Transformation of PPCPs in the environment: Review of knowledge and classification of pathways according to parent molecule structures

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ABSTRACT

Reviewing the transformation pathways and analyzing the reactions undergone according to the matrices and the parent compound chemical structures may help to progress in our understanding of transformation processes of PPCPs. Of the 199 parent molecules initially targeted, 42% had no information on their transformation products (TPs). The transformation of the remaining 116 PPCPs led to 1371 TPs formed by biotic (630), abiotic (568), and both biotic and abiotic (61) reactions in natural (solid waste, natural waters, soils, WWTP effluents, sediments) and/or synthetic matrices. For a small number of TPs (112) no information was found on the conditions of their formation. Eleven main transformation reactions

(hydroxylation, dehydrogenation, cleavage, hydrolysis, dealkylation, oxygenation, dehalogenation, other eliminations, other substitutions, addition and rearrangement) were considered to describe the TPs dataset, that ended up with 3230 individual reactions (one TP can result from several successive reactions). Hydroxylation was the major reaction occurring at 28% followed by dehydrogenation (13%), then cleavage (11%). A majority of studies were performed in synthetic media whereas knowledge on transformation reactions in environmental matrices is very heterogeneous with less information on soils and sediments. Finally, we aimed at assessing the relationship between the transformation reactions and the chemical structures of the parent molecules using 1178 molecular fragments and molecular descriptors. Several clusters composed of sulfonamides, cyclines or macrolides showed trends between functional groups and reactions involved in the transformation pathways. Based on these data and results, some research needs were highlighted.

KEYWORDS PPCP; pharmaceuticals; transformation product; environment; biotransformation; functional groups

1. Introduction

Pharmaceuticals and personal care products (PPCPs) have been increasingly studied over the past twenty years. They contain diverse groups of organic compounds, named according to their pharmacological use or effect, such as antibiotics, hormones, anti-inflammatory drugs, antiepileptic drugs, blood lipid regulators, β-blockers, contrast media, and cytostatic drugs for pharmaceuticals; and antimicrobial agents, synthetic musks, insect repellants, preservatives, fragrance components, and sunscreen UV filters for personal care products (Daughton & Ternes 1999; Kagle et al., 2009). Global world consumption of pharmaceutical active substances was estimated at more than 100,000 tons per year in 2008 (Touraud, 2008), and that of personal care

products at several thousand tons per year (Heath et al., 2006). In 2012, more than 4 000 pharmaceuticals were currently used, and many types for personal care products (Boxall et al., 2012).

For some years, technical advances in analytical chemistry made it possible to monitor and quantify PPCPs in the environment (Kagle et al., 2009). They have evidenced the ubiquitous presence of pharmaceuticals and other so-called 'emerging contaminants', albeit in trace or ultra-trace concentrations (below ng/L), which consequently became of great concern in recent years (Tijani et al., 2016). In particular, questions raised regarding chemical persistence, microbial resistance (Chen et al., 2016), and synergistic effects of the numerous PPCPs encountered in the environment (Vasquez et al., 2014).

The fate of PPCPs in the aquatic environment is governed by several major processes: aerobic and anaerobic biotransformation, abiotic transformation, hydrolysis, photodegradation, and sorption on sediments (Baena-Nogueras et al., 2017). In soils, the fate of PPCPs mainly depends on their sorption and transformation. These processes are controlled by soil properties like organic matter, clays, exchangeable cations, pH, as well as by soil microbial activity related to the abundance and diversity of microbial communities (Xu, et al., 2009).

Understanding the fate and effects of PPCPs in the environment is therefore essential from a human and environmental health perspective. One of the key issues in elucidating the fate of PPCPs in the environment is to better understand their transformation pathways. Indeed, the number of studies on the transformation of PPCPs has increased significantly in recent years. In the literature, both transformation products (TPs) and metabolites originating from PPCPs can be found. Transformation products result from a change in the structure of a molecule after its release in the environment (soil, water…), due to both biotic and abiotic processes (Kümmerer, 2009). Metabolites, as for them, result from changes in the chemical structure of the parent molecule in the body or on the skin of treated humans and animals

(Längin et al., 2008). They can be formed by biological and/or non-biological processes and often result from metabolic pathways in humans and animals (Kümmerer, 2009). They were not retained in this work which is focused on transformations in environmental matrices.

It has already been observed that the transformation of PPCPs varies from one compound to another, as exemplified by the high degree of transformation of oestradiol by comparison to the low one of carbamazepine in waste water treatment plant (WWTP) (Behera et al., 2011). Moreover, the transformation of the parent molecule in the environment and WWTPs could lead to an increase in toxicity, as shown by the example of naproxen which was transformed into more toxic photo-products (Isidori et al., 2005), or by that of diclofenac and its (2-[2-(chlorophenyl)amino]benzaldehyde) TP which has been shown to be ten times more toxic for one species of algae (Diniz et al., 2015).

Better understanding and identification of the general rules of the transformation pathways of PPCPs in various matrices would make it possible to better characterize the fate of PPCP TPs in the environment and in WWTPs which is a crucial issue. Therefore, the objective of this work was to provide a comprehensive review of the available knowledge on the transformation pathways of PPCPs in the environment and in WWTPs. Published data on the detection and identification of TPs in synthetic media, solid wastes, soils, sediments, natural waters and WWTP effluents were compiled in a database and analyzed with respect to the transformation pathways responsible for their formation. In the database, the transformation pathways were described by considering major elementary reactions. The data were then analyzed taking into account the predominant transformation pathways and their occurrence according to the matrices where they took place, and to the chemical structures of the parent molecules.

2. Literature review and bibliometry

2.1 Selection of relevant articles focused on PPCP transformation pathways in the environment

In order to collect data on the transformation of PPCPs in synthetic and non-synthetic matrices and on their corresponding TPs, a literature search was conducted on the Web of Science. First, the list of PPCPs to be studied was defined considering the following criteria: frequent occurrence in environmental matrices and WWTPs, priority substances listed in regulatory texts (AFSSA, 2010; ANSES, 2010), diversity of environmental behaviours, and diversity in the use families. We ended up with a list containing 199 PPCPs (Tables S1 and S2).

Then, the literature search was based on a four-part equation linked by the boolean "AND". The first part contained the name of the molecule being searched for. The second and third parts contained a list of relevant keywords related to the transformation of PPCPs. The last part of the query consisted of keywords related to the different matrices. Therefore, the final equation was as follows: TS/TI=(Molecule name) AND TS/TI=(Keywords 1: Transformation product OR Metabolite OR Microbial degradation OR Degradation OR Biotransformation OR Biodegradation) AND TS=(Keywords 2: Fate OR Emerging contaminant fate OR Drugs OR Micropollutant degradation OR Degradation pathways OR Dissipation OR Anaerobic biotransformation OR Hydrolysis OR Photolysis OR Strain) AND TS=(Keywords 3: Aquatic OR Sediment OR Surface water OR Digestate OR Groundwater OR WWTP OR Treatment plant OR Soil OR Terrestrial OR Agricultural soils OR Wastewater OR Manure OR Biosolids OR Slurry OR Sludge OR Activated sludge OR Incubation OR Membrane bioreactor OR Batch OR Sewage OR Environment).

The used index was SCI-EXPANDED, SSCI, A&HCI, CPCI-S, CPCI-SSH, BKCI-S, ESCI, CCR-EXPANDED, and IC; and the publication types were article, book, book chapter,

data paper, proceedings paper and review. The spanning time for the selection of publications was from 1975 to 2019.

The number of articles varied according to the molecule. Thus, for each molecule, the field tags TS (Subject) and TI (Title) associated to the search were declined in three different combinations considering the number of articles. The higher the number of articles for a molecule, the more the TI field tag was used. It allowed limiting the search to the keywords that made up the title of the article. If the number of articles was large, the TI tag was used in the code, first for the "Molecule name", then for the "Keywords 1". Therefore, the three combinations used during the bibliographic search were the following: (i) for a molecule that has not been studied much and therefore with a low number of articles (< 20): 4 TS (TS = “Molecule name” + TS = “Keywords 1” + TS = “Keywords 2” + TS = “Keywords 3”) ; (ii) for a molecule with moderate number of articles (20-100) : TI + 3 TS (TI = “Molecule name” + TS = “Keywords 1” + TS = “Keywords 2” + TS = “Keywords 3”); (iii) for a molecule with a very large number of articles (>100): 2 TI + 2 TS (TI = “Molecule name” + TI = “Keywords 1” + TS = “Keywords 2” + TS = “Keywords 3”).

Once this step was completed, the results were refined by analyzing the bibliography from the title of the articles and/or of the abstracts. Following this step, the selected articles were read and considered according to the relevance of the information found. In the end, the number of selected publications was 265 (Table S1). Among these articles, 189 were published since 2008, so 71% of our dataset was published in the 2008-2019 period.

Finally, on the 199 initially listed PPCPs, 83 were discarded (Table S2): for 23 molecules, no transformation product was found in the literature, for 60 other ones, there were only data concerning their metabolites. Therefore, the final dataset consisted of 116 PPCPs.

2.2 Data reliability and analysis

For a robust analysis of PPCP transformation pathways, one important point was to determine the analytical confidence level of the identified TPs (Table S3). Therefore, a four-class confidence scale was created: (1) “very good” for TPs that were identified by chromatography coupled to tandem mass spectrometry MS/MS; (2) “good” for TPs identified by MS with a reference or coupled with another method (NMR, X-Ray…); (3) “intermediate” for TPs identified without MS; (4) “bad” for TPs without information (Table S3).

Ninety-three percent of the reviewed TPs were found to have very good or good confidence levels. Considering the "Intermediate" category as acceptable led to 95% of the TPs having an acceptable level of analytical confidence. Only 42 TPs over 1371 (i.e. 3%) had a low level of analytical confidence (Table S3). These 42 TPs were nevertheless considered in this review because they have been studied for a long time and because some related data can be found in existing databases such as EAWAG-BBD (Ellis & Wackett, 2012).

2.3 Description of the dataset

Among the 116 PPCP parent compounds of this study, 101 were pharmaceuticals and 13 were personal care products. Tetrabromobisphenol A and bisphenol A were added to the study because significant information was available on their transformation products and transformation pathways, and they are often classified as PPCPs (Hernandez-Liuz et al. 2012; Dodgen et al. 2014; Qin et al., 2015; Porter et al. 2020). The dataset covers 32 families of use of PPCPs. The most represented pharmaceutical families were antibiotics (26% of the 116 compounds), non-steroidal anti-inflammatory drugs (NSAIDs) (11%), and hormones (9%). For personal care products, the most common families of compounds were flame retardants (8%), excipients (4%), and fragrance components (3%). The representativeness of the collected data was thus heterogeneous, with some families of use much better represented than others. This

could reflect low presence in the environment of the less represented compounds compared to the predominant ones, but more probably less investigations, therefore providing fewer articles in the literature.

All of the TP data were then analyzed according to the different matrices in which the PPCP transformation products were identified and quantified. Six different matrices were reviewed which differed by their physico-chemical conditions (pH, temperature, the concentration of suspended solid...): the most represented matrix, synthetic media, covered 65% of the reviewed data. In addition to the synthetic media, five non-synthetic matrices were distinguished: WWTP effluents (raw and treated wastewater), solid wastes (this medium category contains media with high suspended solids including activated sludge, membrane and anaerobic sludge, manure, compost), soils, natural waters (surface and ground waters), and sediments. The data were distributed as follows: 16% for solid wastes, 9% for natural waters, 5% for WWTP effluents, 4% for soils, and 1% for sediments.

As indicated above, the majority of the studies focused on the transformation of PPCPs in synthetic media, either in biotic or abiotic controlled conditions. A synthetic medium is used with controlled pH, temperature, and redox potential. For biotic transformation, a solution of micro and macronutrients and an inoculum are added to the medium. The most frequently used inocula were bacterial strains (mainly *Sphingonomas, Pseudomonas* and *Rhodococcus* families) (Ivshina et al., 2019; Tanner & Hopper, 2000; Veetil et al., 2012), fungi (*Trametes versicolor*, *Mycobacterium gilvum*) (Adjei et al., 2006; García-Galán et al., 2011), and microalgae (Della Greca et al., 2008; Hom-Diaz et al., 2015). For abiotic transformation, studies were performed in controlled conditions mimicking the physico-chemical processes used in WWTPs or occurring in the environment.

For the studies performed in the non-synthetic matrices, many articles referred to TP identification in solid wastes, i.e. sludge (activated, denitrifying…) (Chiron et al., 2010;

Huntscha et al., 2014), and in manure (Angenent et al., 2008; Spielmeyer et al., 2016). WWTP effluents are also a frequently studied matrix for PPCP transformation (Tran et al., 2018). Indeed, most PPCPs enter WWTPs as household, hospital and industrial components or through runoff (Daughton & Ternes, 1999; Suárez et al., 2008). However, as the removal may be incomplete and may result in the release of these contaminants into receiving waters (Daughton & Ternes, 1999; Heberer, 2002; Suárez et al., 2008), TPs were also searched for and identified in natural waters, including surface water (Henning et al., 2018; Jakimska et al., 2014) and groundwater (Kang et al., 2008). The soil matrix is also impacted by PPCPs because they can be introduced by sludge spreading or landfilling (Daughton & Ternes, 1999), livestock effluent or waste application, and reclaimed water irrigation (Bourdat-Deschamps et al., 2017; Lu et al., 2019). The degradation of PPCPs in soil can be studied in laboratory (Koba et al., 2017) or at the field scale (Topp et al., 2016). In these experiments, soils can be supplemented with organic fertilizers such as raw, digested or composted manure, or biosolids (Zhang et al., 2017). Finally, little information was found for the sediment matrix where the PPCPs transformation has mostly been studied in river sediment samples (Li et al., 2014; Peng et al., 2015).

