reference	Scale	Liquid % Removal
Bezafibrate	226	Full	50-60	Ibuprofen	133	Full	90-99
Caffeine	467	Full	96-98		226	Full	50-90
Carbamazepine	133	Full	0-10		467	Full	77-99
	226	Full	7-91	Ketoprofen	226	Full	50-90
	467	Full	6-31		467	Full	93-100
Diclofenac	133	Full	20-25	Naproxen	133	Full	35-40
DEHP	148	Full	<0–44		226	Full	50-90
	226	Full	50-90		467	Full	66-98
	467	Full	65-96	Nonylphenol	294	Full	<0-50
EE2	421	Full	>69		332	Lab	86.4
E2	211	Full	83	Ranitidine	226	Full	50-91
	391	Full	58.3	Roxithromycin	133	Full	0-40
Estriol	211	Full	90.5	Sulfamethoxazole	133	Full	65-75
	391	Full	57-76.3	Tonalide (AHTN)	133	Full	45-50
Estrone	211	Full	90	Triclosan	491	Full	92.7
	391	Full	96.5		294	Full	75
Galaxolide (HHCB)	133	Full	40-45				
Gemfibrozil	467	Full	72-90				
	226	Full	50-60				

Table C3. Removal efficiencies for selected CECs by SBR treatment.

CEC	Reference	Scale	Liquid % Removal	CEC	Reference	Scale	Liquid % Removal
Bezafibrate	325	Pilot	40-99	Estriol	325	Pilot	20-99
Bisphenol A	325	Pilot	80-99	Estrone	243	Lab	70-100
Carbamazepine	325	Pilot	40-99		258	Full	93.2
	338	Full	>20		325	Pilot	20-99
Diclofenac	325	Pilot	20-70	Galaxolide (HHCB)	43	Full	72
DEHP	85	Lab	95-97	Ibuprofen	325	Pilot	90-99
EE2	243	Lab	<0-50	Musk Ketone	43	Full	60
	325	Pilot	<0-70	Nonylphenol	122	Lab	36.2-75.4
E2	243	Lab	60-100	Sulfamethoxazole	306	Lab	>99
	258	Full	83.3				

Table C4. Removal efficiencies for selected CECs by lagoon treatment.

CEC	Reference	Scale	Liquid % Removal	CEC	Reference	Scale	Liquid % Removal
Acetaminophen	126	Full	>99	Ibuprofen	4	Full	27-74 winter; 6-96 summer
Caffeine	479	Pilot	85-99		121	Full	17-99
	4	Full	23-58 winter; 82-99 summer		126	Full	>99
	126	Full	>99		154	Full	95-96
Carbamazepine	4	Full	24-36 winter; 48 summer		373	Pilot	48-81
	126	Full	51		479	Pilot	17-80
	154	Full	30-47	Ketoprofen	479	Pilot	45-69
	373	Pilot	16-26		154	Full	97-99
Clofibric acid	115	Pilot	<10	Naproxen	154	Full	52-92
	154	Full	32-36		126	Full	>99
Diclofenac	154	Full	73-96		479	Pilot	47-90
	4	Full	17-26 winter; 36-52 summer		4	Full	27-66 winter; 27-83 summer
EE2	204	Pilot	16.9-91.6		121	Full	47-89
E2	204	Pilot	54.7-92.2	Sulfamethoxazole	126	Full	92
Estrone	204	Pilot	13.8-78.2	Tonalide (AHTN)	4	Full	0-65 winter; 30-80 summer
Galaxolide (HHCB)	4	Full	0-65 winter; 30-80 summer		479	Pilot	32-65
	479	Pilot	31-61	Triclosan	294	Full	39
Gemfibrozil	126	Full	95				

APPENDIX D. Chemicals of Emerging Concern

The CECs on this list were originally described by Klečka et al. (2010). Detailed information on the categories, studies reviewed, and findings can be found in that report.

CEC Categories:

- Current use pesticides (CUPs)
- Pharmaceuticals
- Alkylphenol Ethoxylates (APEs)
- Synthetic musks
- Organics wastewater contaminants (OWCs); including Personal care products (PCPs), and Steroids and hormones
- Perfluorinated surfactants (PFOS)
- Polybrominated diphenyl ethers (PBDEs)
- Other flame retardants (FRs)
- Chlorinated paraffins (CPs)

Table D1. Current Use Pesticides (CUPs)

Neutral Herbicides	Acid Herbicides	Insecticides	Fungicides	Parasiticides
Acetochlor	2,4,5-T	Aldicarb	Chloroneb	Oryzalin
Alachlor	2,3,6-TBA	Azinphos-methyl	Chlorothalonil	
Atrazine	2,4,5-TP	Carbaryl	DNOC (Dinitro-o-cresol)	
Barban	2,4-D	Carbofuran		
Benfluralin	2,4-DB	Chlorpyrifos		
Bentazon	2,4-DP	Diazinon		
Benzoylprop-ethyl	Acifluorfen	Dibrom		
Bromacil	Bromoxynil	Dimethoate		
Butylate	Chloramben methyl	Disulfoton		
Cyanazine	Clopyralid	Ethion		
D-Atrazine	Dacthal	Ethoprop		
Deethylatrazine (DEA)	Dicamba	Endosulfan		
Diallate total isomer	MCPA	Fonofos		
Diallate-1	MCPB	Malathion		
Diallate-2	MCPP	Methiocarb		
Dichlobenil	Picloram	Methomyl		
Dichlorprop	Triclopyr	Methoprene		
Diclofop-methyl		Methyl parathion		
Dinoseb		Oxamyl		
Diuron		Parathion		
D-Simazine		cis-Permethrin		
EPTC		trans-Permethrin		
Ethalfluralin		Phorate		
Fenuron		Phosmet		
Fluometuron		Propargite		
Glyphosate - AMPA		Propoxur		
Glyphosate		Terbufos		
Linuron				
Metolachlor				
Metribuzin				