2.4 Statistical analysis

Fingerprints (FPs) are fixed-size Boolean vectors that encode the structural information of a molecule by exploding its structure in all possible sub-structure models (according to a given set of rules) and then processing these models with a hash algorithm (Shemetulskis et al., 1996). The parameters used for fingerprints are 1024 bits for size, 2 bits per pattern with a maximum length of six atoms. The encoding of the sub-structures is not known and therefore the molecular fragments are used to describe the clusters. Molecular fragments are strings of atoms that can reach a maximum length of nine atoms provided with fingerprints which are indicators of the composition of clusters. The molecular descriptors were obtained with the Dragon 7.0 software

(2017). Only molecular descriptors describing functional groups were selected for our dataset. Finally, a total of 1178 variables (1025 fingerprints and 153 molecular descriptors) were provided for each of the 116 PPCPs (Table S4). The dataset was then statistically processed by Hierarchical Clustering on Principal Component (HCPC). The 116 molecules were found to be distributed in nine clusters (Table S5), forming different chemical classes. The variance explained by the first two PCA axes was 40.3%.

Each cluster was characterized by the median values of the molecular descriptors and fragments identified in the PPCP molecules belonging to the cluster. Then, PPCP clusters were related to the chemical reactions identified in their transformation pathways (see 3.1).

3. Transformation pathways of PPCPs and their occurrence in synthetic and non-synthetic matrices

Each TP results from various transformation pathways (Table S6) and can be found in several matrices. As indicated above, human metabolites were not targeted in the review, but information collected on molecules that are both metabolites and TPs was retained for further discussion.

The transformation process can be biotic or abiotic, which makes it possible to distinguish between biotic (BTP) and abiotic (ATP) TPs. A total of 630 BTPs was found in the reviewed articles. These BTPs have been identified in degradation studies with bacterial strains, fungi or microalgae (Čvančarová et al., 2015; Ding et al., 2018; Wetzstein et al., 2006). Some of them can be of both human (MB) or microbial (BTP) origin (Rubirola et al., 2014) as some cytochromes can similarly degrade the parent molecule in humans and in fungi (Marco-Urrea et al., 2009). We also identified 568 ATPs that can be formed in WWTPs or during drinking water treatment (ozonation, chlorination), but also by natural abiotic processes such as hydrolysis, oxidation or photolysis. Some ATPs may be identical to BTPs as shown by Sanchez-

Prado et al. (2006) with triclosan and its 2,4-dichlorophenol TP. Among the 1371 TPs, 61 can be produced both by biotic and abiotic transformations (ABTPs). Finally, for 112 TPs, there was no indication of their biotic or abiotic origin.

3.1 Main chemical reactions involved in the transformation of PPCPs

Transformation pathways were described according to the chemical reactions involved in the transformation of a parent molecule into its TPs. For some TPs of the dataset, these reactions were described in the source articles, whereas for others, we identified the reactions involved according to the observed change in the chemical structure. From the 116 PPCPs and 1371 TPs, 3230 transformation reactions were recorded (since one TP can result from several successive transformation reactions).

Among the various reviewed chemical reactions, eleven of them occurred very frequently (occurrence > 100): hydroxylation, dehydrogenation, cleavage, other eliminations, hydrolysis, other substitutions, dealkylation, oxygenation, addition, dehalogenation, and rearrangement (Table S6 and Figure 1).

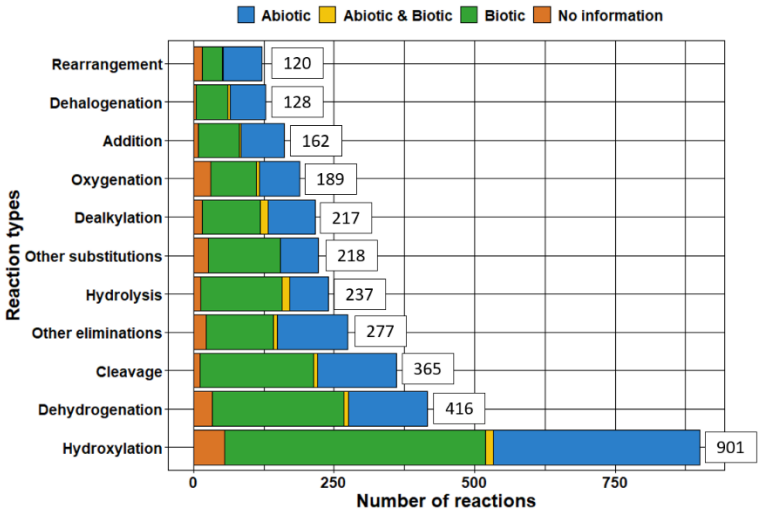

Figure 1. Number of transformation reactions (N=3230 reactions) according to the eleven main reaction types (addition, cleavage, dealkylation, dehalogenation, dehydrogenation, hydrolysis, hydroxylation, other eliminations, other substitutions, oxygenation and rearrangement).

Hydroxylation, more commonly known as mono-oxidation, was the most observed reaction with 901 records that is 28% of the total number of reactions enumerated in the dataset (Figure 1). For biotic processes, the monooxygenase enzyme, which belongs to the cytochrome P450 enzymatic system, catalyzes the formation of a hydroxyl group -OH from an oxygen or dioxygen using NADH or NADPH (Nelson & Cox, 2000).

Dehydrogenation corresponds to the removal of two hydrogen atoms from a molecule. It is also an oxidation sub-reaction. With 416 records (13%), dehydrogenation was the second most occurring reaction.

The third most abundant one (with a total of 365 records, 11%) was cleavage which is a breakdown of carbon-carbon bonds.

Then, the following reactions were observed: other eliminations (277 records), defined by the loss of one functional group, gathers decarboxylation (99), dehydroxylation (39) and other sub-reactions of elimination (139); hydrolysis (237 records) which causes covalent bond breaking by the action of water; other substitutions (218 records) which corresponds to the replacement of a functional group by a hydrogen atom already present on the molecule and include sub-reactions such as alkylation (78) or carboxylation (36); dealkylation (217 records) which removes an alkyl group from a molecule, occurring mainly on a nitrogen (N-dealkylation) or oxygen (O-dealkylation) atom; oxygenation (189 records) where an oxygen atom is transferred from the dioxygen molecule, often associated with dehydrogenation; addition (162 records) grouping together all the reactions that were assimilated to the loss of unsaturated bonds, including mostly hydrogenation and hydration; dehalogenation (128 records), which is the elimination of a halogen (-Cl, -Br); and rearrangements (120 records) corresponding to isomerization reactions of the molecule which will keep the same number of atoms but will change its chemical structure.

The hydroxylation, dehydrogenation, cleavage, hydrolysis, other substitutions, dealkylation and oxygenation reactions mainly occurred under biotic conditions whereas rearrangement occurred under abiotic ones. The other eliminations, dehalogenation and addition reactions, were found in biotic as well as in abiotic conditions (Figure 1).

3.2 Occurrence of transformation pathways in various matrices

To determine whether the transformation in synthetic media reflects the transformation in non-synthetic ones, we compared the corresponding TPs. In general, TPs found in non-synthetic matrices were also found in synthetic matrices. They were counted once and recorded in the synthetic matrices. The main differences between studies using non-synthetic matrices and those using synthetic ones were: (i) the description of the transformation pathways, which was more detailed in synthetic controlled experiments. Consequently, these data could be used in a second step to search for TPs in non-synthetic matrices; (ii) the spiking of parent molecules in synthetic matrices, which was not always representative of environmental concentrations. This could generate transformation pathways that would be found in a lesser extent or not at all in non-synthetic environments.

Several examples of PPCPs with TPs observed in both media can be given. Azithromycin, which has been studied in *in vivo* conditions of agricultural soils as well as in synthetic medium, is one (Terzic et al., 2018; Topp et al., 2016): in both cases, similar TPs, formed by hydrolysis, were identified. For ibuprofen, the 2-hydroxy-ibuprofen TP was characterized in synthetic media (Marco-Urrea et al., 2009), but also in WWTPs (Boix et al., 2016) and sediments (Li et al., 2014).

Figure 2 shows the distribution of biotic vs abiotic reactions according to the matrix in which the transformation takes place. Studies on solid matrices (sediments, solid wastes and soils) mainly focus on biotic transformations whereas studies on liquid matrices (natural waters

and WWTP effluents) mainly concern abiotic transformations, particularly photodegradation studies. Finally, for studies in synthetic media, the proportion of biotic transformations is slightly higher than that of abiotic transformations.

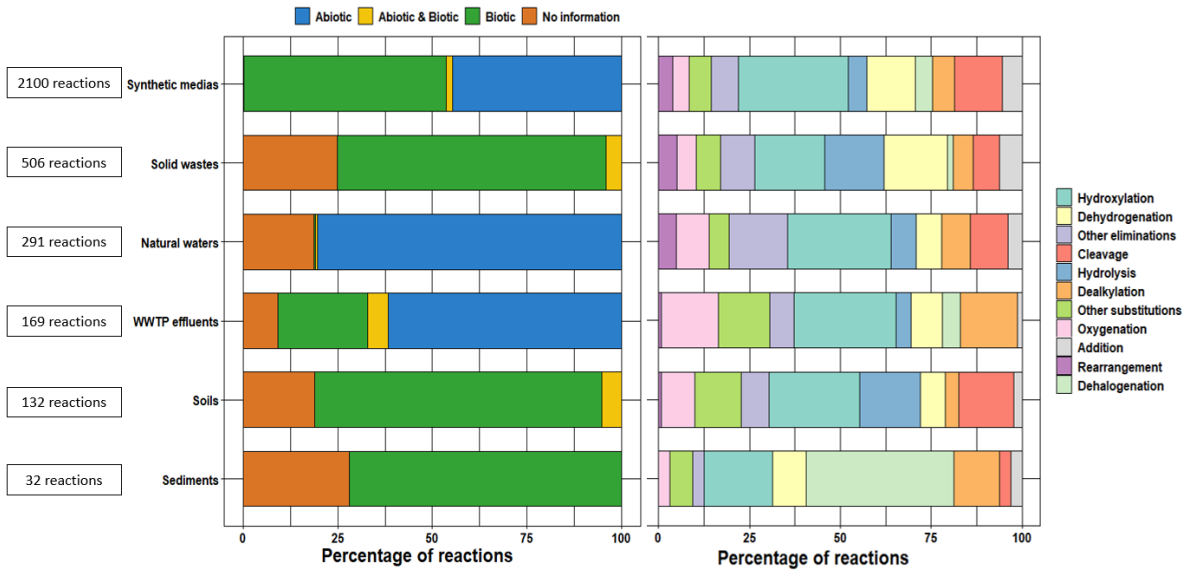

Figure 2. Distribution of reactions involved in the transformation of PPCPs in the different matrices (N=3230 reactions) according to the reaction conditions (biotic, abiotic) (left), and according to the eleven main reaction types (addition, cleavage, dealkylation, dehalogenation, dehydrogenation, hydrolysis, hydroxylation, other eliminations, other substitutions, oxygenation and rearrangement) (right).

The eleven chemical reactions describing the PPCP transformation pathways can be found in both synthetic and non-synthetic matrices but not systematically in the same proportions (Figure 2). Hydroxylation, dehydrogenation, cleavage, and other eliminations corresponded to 70% of the reactions in synthetic matrices. In non-synthetic matrices, except sediments, hydroxylation was the predominant reaction. In solid waste (the first represented matrix with 506 reactions), three main reactions were recorded: hydroxylation (19%), dehydrogenation (17%) and hydrolysis (16%). In natural waters (291 reactions), the most important reactions were other eliminations (16 %), cleavage (11 %) and oxygenation (9 %).

The WWTP effluents group (169 reviewed reactions) mainly involved oxygenation (16 %), dealkylation (16 %) and other substitutions (14 %). Then, the most observed reactions in the soil matrices (132 reactions) were hydrolysis (17 %), cleavage (15 %) and other substitutions (13 %). Finally, in the sediment matrix, which was the least studied matrix (32 reactions), dehalogenation was the predominant reaction (41%). Indeed, in this matrix, anoxic or anaerobic conditions are commonly found and tested (Kagle et al., 2009), and are favourable for dehalogenation. Overall, addition and rearrangement were minor reactions (<6%) in all matrices.

Different trends were observed between solid (solid wastes and soils) and liquid (natural waters and WWTPs) non-synthetic matrices (Figure 2). Hydrolysis, cleavage and dehydrogenation reactions were predominant in the solid matrices. This was observed, for example, for the cladinose and desosamine groups for macrolide molecules in solid waste (Terzic et al., 2018) as well as for sulfamethoxazole in soil (Martin-Laurent et al., 2019). For liquid matrices, the trends were different between natural waters and WWTP effluents. Dealkylation, oxygenation and other substitutions were better represented in the WWTPs, while cleavage and other eliminations were not present, which contrasts with natural waters (Figure 2). For example, cleavage was observed for flumequine transformation in natural waters as well as decarboxylation (Feng et al., 2016). Dealkylation has been observed for azythromycin (Senta et al., 2019), citalopram (Osawa et al., 2019a), and iopromide (Gros et al., 2014) in WWTPs. Oxygenation was found for citalopram (Osawa et al., 2019a), duloxetine (Osawa et al., 2019b), and lamotrigine (Bollmann et al., 2016) in WWTP effluents. Although the predominant reaction was hydroxylation for non-synthetic matrices, there were specificities in the distribution of minor reactions. This specificity could be due to chemical, physical or biological conditions that differed from one matrix to another.

The results which are summarized in Figure 2 show interesting trends, but there is a need of additional information, i.e for one matrix and under similar experimental conditions, to better understand the reaction/matrix relationship. In addition, the largest number of degradation studies have been carried out in synthetic media so additional data on natural matrices are needed. Finally, a molecule-by-molecule comparison in similar matrices would make it possible to compare the formed TPs.

3.3 Case study for two PPCPs well-studied in the literature

To illustrate the various transformation pathways of PPCPs and the associated reactions, and to determine if the matrix influences the reactions undergone by the PPCPs, two representative case-studies, carbamazepine and diclofenac, were selected according to the following criteria: (i) the parent molecules were studied in several matrices and therefore it allowed to gain knowledge on their transformation in the environment, (ii) the parent molecules underwent a majority of the reactions above mentioned.

3.3.1 Carbamazepine

Carbamazepine (CBZ), 5H-dibenzazepine-5-carboxamide, is used as an antiepileptic and in the treatment of mental illness (Fertig & Mattson, 2008). It is one of the most studied and detected pharmaceuticals in the environment. Carbamazepine is recognized as a poorly degraded compound in WWTPs which results in its ubiquitous presence in the different environmental matrices (soil, surface and groundwater) (Clara et al., 2005; Joss et al., 2005; Zhang et al., 2008). Therefore, the degradation of carbamazepine has been frequently investigated and up to 53 TPs were identified in this review (Figures 3 and 4; Table S7).

A significant part of the available information has been provided by laboratory experiments in synthetic media (38 TPs over 53) allowing in depth studies of the driving

mechanisms of abiotic (photodegradation - Calza et al., 2012 ; reductive catalysis - König et al., 2016 ; ozonation - McDowell et al., 2005) or biotic (bacterial - Jelic et al., 2012; fungal - Kang et al., 2008) transformations, and the identification of unknown TPs. In synthetic media, a majority of TPs are of abiotic origin (31/38), and five TPs are of both biotic and abiotic origins. Among the 31 ATPs and 5 ABTPs, 26 were from photodegradation and 10 from catalytic hydrogenation transformations. For the 15 remaining TPs in non-synthetic media, the information on abiotic or biotic origin of the transformation was often not available.

Only eight TPs of carbamazepine, which were identified in synthetic media, were also found in non-synthetic matrices: carbamazepine 10,11-epoxide (CBZ-EP), 2-hydroxycarbamazepine (2OH-CBZ), 3-hydroxycarbamazepine (3OH-CBZ), $C_{14}H_9NO_2$ (TP223A), 10,11-Dhg-CBZ, acridone, 9-CA-acridine and acridine (Figures 3 and 4). Among them, CBZ-EP was the most frequently identified TP within three different matrices (soils, sediments and natural waters). It is pharmacologically active (Tomson & Bertilsson, 1984) and its presence in water bodies is undesirable (Miao & Metcalfe, 2003). In natural waters, the main observed TPs were CBZ-EP, 2OH-CBZ, and 3OH-CBZ, acridone and acridine (López-Serna et al., 2012) (Figure 3). Some other TPs were identified in drinking water following ozonation treatment (McDowell et al., 2005). In these conditions, the transformation pathways involved cleavage, oxygenation, hydration and rearrangement. In soils, Koba et al. (2016) evidenced a slow degradation of carbamazepine leading to six TPs including CBZ-EP and oxcarbazepine (OXC) found in low amounts (Figure 3). Nevertheless, carbamazepine TPs such as CBZ-EP can contribute to soil and water contamination (Paltiel et al., 2016). Finally, despite carbamazepine appeared to be recalcitrant in a water/sediment system (Löffler et al., 2005), CBZ-EP was detected in sediments (Li et al., 2014). In WWTPs and surface waters, five human metabolites (2OH-CBZ, 3OH-CBZ, CBZ-EP 10,11-dihydroxy-CBZ, 10-hydroxy-CBZ) of carbamazepine were found by screening (Miao & Metcalfe, 2003). These compounds are the

same than TPs from biotransformation studies in synthetic media (Jelic et al., 2012; Kang et al., 2008). It could therefore be assumed that the known metabolites of carbamazepine can also be TPs in WWTPs and surface waters, especially because 10,11-dihydroxy-CBZ was found at a concentration three times higher than carbamazepine in all samples (Miao & Metcalfe, 2003).

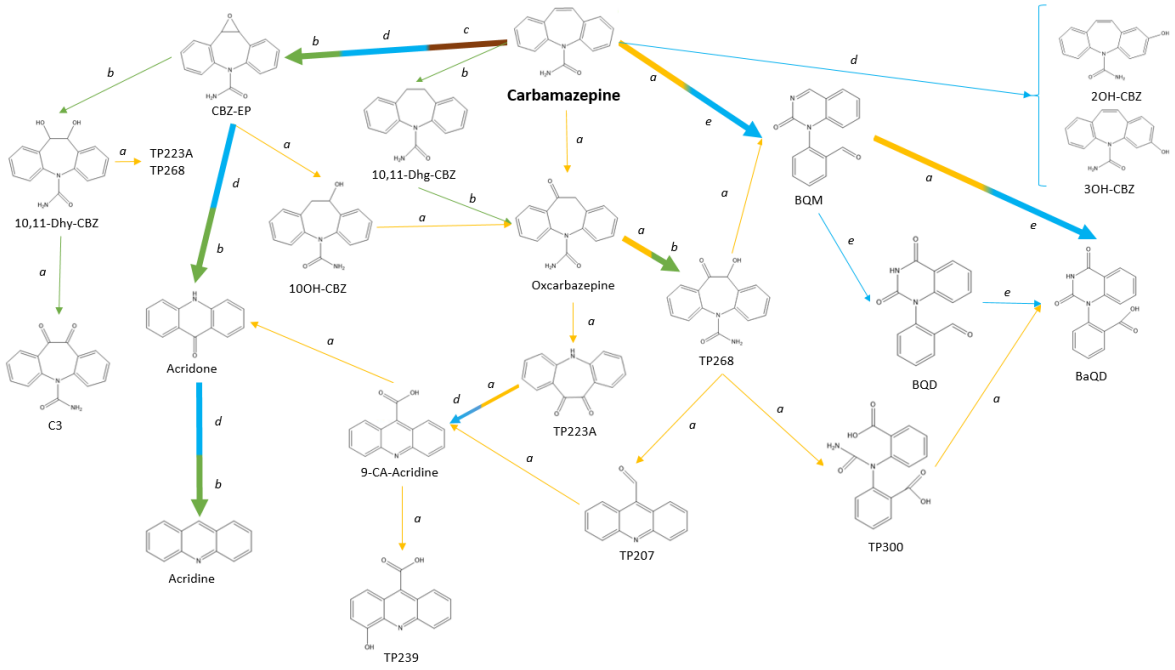

Figure 3. Transformation pathways of carbamazepine in non-synthetic matrices. Arrow in bold: reactions evidenced in two matrices or more; yellow arrow: solid waste; blue arrow: natural waters; green arrow: soils; brown arrow: sediments. (a) Kaiser et al. (2014); (b) Koba et al. (2016); (c) Li et al. (2014); (d) López-Serna et al. (2012); and (e) McDowell et al. (2005).

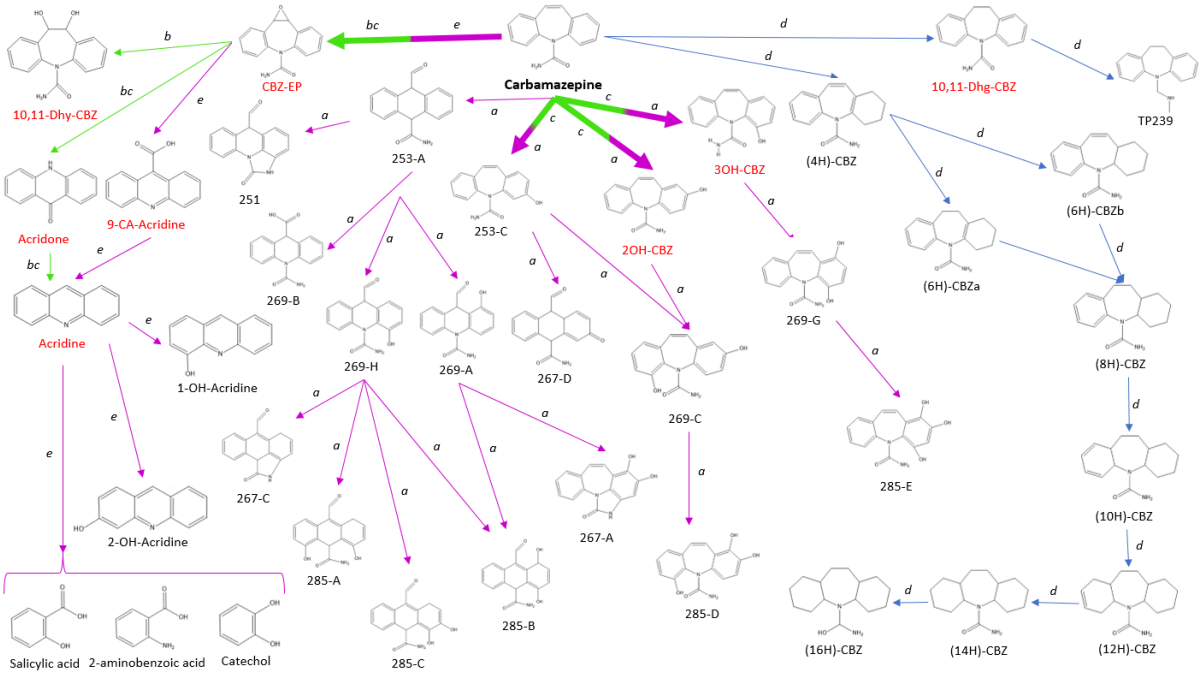

Figure 4. Transformation pathways of carbamazepine in synthetic matrices. In red: transformation products observed in both synthetic and non-synthetic matrices; arrow in bold: reactions evidenced in biotic and abiotic conditions; purple arrow: photodegradation; green arrow: biotic transformation; blue arrow: abiotic transformation except photodegradation (i.e. ozonation, catalysis.). (a) Calza et al. (2012); (b) Jelic et al. (2012); (c) Kang et al., (2008); (d) K€onig et al. (2016); and (e) Vogna et al. (2004).

The main reactions involved in the transformation of carbamazepine in all studied matrices were hydroxylation, addition (hydrogenation + hydration), cleavage, other eliminations, and rearrangement (Table S7). Hydroxylation of carbamazepine was identified in all transformation pathways, whereas dehydrogenation and rearrangement were mostly present in abiotic processes such as photodegradation (Calza et al., 2012). In electrochemical reductive catalysis, carbamazepine is mainly transformed by hydrogenation (König et al., 2016). Carbamazepine can also be degraded by microorganisms like white rot fungi (Marco-Urrea et al., 2009), *Candida elegans* (Kang et al., 2008) or *Trametes versicolor* (Jelic et al., 2012), and specific TPs were identified (10-11-dihydroxy-carbamazepine and acridone). The oxidative

action of extracellular fungal enzymes in liquid media has been demonstrated by comparing the degradation rates obtained with and without CYT P450 inhibitors (Golan-Rozen et al., 2011; Marco-Urrea et al., 2009). CBZ-EP was found as the main oxidation product in presence of white rot fungi.

To conclude, despite the low degradability of carbamazepine, numerous and diverse TPs were described in the literature. Four of them are common to synthetic and non-synthetic media and are formed under both abiotic and biotic conditions. Identification of such common TPs whatever the media and conditions has some implications on research and regulation, i.e. these TPs should be included in the reference lists for environmental survey and impact assessment studies.