Molinate				
Napropamide				
Neburon				
Norflurazon				
Pebulate				
Pendimethalin				
Prometon				
Pronamide				
Propachlor				
Propanil				
Propham				
Simazine				
Tebuthiuron				
Terbacil				
Thiobencarb				
Triallate				
Trifluralin				

Table D2. Pharmaceuticals

Veterinary and Human Antibiotics	Prescription Drugs	Non-prescription Drugs
Azithromycin	Albuterol	Acetaminophen
Carbodox	Atorvastatin	Caffeine
Chloramphenicol	Bezafibrate	Cotinine
Chlortetracycline	Carbamazepine	1,7-Dimethylxanthine
Ciprofloxacin	Cimetidine	Diphenhydramine
Doxycycline	Clofibric acid	Ibuprofen
Enrofloxacin	Codeine	Ketoprofen
Erythromycin	Cyclophosphamide	Miconazole
Lincomycin	Dehydronifedipine	Naproxen
Monensin	Diclofenac	
Norfloxacin	Digoxin	
Oxytetracycline	Digoxigenin	
Roxithromycin	Diltiazem	
Sarafloxacin	Enalaprilat	

Sulfachloropyridazine	Fenoprofen	
Sulfadimethoxine	Fluoxetine	
Sulfamerazine	Gemfibrozil	
Sulfamethazine	Indomethacin	
Sulfamethizole	Meclocycline sulfosalinicylate	
Sulfamethoxazole	Metformin	
Sulfathiazole	Norfluoxetine	
Tetracycline	Paroxetine metabolite	
Thiabendazole	Pentoxifylline	
Trimethoprim	Ranitidine	
Tylosin	Warfarin	
Virginiamycin		

Table D3. Alkylphenol Ethoxylates

Alkylphenol Ethoxylates
NP
NP1EO
NP2EO
NP3-17EO
NPEC
OP
OPEO
OPEC

Table D4. Synthetic Musk

Synthetic Musks
AHTN
HHCB
ATII
ADBI
AHMI
DPMI
Musk Ketone
Musk Xylene

Table D5. Organic Wastewater Constituents (OWCs)

Anticorrosives/ antioxidants	Deodorizer/fragrance	Disinfectants	Insect Repellant
Butylated hydroxy toluene	Acetophenone	4-Methyl phenol	N,N-Diethyl-toluamide
3-tert-Butyl-4-hydroxy anisole	Acetyl hexamethyl tetrahydronaphthalene (AHTN)	Phenol	
2,6-Di-tert-p-benzoquinone	Camphor	Triclosan	
2,6-Di-tert-butyl-phenol	1,4-Dichlorobenzene		
5-Methyl-1H-benzo-triazole	Hexahydrohexamethylcyclopentabenzopyran (HHCB)		
	Indole		
	Isoborneol		
	Isoquinoline		
	d-Limolene		
	Menthol		
	3-Methyl Indole		
Plasticizers/plastic manufacture	**Polycyclic Aromatic Hydrocarbons**	**Solvents**	**Steroids/ hormones**
Anthraquinone	Anthracene	Isophorone	cis-Androsterone
Benzophenone	Benzo (a) pyrene	Tetrachloroethylene	Cholesterol
Benzylbutylphthalate	2,6-Dimethylnaphthalene		Coprostanol
Bis (2-ethylhexyl) adipate	Fluoranthene		Equilenin
Bis (2-ethylhexyl) phthalate	1-Methylnaphthalene		Equilin
Bis (isononyl) phthalate	2-Methylnaphthalene		17a-Estradiol
Bisphenol A	Naphthalene		17a-Ethynyl estradiol
Carbazole	Phenanthrene		17b-Estradiol
4-Cumylphenol	Pyrene		Estriol
Diethyl phthalate			Estrone
Ethanol, 2-butoxy phosphate			Mestranol
Isopropylbenzene			19-Norethisterone
Phthalic anhydride			Progesterone
2,2,4,4-Tetrabromodiphenylether			ß-Sitosterol
Tributylphosphate			ß-Stigmastanol
Triphenyl phosphate			Testosterone
Tris(2-butoxyethyl) phosphate			
Tris(dichloroisopropyl)phosphate			

Table D6. Perfluorinated Surfactants

PFS	PFA
PFHxS	TFA
PFOS	PFPrA
PFOSulfinate	PFBA
PFOSA	PFPeA
PFOSAA	PFHxA
N-EtFOSA	PFHpA
N-EtFOSAA	PFOA
N-EtFOSE	PFNA
	PFDA
	PFUnA
	PFDoA
	PFTrA
	PFTeA
	PFPA

PFS – Perfluorinated surfactants
PFA – Perfluoroalkylated surfactants

Table D7. Polybrominated Diphenyl Ethers

Polybrominated Diphenyl Ethers
Br_3 BDE
Br_4 BDE
Br_5 BDE
Br_6 BDE
Br_7 BDE
Br_8 BDE
Br_9 BDE
Br_{10} BDE or BDE-209

BDE – Brominated diphenyl ether

Table D8. Other Flame Retardants

Other Flame Retardants
BTBPE
HBB
PBEB
PBT
TBE
Total DP
Total HBCD
Tri (2-chloro-ethyl) phosphate
Tri (di-chloro-isopropyl) phosphate
Tri(dichloro-propyl phosphate)

Table D9. Chlorinated Paraffins

SCCP	MCCP
C10	C14
C11	C15
C12	C16
C13	C17

SCCP – short chained chlorinated paraffins.
MCCP – medium chained chlorinated paraffins.