3.3.2 Diclofenac

Diclofenac (DCF) (2-{2-[(2,6-dichlorophenyl)amino]phenyl}acetic acid) is a non-steroidal inflammatory drug (NSAID), having an analgesic, antiarthritic and antirheumatic action with a worldwide consumption of 940 t per year (Zhang et al., 2008). It is the most widely consumed pharmaceutical in the world and it has been often found in high concentrations in WWTPs (0.1 to 10 µg/L in raw influent according to Verlicchi et al., (2012). Photolytic degradation has been shown to be an important abiotic degradation process for such NSAIDs (Diniz et al., 2015; Li et al., 2017), and it has been demonstrated that the photoproducts of diclofenac were more toxic than the parent molecule (Barra Caracciolo et al., 2015). The degradation of diclofenac led to at least 64 TPs (Table S8) of biotic and/or abiotic origins in synthetic media, soils, solid wastes and sediments (Figures S1 and S2). Diclofenac undergoes hydroxylation, cleavage, addition, dehydrogenation, hydrolysis, other substitutions, other eliminations, and rearrangement reactions

In synthetic media, contrary to carbamazepine, a majority of TPs of biotic origin has been observed (25 over 43). Diclofenac can be degraded by various microorganisms, in particular the fungus *Trametes versicolor* (Marco-Urrea et al., 2010) or bacterial strains such as *Labrys portucalensis* F11 (Moreira et al., 2018), *Klebsiella* sp. KSC (Stylianou et al., 2018) or *Rhodococcus ruber* IEGM 346 (Ivshina et al., 2019). The transformation pathways seemed to be similar regardless of the microorganism: they led to TPs such as 5-OH-DCF-Q (5-hydroxydiclofenac-quinone imine) or DCF7 (2-[1-(5-oxocyclohexa-1,3-dienyl-2-(3′,4′-dihydroxy-2′,6′-dichlorophenyl)imino]acetic acid 4-(2,6-D)-1,3B) (Ivshina et al., 2019; Jewell et al., 2016; Kosjek et al., 2008; Moreira et al., 2018; Stylianou et al., 2018; Wu et al., 2019) (Figure S2). Biotic transformation studies showed that some TPs were also human metabolites (Marco-Urrea et al., 2010; Stylianou et al., 2018; Ivshina et al., 2019). The 18 TPs of abiotic origin were produced by photodegradation excepted MW 261 ($C_{14}H_{11}ClNO_2$) which is produced by reductive dechlorination (Yu et al., 2013) (Figure S2). Only two TPs are attributable to both biotic and abiotic transformations: 4'-hydroxy-diclofenac and 5-hydroxy-diclofenac (Webster et al., 1998; Marco-Urrea et al., 2010; Yu et al., 2013; Poirier-larabie et al., 2016; Moreira et al., 2018; Stylianou et al., 2018; Ivshina et al., 2019).

The majority of the diclofenac TPs which were observed in non-synthetic matrices (Figure S1) was found in solid wastes (22 over 25) (Jewell et al., 2016; Wang et al., 2019). Then, Dodgen et al. (2014) identified three TPs (2,4-dichlorobenzoic acid, 2,6-dichlorobenzoic acid and 3,5-dichlorobenzoic acid) which were only found in soils (Figure S1). Finally, three other TPs were found to be common to soils/sediments and solid wastes: 5-hydroxy-diclofenac quinone imine (5-OH-DCF-Q), 4'-hydroxy-diclofenac (4'-OH-DCF) and 5-hydroxy-diclofenac (5-OH-DCF) (Dodgen et al., 2014; Gröning et al., 2007; Jewell et al., 2016; Kosjek et al., 2008; Wu et al., 2019) (Figure S1).

In both synthetic (Figure S2) and non-synthetic media (Figure S1), four common TPs (4'-hydroxy-diclofenac, 5-hydroxy-diclofenac, diclofenac-lactam, 5-hydroxy-diclofenac quinone imine) were found. The 4'-hydroxy-diclofenac and 5-hydroxy-diclofenac TPs also have the particularity to be observed in biotic and abiotic conditions (Figure S2), and in several matrices (Figure S1).

As for carbamazepine, the identification of diclofenac TPs that have been observed in various media and experimental conditions is challenging for environmental monitoring and impact assessment studies of diclofenac.

4. Relationship between the functional groups of PPCPs and their transformation pathways

To better understand the transformation pathways of PPCPs in the environment, we created chemical classes to examine the relationship between the chemical structures and the reviewed transformation reactions. To discriminate molecules according to their chemical structure, we used molecular fragments from fingerprints and molecular descriptors.

4.1 Clusters composition

Cluster 1 is composed of 18 molecules which were characterized by the smallest number of atoms (22) (Table S5). Beside this characteristic of low molecular size, molecules had no specific features in terms of molecular fragment or descriptor. Most fragments were aromatic carbon chains that were found in other families. The number of aromatic sp^2 carbon (6), unsubstituted benzenic sp^2 carbon (4), and the number of acceptor atoms for H-bonds (3) were the predominant descriptors in this group, but they were also common to other clusters. Some molecules of the cluster, such as ortho-cresol, para-cresol or indole, had similar chemical

structures while other molecules, such as thiabendazole, sotalol or lamotrigine, shared specific functions such as halogen or sulphur ones.

The Cluster 2 contained eight molecules, almost all belonging to the sulfonamide antibiotic family. Of all the sulphonamides, only furosemide was absent in this cluster (Table S5). The predominant fragments and descriptors are those related to the sulphonamide group -SO_2N-R (1) and to the aromatic primary amines -$ArNH_2$ (1) which were only present in this cluster. An important feature was the absence of secondary and tertiary carbon on aromatic rings (Crs and Crt). There were 78 unique fragments which were specific to this cluster. The most frequent fragments among the eight molecules were composed of -SNO-R or -SN-R descriptor.

The 11 molecules of Cluster 3 had the lowest molecular weight median value of all clusters (176.2 g/mol^{-1}) (Table S5). As for Cluster 1, there were no preponderant fragments or descriptors. Nevertheless, ketone -C=O, secondary amine and aromatic functions were redundant for several molecules of this group such as caffeine, camphor or nitrofurantoin.

Cluster 4 was the one with the highest number of molecules (34), but which were poorly discriminated by specific characteristics (Table S5). The main fragments or descriptors were aliphatic or aromatic carbon chains that were also present in all clusters. This group gathered compounds of several use families: six of the seven NSAID molecules, bisphenol A and tetrabromobisphenol A, antihypertensives (irbesartan and valsartan), and the antimicrobials triclosan and triclocarban.

Cluster 5 are composed of 11 molecules (Table S5). The descriptors characterizing this group were the number of aromatic secondary amine -ArNHR (1), the number of sp^2 conjugated non-aromatic carbon (1) and the number of hydroxyl group -OH (1). Examples of molecules composing this group are iopromide, methotrexate or amoxicillin.

Composed of nine molecules, Cluster 6 only contained fluoroquinolones (Table S5). Several descriptors characterized this group: the number of aromatic tertiary amine -$ArNR_2$ (2), the number of aromatic ketone -ArCO (1), the number of aromatic halogen -ArX (1), the number of tertiary aliphatic carbon sp^2 (1), the number of carboxylic acids -COOH (1), the number of primary amine -RNH_2 (1), and the number of hydroxyl -OH (1). There was no tertiary ring carbon as for Cluster 2. This cluster was characterized by a high number of molecular fragments (221) which were not found in the other clusters and specific for the fluoroquinolones.

Among the 14 molecules composing Cluster 7, there were the five hormones (17β-estradiol, 17-ethinylestradiol, cholesterol, estriol, estrone) (Table S5). The descriptors characterizing this cluster were the number of secondary alcohol -OHs (1), the number of hydroxyl groups -OH (1), the total number of quaternary carbon sp^3 (1), the number of cyclic quaternary carbon sp^3 (1) and the number of primary aliphatic amine -RNH_2 (0.5). There were 27 unique molecular fragments, which is a rather small number. The most abundant fragments were aliphatic chains combined with aromatic rings.

Cluster 8 contained only four molecules, all from the tetracycline family (chlortetracycline, doxycycline, oxytetracycline, tetracycline) (Table S5). The molecular descriptors that described these four molecules were the number of aromatic hydroxyl groups -ArOH (4), the number of tertiary alcohols -OHt (2), the number of aliphatic sp^2 secondary carbon (2), the number of ketones -RCO (2), the number of primary amides -$RCONH_2$ (1), and the number of primary amines -RNH_2 (1). This cluster has the highest number of unique fragments (682).

Finally, Cluster 9 was characterized by the largest number of atoms (median value = 124) (Table S5). The seven molecules were mostly macrolides (azithromycin, clarithromycin, erythromycin, roxithromycin and tylosin) in addition to ivermectin and monensin. The

molecular descriptors that best defined these molecules were the number of hydroxyl groups -OH (5), the number of secondary alcohols -OHs (3), the number of tertiary alcohols -OHt (1), the number of aliphatic esters -RCOOR (1), and the number of aliphatic primary amines – RNH_2(1). There were 233 fragments unique to this cluster.

4.2 Relationships between chemical structures and transformation reactions

From the cluster compositions, relationships between the transformation pathways undergone by the 116 PPCPs and their predominant chemical structures were analysed (Figure 5). First of all, the least discriminated clusters (1, 3 and 4) were shown to have similar reaction distributions with hydroxylation (~30%) as the main reaction. The only significant difference between these clusters is the second most frequent reaction, which was dehydrogenation for Clusters 1 and 3, and other eliminations for Cluster 4. These three clusters accounted for 64 molecules, that is 55% of the dataset. We assume that the lack of discrimination of these clusters was due to the absence of representativeness of certain chemical structures of PPCPs. It is important to note that, in this review, the selection of molecules was firstly made according to the availability of the data, and not with a view to the representativeness of the different chemical structures composing the PPCPs.

Clusters 2, 5, 6, 7, 8 and 9 were quite well discriminated by several specific fingerprints or molecular descriptors and it appeared that the distribution of the reactions was partly explained by chemical structures (Figure 5). For compounds of Cluster 2, gathering only sulfonamides, hydroxylation was the most frequent transformation reaction, followed by cleavage (14 %), hydrolysis (14 %), other eliminations (14 %), and other substitutions (12 %) (there were few addition and no dealkylation reactions). This cluster has the particularity of being characterized by S-N, C-N, C-S bonds. Cleavage and hydrolysis reactions seemed to be in greater proportion due to the presence of these bonds which are sites that could be attacked

in priority during the transformation of sulfonamides. Indeed, the presence of the S-N, C-N, C-S bonds in the functional sulphonamide moieties is linked to certain reactions that break down the bonds either by hydrolysis (Olvera-Vargas et al., 2016; Zhang et al., 2017) or cleavage (Liu et al., 2018; Xiong et al., 2019; Zhang et al., 2017). Once the molecules are breakdown, the transformation involves further eliminations (García-Galán et al., 2011) or hydrolysis reactions (Olvera-Vargas et al., 2016; Zhang et al., 2017). During acid hydrolysis, the breakdown of the sulphonamide bond leads to sulphanilic acid and amino derivatives (Sukul et al., 2008). For this Cluster 2, the relationship between the reactions undergone (hydrolysis and cleavage) and chemical structures (molecular fragment composed of S-N, C-N and S-C bonds) was well demonstrated.

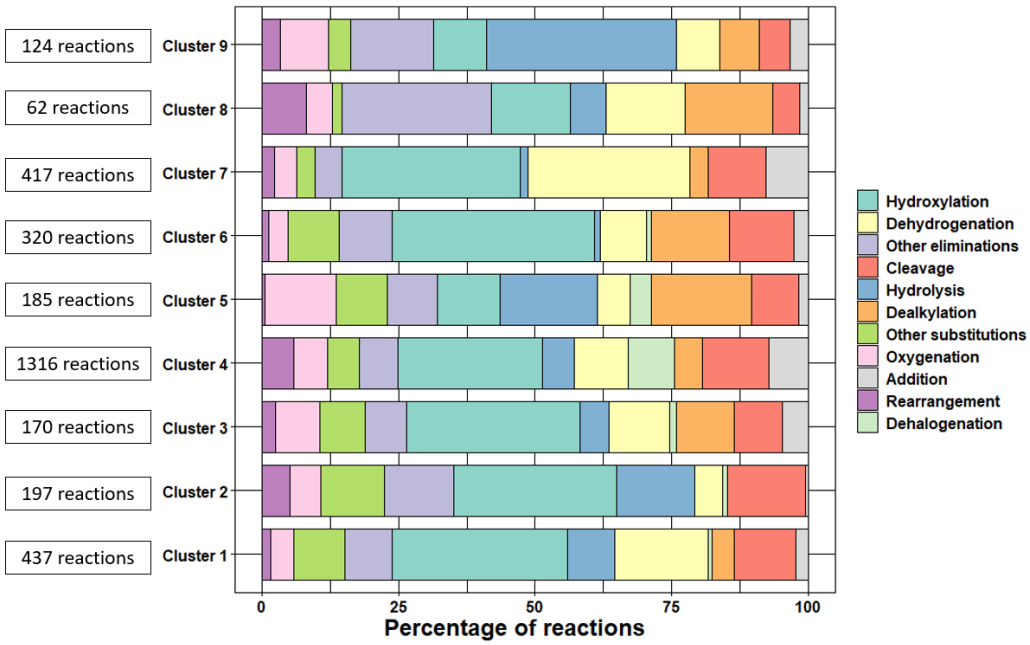

Figure 5. Distribution of the reactions involved in the transformation of PPCPs according to the different clusters based on chemical structure information (molecular fragments and molecular descriptors).

The transformation pathways of Cluster 5 compounds involved several reactions with similar occurrences (Figure 5): dealkylation (19%), hydrolysis (18%), oxygenation (14%), hydroxylation (12%), and other eliminations (11%). This balanced distribution could be explained by the heterogeneity of the chemical structures of the compounds belonging to this group. This cluster was also characterized by the lowest percentage of rearrangement reactions (1 %). The 11 compounds of Cluster 5 could be split in three sub-clusters. The first one is composed of amisulpiride, furosemide, glibenclamide, sildenafil and sulpiride. These molecules had in common a sulphonamide function. The second sub-cluster would be amoxicillin, ampicillin and ceftiofur which were all antibiotics of the β-lactamine family. They had a cyclic amide function (β-lactam), and sulphur and nitrogen atoms in the β position in their cycle. The last sub-cluster would contain trimethoprim and methotrexate, which have a diaminopyrimidine in common, and iopromide, which has nothing in common with the other molecules. For this sub-cluster, dealkylation occurred exclusively on the nitrogen atom of an aromatic amine. Steric hindrance could favour this reaction which was predominant.

In Cluster 6, fluoroquinolones were mainly concerned with hydroxylation (38 %), but dealkylation (14 %), other eliminations (13 %) and cleavage (12 %) were also frequently observed (Figure 5). Fluoroquinolone antibiotics form a large group of compounds with a wide diversity of functions with halogens, ketone, primary amine, carboxylic acid, and hydroxyl. The reaction of hydroxylation is observed with enrofloxacin (Wetzstein et al., 2006), flumequine (Feng et al., 2016), ofloxacin (Amorim et al., 2014), and norfloxacin (Kim et al., 2011). Dealkylation seemed to be favoured by the presence of fluorinated functional groups which could induce steric properties. Moreover, fluroroquinolones have in common a piperazine group (cyclic fragments composed of carbon and nitrogen) which is conducive to specific transformations (Čvančarová et al., 2015). Indeed, dealkylation on the piperazine moiety is observed for ciprofloxacin, ofloxacin and norfloxacin (Čvančarová et al., 2015; Vasquez &

Hapeshi, 2013). Decarboxylation (in "other eliminations" reactions) could also be favoured by the steric property of fluorine. Vasquez & Hapeshi (2013) mentions that the main abiotic reactions found for ofloxacin are opening of the piperazinyl ring and decarboxylation. Decarboxylation is found in several other biotransformation studies as well (Amorim et al., 2014; Čvančarová et al., 2013). Hydrolysis was not a predominant reaction for this cluster, possibly due to the absence of reaction-promoting moieties such as those found in macrolides (Cluster 9) which have cladinose and desosamine moeity or sulphonamides function (Cluster 2). This is consistent with the low performances of hydrolysis observed in studies on fluoroquinolones (Thiele-Bruhn, 2003). It has also been reported that oxolinic acid and flumequine are not hydrolysed in three types of water (deionised water, fresh water and seawater) (Pouliquen et al., 2007).

Cluster 7 transformation pathways mainly involved oxidation reactions: hydroxylation and dehydrogenation (65 %) (Figure 5). Other types of reaction were infrequent, less than 10%, apart cleavage (11%). Hydrolysis had rarely been observed (1%): the explanation given above for fluoroquinolones could also be applicable for this cluster and, for example, it is indeed well-know that steroid hormones do not undergo hydrolysis (Ying et al., 2013). The particularity of this cluster, with compounds having a large number of quaternary carbon sp^3 (median =1), could limit certain reactions because the quaternary carbons at the end of an alkyl chain prevent degradation (Knapp & Bromley-Challoner, 2003; Touraud & Roig, 2008). In addition, there are a large number of hydroxyl, ester and carbonyl groups that can undergo oxidation reactions. This two structural information could explain the high proportion of hydroxylation and dehydrogenation for this cluster.

The most frequent reactions identified in Cluster 8 (gathering cyclines) were other eliminations (27%), followed by dealkylation (16%), dehydrogenation (15%) and hydroxylation (15 %) (Figure 5). This cluster was also characterized by the highest occurrence

of rearrangements (8 %). Cyclines family had a specific structure with four rings (family with the greatest number of similar fragments) that caused a steric hindrance of these molecules and therefore played an important role in the reactions they underwent. These observations seems to give the following order of elimination: dealkylation of the methyl groups on the nitrogen, carbonyl group, and then the amine (Leng et al., 2016). In the other eliminations, in addition to decarbonylation, there is dehydration (Liu et al., 2016). The steric hindrance also seems to favour rearrangement with the aryl alcohol and ketone functional groups. Certain reactions seemed to be enhanced in biotic conditions such as cleavage or hydrolysis while hydroxylation was mainly present in abiotic conditions. This result seems essential because the TPs resulting from photolysis (Guo & Chen, 2012; Jiao et al., 2008) are more toxic than those resulting from fungi biotransformation (Suda et al., 2012) when compared to the toxicity of the parent compound. Nevertheless, dealkylation, hydroxylation and other eliminations were found in both conditions for the same molecules of cyclines.

Cluster 9 stood out from the other clusters by the predominant occurrence of hydrolysis (36 %) (Figure 5). Other eliminations had also been frequently identified in transformation pathways (15.7%) whereas other reactions had a low occurrence, less than 10%. Hydrolysis was probably favoured by the sequence of atoms in the molecular fragments corresponding to O=C-R-CHOH-R or OH-R-C-NH_2. This chemical family is characterized by its macrocyclic lactone structure to which several types of function are substituted such as hydroxyl, alkyl and especially the desososamine and cladinose fractions. The bonds of these two fractions were the ones affected by the hydrolysis reactions. Moreover, these reactions only take place in biotic conditions, which reduces their antibiotic activity and residual toxicity (Terzic et al., 2018). Elimination reactions are mainly due to β-oxidation after the main cycle had been hydrolysed (Terzic et al., 2018). These reactions appear to be in conjunction with hydrolysis. Finally, microbial phosphorylation is a known reaction for the inactivation of macrolide antibiotics

(D'Costa & Wright, 2017). This reaction was only found four times; it was part of other substitutions.

The classification allowed us to discriminate nine clusters which can be separated into two main groups. This first one is composed of Clusters 1, 3 and 4 which seemed to be poorly discriminated by fingerprints and molecular descriptors. The second one is composed by Clusters 2, 5, 6, 7, 8 and 9, which were better discriminated. In particular, Clusters 2, 6, 8 and 9 only consisted in sulfonamides, fluoroquinolones, cyclines and macrolides which had specific chemical structures that explain their transformation reactions.

However, this classification did not make it possible to describe all the data. Two hypotheses could explain this result: first, the fingerprints that encoded the molecular fragments were not sufficient to discriminate all molecules; second, the number of molecules for certain chemical structures was too low. In the dataset, some chemical structures were not poorly represented to form fully-fledged clusters as molecules in cluster not-welled discriminate. This analysis should be deepened by using a larger number of molecules with similar structures. Nevertheless, the difficulty is the lack of data on transformation pathways for molecules not or poorly studied.

5. Conclusion and research needs

This work aimed at reviewing the existing knowledge on the transformation in the environment of frequently used PPCPs to better understand the formation of their TPs and the corresponding transformation pathways. New findings emerged from the data analysis which also allowed to highlight several data gaps and research needs (**in bold**):

No information on TP was found for 42% of the 199 parent molecules initially targeted. Molecules with missing data gathered 81 pharmaceuticals and 2 PCPs. Among the less studied pharmaceuticals, we found families of use such as sartans, antidepressants, psychotropic drugs

or antibiotics (aminosides...). **Further investigations on PPCP transformations should therefore target these types of compounds.** For the remaining 116 compounds, the available data were also heterogeneous, as only 15 of them were PCPs, and some pharmaceuticals such as antidiabetics or antihelmintics were less represented. Indeed, some families of PPCP use were more studied than others, such as antibiotics, NSAIDs or hormones, which accounted for 44% of the transformation reactions examined. This over-representation of some families of use may have introduced biases in the results and in their interpretation. A total of 1371 TPs was inventoried for the 116 studied PPCPs which were formed in various matrices and following several transformation reactions. Among them, eleven main reactions were identified: addition, cleavage, dehalogenation, dealkylation, dehydrogenation, hydrolysis, hydroxylation, other eliminations, other substitutions, oxygenation, and rearrangement. Hydroxylation was the main reaction involved in the transformation of PPCPs, with 28% of the total reactions, followed by dehydrogenation (13%), and cleavage (11%). This shows genericity in the reactions disregarding the biotic/abiotic conditions, matrices and chemical families composing the set of transformation studies.

The majority of PPCP transformation reactions have been retrieved from studies conducted in synthetic media (65%). These studies are very useful to provide accurate identification of the TPs, reaction mechanisms and their controlling factors. Some TPs identified in synthetic media have also been found in non-synthetic media, which underlines the genericity of some transformation pathways between both matrices. However, the majority of the transformation pathways in synthetic studies are different from those found in non-synthetic studies. Indeed, such experiments are sometimes performed under non-realistic environmental conditions and concentrations.

There is a strong heterogeneity of available information on transformation reactions according to the non-synthetic media studied: only 1% of reactions were found in sediments,

4% in soils, 5% in wastewater treatment plant effluents, 9% in natural waters and 16% in solid wastes. In addition, different predominant secondary reactions were observed in the solid (solid wastes and soils) versus liquid (natural waters and sewage treatment plant effluents) matrices, implying different TPs according to the matrices. **To fill in knowledge gaps on TPs, there is a critical need for mechanistic studies carried out at realistic concentrations for the less investigated matrices (sediments, soils, wastewater effluents).**

Among the reviewed TPs, we were able to distinguish those formed by biotic reactions (629 BTPs) from those formed by abiotic reactions (568 ATPs). A few number of TPs can be formed by both biotic and abiotic reactions (61 ABTP). For 113 TPs, the type of reaction could not be identified due to the absence of controls. ABTPs should be monitored as a priority because they are more likely to be formed in the environment. **Further studies have to be conducted to confirm the higher occurrence of these compounds, e.g. by monitoring different environmental compartments.**

Regarding the carbamazepine and diclofenac case studies, five TPs (carbamazepine-10,11-epoxide, 1-hydroxy-CBZ, 2-hydroxy-CBZ 3-hydroxy-CBZ, and acridine) of carbamazepine and two TPs (4'-hydroxy-DCF and 5-hydroxy-DCF) of diclofenac were found to have the particularity of being formed under both biotic and abiotic conditions. These TPs would therefore be ubiquitous since they were produced under various conditions and in several matrices. These compounds should be placed on priority lists for environmental monitoring. Nevertheless, the majority of the TPs identified for carbamazepine (89%) and diclofenac (95%) was very specific to the conditions of the degradation experiments.

Finally, *in silico* approaches appeared to be relevant to link the chemical structure of PPCPs to their transformation pathways. **To go further, it would be necessary to integrate more data (molecular fragments and functional descriptors) on a broader number of molecules in order to increase the robustness and understanding of structures/reactions**

relationships. In addition, the eleven transformation reactions could be divided into sub-reactions, depending on the type and hybridization of the atom on which the reaction occurs, thus creating more subgroups. This could deepen the knowledge on the relationship between molecular structures and reactions undergone by PPCP molecules.

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Supplementary material

Table S1. List of the 116 PPCP compounds and their 1371 TPs with article references (Name of TPs are from articles). "-": No referenced CAS number.

Parent compound	CAS number	Transformation product	TP CAS number	Reference
17β-estradiol (E2)	50-28-2	10ε-17β-dihydroxy-1,4-estradieno-3-one	-	(Bila et al., 2007)
17β-estradiol (E2)	50-28-2	2-hydroxyestradiol	362-05-0	(Bila et al., 2007)
17β-estradiol (E2)	50-28-2	Estrone sulfate	481-97-0	(Goeppert et al., 2015)
17β-estradiol (E2)	50-28-2	Estrone	53-16-7	(Goeppert et al., 2015)
17β-estradiol (E2)	50-28-2	E2/A	-	(Mazellier et al., 2008)
17β-estradiol (E2)	50-28-2	E2/B	-	(Mazellier et al., 2008)
17β-estradiol (E2)	50-28-2	E2/C	-	(Mazellier et al., 2008)
17β-estradiol (E2)	50-28-2	TP 286	-	(Wang et al., 2019)
17β-estradiol (E2)	50-28-2	TP 292	-	(Wang et al., 2019)
17β-estradiol (E2)	50-28-2	TP 320-2	-	(Wang et al., 2019)
17β-estradiol (E2)	50-28-2	TP266	-	(Wang et al., 2019)
17β-estradiol (E2)	50-28-2	TP268	-	(Wang et al., 2019)
17β-estradiol (E2)	50-28-2	TP288	-	(Wang et al., 2019)
17β-estradiol (E2)	50-28-2	TP320-1	-	(Wang et al., 2019)
17β-estradiol (E2)	50-28-2	III	-	(Yu et al., 2016)
17β-estradiol (E2)	50-28-2	IV	-	(Yu et al., 2016)
17β-estradiol (E2)	50-28-2	M1	-	(Yu et al., 2016)
17β-estradiol (E2)	50-28-2	M2	-	(Yu et al., 2016)
17β-estradiol (E2)	50-28-2	V	-	(Yu et al., 2016)
17β-estradiol (E2)	50-28-2	VI	-	(Yu et al., 2016)
17β-estradiol (E2)	50-28-2	VII	-	(Yu et al., 2016)
17-Ethinylestradiol (EE2)	57-63-6	19-nor-17α-pregna-1,3,5 (10)-trien-20-yne-3,11α,17β -triol	-	(Choudhary et al., 2004)

17-Ethinylestradiol (EE2)	57-63-6	19-nor-17α-pregna-1,3,5 (10)-trien-20-yne-3,17β -diol-3β -methoxy	-	(Choudhary et al., 2004)
17-Ethinylestradiol (EE2)	57-63-6	19-nor-17α-pregna-1,3,5 (10)-trien-20-yne-3,6β ,17β -triol	-	(Choudhary et al., 2004)
17-Ethinylestradiol (EE2)	57-63-6	19-nor-17α-pregna-1,3,5(10)-trien-20-yne-3,7α,17β-triol	-	(Choudhary et al., 2004)
17-Ethinylestradiol (EE2)	57-63-6	17α-ethinyl-1,4-estradien-10,17 β-diol-3-one	-	(Della Greca et al., 2008)
17-Ethinylestradiol (EE2)	57-63-6	3- β -D-glucopyranosyl-2-hydroxyethinylestradiol	-	(Della Greca et al., 2008)
17-Ethinylestradiol (EE2)	57-63-6	3-β-D-glucopyranosyl-6β -hydroxyethinyl estradiol	-	(Della Greca et al., 2008)
17-Ethinylestradiol (EE2)	57-63-6	6- α -hydroxy-ethinylestradiol	-	(Della Greca et al., 2008)
17-Ethinylestradiol (EE2)	57-63-6	Ethinylestradiol glucoside	-	(Della Greca et al., 2008)
17-Ethinylestradiol (EE2)	57-63-6	2,4-nitro-EE2	-	(Gaulke et al., 2008)
17-Ethinylestradiol (EE2)	57-63-6	2-hydroxy-2,4-diene-1,6-dioic acid	-	(Haiyan et al., 2007)
17-Ethinylestradiol (EE2)	57-63-6	2-hydroxy-2,4-dienevaleric	-	(Haiyan et al., 2007)
17-Ethinylestradiol (EE2)	57-63-6	3,4-dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9.17-dione	-	(Haiyan et al., 2007)
17-Ethinylestradiol (EE2)	57-63-6	Estrone	53-16-7	(Haiyan et al., 2007)
17-Ethinylestradiol (EE2)	57-63-6	EE2 TP11	-	(Hom-Diaz et al., 2015)
17-Ethinylestradiol (EE2)	57-63-6	EE2 TP6	-	(Hom-Diaz et al., 2015)
17-Ethinylestradiol (EE2)	57-63-6	EE2 TP8	-	(Hom-Diaz et al., 2015)
17-Ethinylestradiol (EE2)	57-63-6	EE2 TP9	-	(Hom-Diaz et al., 2015)
17-Ethinylestradiol (EE2)	57-63-6	EE2 - 1	-	(Śliwka-Kaszyńska et al., 2019)
17-Ethinylestradiol (EE2)	57-63-6	EE2 - 2	-	(Śliwka-Kaszyńska et al., 2019)
17-Ethinylestradiol (EE2)	57-63-6	EE2 - 3	-	(Śliwka-Kaszyńska et al., 2019)
17-Ethinylestradiol (EE2)	57-63-6	TP306	-	(Wang et al., 2019)
17-Ethinylestradiol (EE2)	57-63-6	TP328	-	(Wang et al., 2019)
17-Ethinylestradiol (EE2)	57-63-6	TP344	-	(Wang et al., 2019)
4-Nonylphenol (NP)	104-40-5	Hydroquinone	123-31-9	(Gabriel et al., 2005)
4-Nonylphenol (NP)	104-40-5	3,6-dimethylheptan-3-ol	1573-28-0	(Gabriel et al., 2005)
Acetaminophen	103-90-2	Dichloro-4-acetamido-phenol	-	(Bedner & MacCrehan, 2006)
Acetaminophen	103-90-2	Chloro-4-acetamidophenol	3964-54-3	(Bedner & MacCrehan, 2006)
Acetaminophen	103-90-2	N-acetyl-p-benzoquinone imine	50700-49-7	(Bedner & MacCrehan, 2006)
Acetaminophen	103-90-2	3,5-dinitroacetaminophen	-	(Chiron et al., 2010)

Acetaminophen	103-90-2	3-chloro-5-nitro-acetaminophen	-	(Chiron et al., 2010)
Acetaminophen	103-90-2	3-chloroacetaminophen	-	(Chiron et al., 2010)
Acetaminophen	103-90-2	3-nitroacetaminophen	-	(Chiron et al., 2010)
Acetaminophen	103-90-2	p-Aminophenol	123-30-8	(Hart & Orr, 1975)
Acetaminophen	103-90-2	Acetate	64-19-7	(Hart & Orr, 1975)
Acetaminophen	103-90-2	Hydroquinone	123-31-9	(Li et al., 2014)
Acetaminophen	103-90-2	2-hexenoic acid	13419-69-7	(Li et al., 2014)
Acetaminophen	103-90-2	4-methoxyphenol	150-76-5	(Li et al., 2014)
Acetaminophen	103-90-2	1,4-dimethoxybenzene	150-78-7	(Li et al., 2014)
Acetaminophen	103-90-2	3-hydroxyacetaminophen	37519-14-5	(Li et al., 2014)
Acetaminophen	103-90-2	p-acetanisidide	51-66-1	(Li et al., 2014)
Acetaminophen	103-90-2	p-benzoquinone	106-51-4	(Zhao et al., 2000)
Acetophenone	98-86-2	Acetate de benzoyle	2819-08-1	(Jobst et al., 2010)
Acetophenone	98-86-2	2-hydroxyacetophenone	582-24-1	(Lee & Gibson, 1996)
Acetyl-sulfamethoxazole	21312-10-7	Sulfamethoxazole	723-46-6	(Helbling et al., 2010)
Amisulpride	71675-85-9	TP 166	-	(Gros et al., 2015)
Amisulpride	71675-85-9	TP 249	-	(Gros et al., 2015)
Amisulpride	71675-85-9	TP 258	-	(Gros et al., 2015)
Amisulpride	71675-85-9	TP 277	-	(Gros et al., 2015)
Amisulpride	71675-85-9	TP 291	-	(Gros et al., 2015)
Amisulpride	71675-85-9	TP 293	-	(Gros et al., 2015)
Amisulpride	71675-85-9	TP 323	-	(Gros et al., 2015)
Amisulpride	71675-85-9	TP 339	-	(Gros et al., 2015)
Amisulpride	71675-85-9	TP 357	-	(Gros et al., 2015)
Amisulpride	71675-85-9	D2	-	(Trawiński & Skibiński, 2017)
Amitriptyline	50-48-6	m/z 294.3-1	-	(Chen et al., 2016)
Amitriptyline	50-48-6	m/z 294.3-2	-	(Chen et al., 2016)
Amitriptyline	50-48-6	m/z 233	-	(Li et al., 2013)
Amitriptyline	50-48-6	Amitriptyline N-oxide	4317-14-0	(Li et al., 2013)

Amitriptyline	50-48-6	Nortriptyline	72-69-5	(Li et al., 2013)
Amoxicillin	26787-78-0	Amoxicillin penilloic acid	-	(Franski et al.,2014)
Amoxicillin	26787-78-0	Amoxicilloic acid methyl ester	-	(Franski et al.,2014)
Amoxicillin	26787-78-0	Amoxicilloic penicilloic acid	-	(Franski et al.,2014)
Amoxicillin	26787-78-0	AMX desaminated	-	(Franski et al.,2014)
Amoxicillin	26787-78-0	Diketopiperazine amoxicillin	-	(Franski et al.,2014)
Amoxicillin	26787-78-0	2-[amino(carboxy)-methyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxylic acid	-	(Hirte et al., 2016)
Amoxicillin	26787-78-0	2-[amino(carboxy)-methyl]-5,5-dimethyl-1,3-thiazolidine-4-carboxylic acid dehydrocarboxylated AMX penilloic acid	-	(Hirte et al., 2016)
Amoxicillin	26787-78-0	Amino-(4-hydroxyphenyl)acetic acid	-	(Hirte et al., 2016)
Amoxicillin	26787-78-0	Dehydrocarboxylated AMX penilloic acid	-	(Hirte et al., 2016)
Amoxicillin	26787-78-0	L-5,5-dimethylthiazolidin-4 carbonic acid	-	(Hirte et al., 2016)
Amoxicillin	26787-78-0	Penicillamine disulfide	20902-45-8	(Hirte et al., 2016)
Amoxicillin	26787-78-0	AMX-S-oxide	-	(Jung et al., 2012)
Amoxicillin	26787-78-0	m/z 307	-	(Längin et al., 2008)
Amoxicillin	26787-78-0	6-aminopenicillanic acid	-	(Trovo et al., 2011)
Amoxicillin	26787-78-0	Thiazolidinecarboxylic acid	34592-47-7	(Trovo et al., 2011)
Amoxicillin	26787-78-0	4-hydroxyphenylglycine	938-97-6	(Trovo et al., 2011)
Ampicillin	69-53-4	AMP desaminated	-	(Li et al., 2014)
Ampicillin	69-53-4	AMP diketopiperazines	-	(Li et al., 2014)
Ampicillin	69-53-4	AMP penicilloic acid	-	(Li et al., 2014)
Ampicillin	69-53-4	AMP penilloic acid	-	(Li et al., 2014)
Ampicillin	69-53-4	Ampicilloic acid methyl ester	-	(Li et al., 2014)
Atenolol	29122-68-7	A1	-	(Koba et al., 2016)
Atenolol	29122-68-7	A2	-	(Koba et al., 2016)
Atenolol	29122-68-7	Atenolol acid	56392-14-4	(Krah et al., 2016)
Atenolol	29122-68-7	?-hydroxy-4-[2-hydroxy-3-(isopropylamino)propoxy]benzaldehyde	-	(Salgado et al., 2013)
Atenolol	29122-68-7	2-(?-hydroxy-4-(2-hydroxy-3-isopropylamino)propoxy)phenyl)acetamide	-	(Salgado et al., 2013)
Atenolol	29122-68-7	4-[(2-amino-2-oxoethyl)phenyl-2-hydroxy-3-(isopropylamino)]propanoate	-	(Salgado et al., 2013)

Atenolol	29122-68-7	4-[2-hydroxy-3-(isopropylamino)propoxy]benzaldehyde	29122-74-5	(Salgado et al., 2013)
Atenolol	29122-68-7	1-isopropylamino-2-propanol	41063-31-4	(Xu et al., 2017)
Atenolol	29122-68-7	1-amino-3-phenoxy-2-propanol	4287-19-8	(Xu et al., 2017)
Atorvastatin	134523-00-5	5-(4-fluoro-phenyl)-1-(3-hydroxy-5-oxo-pentyl)-2-isopropyl-4-phenyl-1H-pyrrole-3-carboxylic acid (4-hydroxy-phenyl)-amide	-	(Sulaiman et al., 2015)
Atorvastatin	134523-00-5	7-[4-(2,4-dihydroxy-phenylcarbamoyl)-2-(4-fluoro-phenyl)-3-phenyl-pyrrol-1-yl]-5-hydroxy-3-oxo-heptanoic acid	-	(Sulaiman et al., 2015)
Atorvastatin	134523-00-5	Ortho-, para-dihydroxy atorvastatin	-	(Sulaiman et al., 2015)
Atorvastatin	134523-00-5	Ortho-hydroxy atorvastatin	214217-86-4	(Sulaiman et al., 2015)
Atorvastatin	134523-00-5	Para-dihydroxy atorvastatin	265989-44-4	(Sulaiman et al., 2015)
Atorvastatin	134523-00-5	P313	-	(Wang et al., 2018)
Atorvastatin	134523-00-5	P416	-	(Wang et al., 2018)
Atorvastatin	134523-00-5	P432	-	(Wang et al., 2018)
Atorvastatin	134523-00-5	P438	-	(Wang et al., 2018)
Atorvastatin	134523-00-5	P456	-	(Wang et al., 2018)
Atorvastatin	134523-00-5	P557	-	(Wang et al., 2018)
Atorvastatin	134523-00-5	P573	-	(Wang et al., 2018)
Atorvastatin	134523-00-5	P575	-	(Wang et al., 2018)
Atorvastatin	134523-00-5	P591	-	(Wang et al., 2018)
Azithromycin	83905-01-5	N-demethyl azithromycin	-	(Senta et al., 2019)
Azithromycin	83905-01-5	Decladinose azithromycin	117693-41-1	(Senta et al., 2019)
Azithromycin	83905-01-5	N'-demethyl azithromycin	172617-84-4	(Senta et al., 2019)
Azithromycin	83905-01-5	Azithromycin N-oxide	90503-06-3	(Senta et al., 2019)
Azithromycin	83905-01-5	AZI TP 374a	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 374b	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 374c	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 376a	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 376b	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 392	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 394	-	(Terzic et al., 2018)

Azithromycin	83905-01-5	AZI TP 434	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 450	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 452	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 592	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 608	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 610	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 765a	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	AZI TP 767	-	(Terzic et al., 2018)
Azithromycin	83905-01-5	Phosphoryle azithromycin	-	(Terzic et al., 2011)
Azithromycin	83905-01-5	AZI product A	-	(Topp et al., 2016)
Azithromycin	83905-01-5	AZI product B	-	(Topp et al., 2016)
Azithromycin	83905-01-5	AZI product C	-	(Topp et al., 2016)
Azithromycin	83905-01-5	AZI product D	-	(Topp et al., 2016)
Benzotriazole	95-14-7	1-hydroxy-benzotriazole	-	(Felis et al., 2016)
Benzotriazole	95-14-7	5-OH-1,2,3-T	-	(Felis et al., 2016)
Benzotriazole	95-14-7	TP1-BTA	-	(Felis et al., 2016)
Benzotriazole	95-14-7	4-methyl-benzotriazole	-	(Huntscha et al., 2014)
Benzotriazole	95-14-7	5-COOH-Benzotriazole	-	(Huntscha et al., 2014)
Benzotriazole	95-14-7	1-methyl-benzotriazole	13351-73-0	(Huntscha et al., 2014)
Benzotriazole	95-14-7	5-methyl-benzotriazole	136-85-6	(Huntscha et al., 2014)
Benzotriazole	95-14-7	4-hydroxy-benzotriazole	26725-51-9	(Huntscha et al., 2014)
Benzotriazole	95-14-7	1H-benzotriazole 4-methoxy	-	(Liu et al., 2010)
Benzotriazole	95-14-7	1H-benzotriazole 5-methoxy	-	(Liu et al., 2010)
Benzotriazole	95-14-7	Dimethyl benzylamine	-	(Liu et al., 2010)
Benzotriazole	95-14-7	Phtalic acid	-	(Liu et al., 2010)
Benzotriazole	95-14-7	Phenol	108-95-2	(Liu et al., 2010)
Benzotriazole	95-14-7	Carbazole	86-74-8	(Liu et al., 2010)
Bezafibrate	41859-67-0	BEZ 224	-	(Helbling et al., 2010)
Bezafibrate	41859-67-0	BEZ 256	-	(Helbling et al., 2010)

Bezafibrate	41859-67-0	BEZ 360	-	(Helbling et al., 2010)
Bezafibrate	41859-67-0	4-hydroxybenzoic acid	99-96-7	(Helbling et al., 2010)
Bezafibrate	41859-67-0	Bez 238	-	(Li et al., 2014)
Bezafibrate	41859-67-0	4-chlorobenzoic acid	74-11-3	(Quintana et al., 2005)
Bisphenol A	80-05-7	4-hydroxybenzoate	456-23-5	(Bossert et al., 1989)
Bisphenol A	80-05-7	p-benzoquinone	106-51-4	(Chauhan et al., 2000)
Bisphenol A	80-05-7	2-hydroxy-1,4-benzoquinone	2474-72-8	(Chauhan et al., 2000)
Bisphenol A	80-05-7	1,2,4-benzenetriol	533-73-3	(Eppink et al., 2000)
Bisphenol A	80-05-7	Hydroquinone	123-31-9	(Gabriel et al., 2007)
Bisphenol A	80-05-7	4-isopropylcatechol	2138-43-4	(Gabriel et al., 2007)
Bisphenol A	80-05-7	4-(2-hydroxypropan-2-yl)phenol	2948-47-2	(Gabriel et al., 2007)
Bisphenol A	80-05-7	4-isopropylphenol	99-89-8	(Gabriel et al., 2007)
Bisphenol A	80-05-7	Styrene	100-42-5	(Han et al., 2015)
Bisphenol A	80-05-7	Maleic acid	110-16-7	(Han et al., 2015)
Bisphenol A	80-05-7	4'-methylacetophenone	122-00-9	(Han et al., 2015)
Bisphenol A	80-05-7	1,4-pentadien-3-one	1890-28-4	(Han et al., 2015)
Bisphenol A	80-05-7	2-phenylpropenal	4432-63-7	(Han et al., 2015)
Bisphenol A	80-05-7	2-phenyl-2-propanol	617-94-7	(Han et al., 2015)
Bisphenol A	80-05-7	2-methyl-1,1-diphenylpropene	781-33-9	(Han et al., 2015)
Bisphenol A	80-05-7	α-methylstyrene	98-83-9	(Han et al., 2015)
Bisphenol A	80-05-7	Maleylacetate	24740-88-3	(Jain et al., 1994)
Bisphenol A	80-05-7	3-oxoadipate	689-31-6	(Kaschabek & Reineke, 1995)
Bisphenol A	80-05-7	3,4-dihydroxybenzoate	99-50-3	(Lah, et al., 1994)
Bisphenol A	80-05-7	4,4'-dihydroxy-alpha-methylstilbene	72108-22-6	(Peng et al.,2015)
Bisphenol A	80-05-7	2,2-bis(4-hydroxyphenyl)propanoic acid	92549-67-2	(Peng et al.,2015)
Bisphenol A	80-05-7	cis,cis-4-hydroxymuconic semialdehyde	-	(Spain & Gibson, 1991)
Bisphenol A	80-05-7	2,2-bis (4-hydroxyphenyl) -1-propanoate	-	(Spivacks et al., 1994)
Bisphenol A	80-05-7	Alcool 4-hydroxyphenacylique	-	(Spivacks et al., 1994)
Bisphenol A	80-05-7	4-hydroxybenzaldehyde	123-08-0	(Spivacks et al., 1994)

Bisphenol A	80-05-7	2,3-bis (4-hydroxyphenyl) -1,2-propanediol	139755-03-6	(Spivacks et al., 1994)
Bisphenol A	80-05-7	2,2-bis(4-hydroxyphenyl)-1-propanol	142648-65-5	(Spivacks et al., 1994)
Bisphenol A	80-05-7	1,2-bis(4-hydroxyphenyl)-2-propanol	154928-56-0	(Spivacks et al., 1994)
Bisphenol A	80-05-7	4-isopropenylphenol	4286-23-1	(Spivacks et al., 1994)
Bisphenol A	80-05-7	4-hydroxyacetophenone	99-93-4	(Spivacks et al., 1994)
Bisphenol A	80-05-7	Acetate de 4-hydroxyphenyle	3233-32-7	(Tanner & Hopper, 2000)
Bisphenol A	80-05-7	Acetate	71-50-1	(Tanner & Hopper, 2000)
Bisphenol A	80-05-7	Pyruvate	127-17-3	(Toyama et al., 2010)
Bisphenol A	80-05-7	3-methyl-2-butanone	563-80-4	(Toyama et al., 2010)
Bisphenol A	80-05-7	2-hydroxy-3-hydroxymethy-BPA	-	(Wang et al., 2017)
Bisphenol A	80-05-7	2-hydroxy-3-hydroxymethy-BPA glycoside	-	(Wang et al., 2017)
Bisphenol A	80-05-7	3-hydroxymethyl-4-(1-hydroxy1-methyl-ethyl)-benzene-1, 2-diol	-	(Wang et al., 2017)
Bisphenol A	80-05-7	4-isopropanol-benzene-1,2-diol	-	(Wang et al., 2017)
Bisphenol A	80-05-7	4-isopropenyl-benzene-1,2-diol	-	(Wang et al., 2017)
Bisphenol A	80-05-7	Bisphenol A glycoside	-	(Wang et al., 2017)
Bisphenol A	80-05-7	Monohydroxy-BPA glycoside	-	(Wang et al., 2017)
Bisphenol A	80-05-7	5-hydroxybisphenol	79371-66-7	(Wang et al., 2017)
Bisphenol A	80-05-7	Phenol	108-95-2	(Wang et al., 2010)
Bisphenol A	80-05-7	Butenedioic acid	110-17-8	(Wang et al., 2010)
Bisphenol A	80-05-7	Oxalic acid	144-62-7	(Wang et al., 2010)
Caffeine	58-08-2	Xanthine	69-89-6	(Asano et al., 1993)
Caffeine	58-08-2	3-methylxanthine	1076-22-8	(Hakil et al., 1998)
Caffeine	58-08-2	Theophylline	58-55-9	(Hakil et al., 1998)
Caffeine	58-08-2	N,N'-dimethylurea	1320-50-9	(Madyastha et al., 1999)
Caffeine	58-08-2	Glyoxylate	298-12-4	(Madyastha et al., 1999)
Caffeine	58-08-2	3,6,8-trimethylallantoïne	42794-72-9	(Madyastha et al., 1999)
Caffeine	58-08-2	1,3,7-trimethyluric acid	5415-44-1	(Madyastha et al., 1999)
Caffeine	58-08-2	N-methylurea	598-50-5	(Madyastha et al., 1999)
Caffeine	58-08-2	3,7-dimethyluric acid	13087-49-5	(Mazzafera, 2004)

Caffeine	58-08-2	Acide 1,7-dimethylurique	33868-03-0	(Mazzafera, 2004)
Caffeine	58-08-2	7-methylxanthine	552-62-5	(Mazzafera, 2004)
Caffeine	58-08-2	Paraxanthine	611-59-6	(Mazzafera, 2004)
Caffeine	58-08-2	7-methyluric acid	612-37-3	(Mazzafera, 2004)
Caffeine	58-08-2	1-methylxanthine	6136-37-4	(Mazzafera, 2004)
Caffeine	58-08-2	Theobromine	83-67-0	(Mazzafera, 2004)
Camphor	76-22-2	2-oxo-delta 3 -4,5,5-trimethylcyclopentenylacetate	1130-49-0	(Jones et al., 1993)
Camphor	76-22-2	2,5-diketocamphane	4230-32-4	(Jones et al., 1993)
Camphor	76-22-2	5-exo-hydroxycamphor	13948-58-8	(Poulos, 1992)
Carbamazepine	298-46-5	251	-	(Calza et al., 2012)
Carbamazepine	298-46-5	253-A	-	(Calza et al., 2012)
Carbamazepine	298-46-5	253-D	-	(Calza et al., 2012)
Carbamazepine	298-46-5	267-A	-	(Calza et al., 2012)
Carbamazepine	298-46-5	267-B	-	(Calza et al., 2012)
Carbamazepine	298-46-5	267-C	-	(Calza et al., 2012)
Carbamazepine	298-46-5	267-D	-	(Calza et al., 2012)
Carbamazepine	298-46-5	269-A	-	(Calza et al., 2012)
Carbamazepine	298-46-5	269-B	-	(Calza et al., 2012)
Carbamazepine	298-46-5	269-C	-	(Calza et al., 2012)
Carbamazepine	298-46-5	269-G	-	(Calza et al., 2012)
Carbamazepine	298-46-5	269-H	-	(Calza et al., 2012)
Carbamazepine	298-46-5	285-A	-	(Calza et al., 2012)
Carbamazepine	298-46-5	285-B	-	(Calza et al., 2012)
Carbamazepine	298-46-5	285-C	-	(Calza et al., 2012)
Carbamazepine	298-46-5	285-D	-	(Calza et al., 2012)
Carbamazepine	298-46-5	285-E	-	(Calza et al., 2012)
Carbamazepine	298-46-4	Acridine	260-94-6	(Jelic et al., 2012)
Carbamazepine	298-46-4	Acridone	578-95-0	(Jelic et al., 2012)
Carbamazepine	298-46-5	10-hydroxycarbamazepine	29331-92-8	(Kaiser et al., 2014)

Carbamazepine	298-46-4	2-hydroxycarbamazepine	68011-66-5	(Su Il Kang et al., 2008)
Carbamazepine	298-46-4	3-hydroxycarbamazepine	68011-67-6	(Su Il Kang et al., 2008)
Carbamazepine	298-46-4	9-carboxylic acid-acridine	5336-90-3	(Su Il Kang et al., 2008)
Carbamazepine	298-46-5	Oxcarbamazepine	28721-07-5	(Koba et al., 2016)
Carbamazepine	298-46-4	10,11-dihydroxy carbamazepine	35079-97-1	(Koba et al., 2016)
Carbamazepine	298-46-4	10,11-dihydrocarbamazepine	3564-73-6	(Koba et al., 2016)
Carbamazepine	298-46-4	Carbamazepine 10,11-epoxide	36507-30-9	(Koba et al., 2016)
Carbamazepine	298-46-4	(10H)-carbamazepine	-	(König et al., 2016)
Carbamazepine	298-46-4	(12H)-carbamazepine	-	(König et al., 2016)
Carbamazepine	298-46-4	(14H)-carbamazepine	-	(König et al., 2016)
Carbamazepine	298-46-4	(16H)-carbamazepine	-	(König et al., 2016)
Carbamazepine	298-46-4	(2H)-carbamazepine	-	(König et al., 2016)
Carbamazepine	298-46-4	(4H)-carbamazepine	-	(König et al., 2016)
Carbamazepine	298-46-4	(6H)-carbamazepine	-	(König et al., 2016)
Carbamazepine	298-46-4	(6H)-carbamazepine a	-	(König et al., 2016)
Carbamazepine	298-46-4	(8H)-carbamazepine	-	(König et al., 2016)
Carbamazepine	298-46-4	TP 239	-	(König et al., 2016)
Carbamazepine	298-46-4	1-(2-benzaldehyde)-(1H, 3H)-quinazoline- 2,4-dione	-	(McDowell et al., 2005)
Carbamazepine	298-46-4	1-(2-benzaldehyde)-4-hydro-(1H, 3H)- quinazoline-2-one	-	(McDowell et al., 2005)
Carbamazepine	298-46-4	1-(2-benzoic acid)-(1H,3H)-quinazoline-2,4- dione	-	(McDowell et al., 2005)
Carbamazepine	298-46-4	2-aminobenzoic acid	118-92-3	(Vogna et al., 2004)
Carbamazepine	298-46-4	Catechol	120-80-9	(Vogna et al., 2004)
Carbamazepine	298-46-4	2-OH-acridine	22817-17-0	(Vogna et al., 2004)
Carbamazepine	298-46-4	1-OH-acridine	5464-73-3	(Vogna et al., 2004)
Carbamazepine	298-46-4	Salicylic acid	69-72-7	(Vogna et al., 2004)
Carbamazepine	298-46-4	Acridine-9-CA	885-23-4	(Vogna et al., 2004)
Ceftiofur	80370-57-6	Cef-aldehyde	-	(Li et al., 2011)
Ceftiofur	80370-57-6	Desfuroylceftiofur	120882-22-6	(Li et al., 2011)
Ceftiofur	80370-57-6	Furoic acid	88-14-2	(Li et al., 2011)

Cetirizine	83881-51-0	Cetirizine N-oxyde	1076199-80-8	(Borowska et al., 2016)
Cetirizine	83881-51-0	4-chlorobenzophenone	134-85-0	(Borowska et al., 2016)
Cetirizine	83881-51-0	Norchlorcyclizine	303-26-4	(Borowska et al., 2016)
Chlortetracycline	57-62-5	N-didesmethyl-chlortetracycline	-	(Chen et al., 2011)
Chlortetracycline	57-62-5	Keto-chlortetracycline	-	(Halling-Sørensen et al., 2002)
Chlortetracycline	57-62-5	N-desmethyl-chlortetracycline	-	(Halling-Sørensen et al., 2002)
Chlortetracycline	57-62-5	Anhydrochlortetracycline	4497-08-9	(Halling-Sørensen et al., 2002)
Chlortetracycline	57-62-5	Iso-chlortetracyclines (iso-CTC)	514-53-4	(Halling-Sørensen et al., 2002)
Cholesterol	57-88-5	2-hydroxyhexa-2,4-dienoate	-	(Merino et al., 2012)
Cholesterol	57-88-5	4,5,9,10-diseco-3-hydroxy-5,9,17-trioxandrosta-1(10)-2-diene-4-oate	-	(Merino et al., 2012)
Cholesterol	57-88-5	9,17-dioxo-1,2,3,4,10,19-hexanorandrostan-5-oate	-	(Merino et al., 2012)
Cholesterol	57-88-5	3-hydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione	2394-69-6	(Merino et al., 2012)
Cholesterol	57-88-5	4-androsten-3,17-dione	63-05-8	(Merino et al., 2012)
Cholesterol	57-88-5	7-β-hydroxycholesterol	-	(Pang et al., 2016)
Cholesterol	57-88-5	7-oxocholesterol	566-28-9	(Pang et al., 2016)
Cholesterol	57-88-5	1,17-dioxo-2,3-seco-androstan-3-oic acid	-	(Wei et al., 2018)
Cholesterol	57-88-5	17-hydroxy-1-oxo-2,3-seco-androstan-3-oic acid	-	(Wei et al., 2018)
Cholesterol	57-88-5	1-hydroxyandrostan-3,17-dione	-	(Wei et al., 2018)
Cholesterol	57-88-5	2,5-seco-3,4-dinorandrost-1,5,17-trione	-	(Wei et al., 2018)
Cholesterol	57-88-5	25-hydroxycholest-4en-3one	-	(Wei et al., 2018)
Cholesterol	57-88-5	Androst-1,4-en-3,17-dione	-	(Wei et al., 2018)
Cholesterol	57-88-5	Androstan-1,3,17-trione	-	(Wei et al., 2018)
Cholesterol	57-88-5	Cholest-1,4-diene-3one	-	(Wei et al., 2018)
Cholesterol	57-88-5	Cholest-4-3-one	-	(Wei et al., 2018)
Cholesterol	57-88-5	Cholest-4-en-3-one-24-oic acid	-	(Wei et al., 2018)
Cholesterol	57-88-5	Cholest-4-en-3-one-26-oic acid	-	(Wei et al., 2018)
Cholesterol	57-88-5	Preg-4-en-3-one-20-carboxylic acid	-	(Wei et al., 2018)
Cholesterol	57-88-5	26-hydroxycholest-4-en-3-one	19257-21-7	(Wei et al., 2018)
Cholesterol	57-88-5	Androst-1-en-3,17-dione	571-40-4	(Wei et al., 2018)

Cholesterol	57-88-5	Androst-4-en-3,17-dione	63-05-8	(Wei et al., 2018)
Cholesterol	57-88-5	4-cholestene-3-one	601-57-0	(Yazdi et al., 2000)
Cimetidine	51481-61-9	β-sultam	-	(Buth et al., 2007)
Cimetidine	51481-61-9	δ-sultam	-	(Buth et al., 2007)
Cimetidine	51481-61-9	4-hydroxymethyl-5-methyl-1H-imidazole	29636-87-1	(Buth et al., 2007)
Cimetidine	51481-61-9	4-chloro-5-methyl-1H-imidazole	86604-94-6	(Buth et al., 2007)
Ciprofloxacin	85721-33-1	7-amino-1-cyclopropyl- 6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid	-	(Čvančarová et al., 2015)
Ciprofloxacin	85721-33-1	Hydroxymethyl-N-ciprofloxacine	-	(Čvančarová et al., 2015)
Ciprofloxacin	85721-33-1	Desethylene-N-ciprofloxacine (C1)	103222-12-4	(Čvančarová et al., 2015)
Ciprofloxacin	85721-33-1	Desethylene-N-formylciprofloxacine	93594-39-9 (Formyl ciprofloxacin)	(Čvančarová et al., 2015)
Ciprofloxacin	85721-33-1	Desethylene-N-acetylciprofloxacine	-	(Parshikov et al., 2001)
Ciprofloxacin	85721-33-1	N- formylciprofloxacine	-	(Parshikov et al., 2001)
Ciprofloxacin	85721-33-1	N-acetylciprofloxacine	-	(Parshikov et al., 2001)
Ciprofloxacin	85721-33-1	M19	-	(Parshikov et al., 2001)
Ciprofloxacin	85721-33-1	M6	-	(Prieto et al., 2011)
Ciprofloxacin	85721-33-1	M20	-	(Terzic et al., 2011a)
Ciprofloxacin	85721-33-1	M21	-	(Terzic et al., 2011a)
Ciprofloxacin	85721-33-1	F-1	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-12	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-2	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-3	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-4	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-5	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-6	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-7	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-8	-	(Wetzstein et al., 1999)
Ciprofloxacin	85721-33-1	F-9	-	(Wetzstein et al., 1999)

Ciprofloxacin	85721-33-1	Piperazine	110-85-0	(Wetzstein et al., 1999)
Citalopram	59729-33-8	N-desmethylcitalopram amide	-	(Beretsou et al., 2016)b
Citalopram	59729-33-8	N-desmethylcitalopram carboxylic acid	-	(Beretsou et al., 2016)
Citalopram	59729-33-8	3-oxocitalopram	372941-54-3	(Beretsou et al., 2016)
Citalopram	59729-33-8	Citalopram carboxylic acid	440121-09-5	(Beretsou et al., 2016)
Citalopram	59729-33-8	Citalopram amide	64372-56-1	(Beretsou et al., 2016)
Citalopram	59729-33-8	N-desmethylcitalopram	62498-67-3	(Kwon & Armbrust, 2005)
Citalopram	59729-33-8	Citalopram N-oxide	63284-72-0	(Kwon & Armbrust, 2005)
Citalopram	59729-33-8	TP-245	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-261	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-311	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-323	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-325	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-327	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-337	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-339A	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-339B	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-341-A2	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-341-B	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-343	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-353	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-355B	-	(Osawa et al.,2019)
Citalopram	59729-33-8	TP-359	-	(Osawa et al.,2019)
Clarithromycin	81103-11-9	14-hydroxy-decladinosyl-clarithromycin	-	(Buchicchio et al., 2016)
Clarithromycin	81103-11-9	Decladinosyl clarithromycin	-	(Buchicchio et al., 2016)
Clarithromycin	81103-11-9	N-desmethyl clarithromycin	101666-68-6	(Buchicchio et al., 2016)
Clarithromycin	81103-11-9	14-OH-clarithromycin	110671-78-8	(Buchicchio et al., 2016)
Clarithromycin	81103-11-9	TP 746	-	(Calza et al., 2012)
Clarithromycin	81103-11-9	TP 764	-	(Calza et al., 2012)

Clarithromycin	81103-11-9	TP 780	-	(Calza et al., 2012)
Clarithromycin	81103-11-9	TP 796	-	(Calza et al., 2012)
Clarithromycin	81103-11-9	TP 812	-	(Calza et al., 2012)
Clarithromycin	81103-11-9	Acetalized clarithromycin	-	(Lange et al., 2006)
Clarithromycin	81103-11-9	Deaminated clarithromycin	-	(Lange et al., 2006)
Clarithromycin	81103-11-9	Phosphorylated clarithromycin	-	(Senta et al., 2019)
Clarithromycin	81103-11-9	Clarithromycin N-oxide	118074-07-0	(Senta et al., 2019)
Clindamycin	18323-44-9	Hydroxy clindamycin sulfoxide	-	(Koba et al., 2017)
Clindamycin	18323-44-9	N-desmethyl clindamycin	-	(Koba et al., 2017)
Clindamycin	18323-44-9	S-desmethyl clindamycin	-	(Koba et al., 2017)
Clindamycin	18323-44-9	Clindamycin sulfoxide	22431-46-5	(Koba et al., 2017)
Clofibric acid	882-09-7	Hydroxy-clofibric acid	-	(Cruz-Morató et al., 2013)
Clofibric acid	882-09-7	1-chloro-4-isopropoxybenzene	-	(Maldonado-Torres et al., 2018)
Clofibric acid	882-09-7	P6	-	(Rosal et al., 2009)
Clofibric acid	882-09-7	P7	-	(Rosal et al., 2009)
Clofibric acid	882-09-7	P8	-	(Rosal et al., 2009)
Clofibric acid	882-09-7	Hydroquinone	123-31-9	(Rosal et al., 2009)
Clofibric acid	882-09-7	4-chlorophenol	106-48-9	(Salgado et al., 2012)
Clofibric acid	882-09-7	Lactic acid	50-21-5	(Salgado et al., 2012)
Clofibric acid	882-09-7	α-hydroxyisobutyric acid	594-61-6	(Salgado et al., 2012)
Codeine	76-57-3	Hydrocodone	125-29-1	(Long et al., 1995)
Codeine	76-57-3	Codeinone	467-13-0	(Long et al., 1995)
Codeine	76-57-3	Norcodeine	467-15-2	(Niknam et al., 2009)
Codeine	76-57-3	Morphine	57-27-2	(Niknam et al., 2009)
Codeine	76-57-3	6-acetylcodeine	6703-27-1	(Niknam et al., 2009)
Codeine	76-57-3	Oxycodone	76-42-6	(Niknam et al., 2009)
Cotinine	486-56-6	70	-	(Medana et al., 2016)
Cotinine	486-56-6	106	-	(Medana et al., 2016)
Cotinine	486-56-6	114	-	(Medana et al., 2016)

Cotinine	486-56-6	144	-	(Medana et al., 2016)
Cotinine	486-56-6	163	-	(Medana et al., 2016)
Cotinine	486-56-6	193	-	(Medana et al., 2016)
Cotinine	486-56-6	209	-	(Medana et al., 2016)
Cotinine	486-56-6	6-hydroxy-3-succinolpyridine	-	(Qiu et al., 2018)
Cotinine	486-56-6	6-hydroxy-cotinine	-	(Qiu et al., 2018)
Cotinine	486-56-6	2,3,6-trihydroxypyridine	39954-19-3	(Qiu et al., 2018)
Danofloxacin	112398-08-0	7-amino danofloxacin	-	(Chen et al., 1997)
Danofloxacin	112398-08-0	N-desmethyl danofloxacin	108461-04-7	(Chen et al., 1997)
Diazepam	439-14-5	Nordiazepam	1088-11-5	(Ambrus et al., 1975)
Diazepam	439-14-5	2-amino-N-(benzoyl-4-chlorophenyl)-N-methylacetamid	6021-21-2	(Ambrus et al., 1975)
Diazepam	439-14-5	TP-303	-	(Kosjek et al., 2012)
Diazepam	439-14-5	TP-A-301	-	(Kosjek et al., 2012)
Diazepam	439-14-5	TP-C-301	-	(Kosjek et al., 2012)
Diazepam	439-14-5	TP-C-317	-	(Kosjek et al., 2012)
Diazepam	439-14-5	Oxazepam	604-75-1	(Kosjek et al., 2012)
Diazepam	439-14-5	Temazepam	846-50-4	(Kosjek et al., 2012)
Diazepam	439-14-5	4-chloro-10-methylacridin-9-one	-	(West & Rowland, 2012)
Diazepam	439-14-5	5-chloro-2-(methylamino)benzophenone	1022-13-5	(West & Rowland, 2012)
Diazepam	439-14-5	2-amino-5-chlorobenzophenone	719-59-5	(West & Rowland, 2012)
Diazepam	439-14-5	4-chloro-10-H-acridin-9-one	7497-52-1	(West & Rowland, 2012)
Diclofenac	15307-86-5	2,6-dichlorobenzoic acid	50-30-6	(Dodgen et al., 2014)
Diclofenac	15307-86-5	2,4-dichlorobenzoic acid	50-84-0	(Dodgen et al., 2014)
Diclofenac	15307-86-5	3,5-Dichlorobenzoic acid	51-36-5	(Dodgen et al., 2014)
Diclofenac	15307-86-5	TPGG1-2019	-	(Gonzalez-Gil et al., 2019)
Diclofenac	15307-86-5	TPGG2-2019	-	(Gonzalez-Gil et al., 2019)
Diclofenac	15307-86-5	2-(1-(5-oxo-cyclohexa-1,3-dienyl-2-(2′,6′-dichloro-phenylimino)acetic acid	-	(Ivshina et al., 2019)
Diclofenac	15307-86-5	2-(p-benzoquinone-2)acetic acid	-	(Ivshina et al., 2019)

Diclofenac	15307-86-5	2-[1-(5-oxocyclohexa-1,3-dienyl-2-(3′,4′-dihydroxy-2′,6′-dichlorophenyl)imino]acetic acid	-	(Ivshina et al., 2019)
Diclofenac	15307-86-5	3-oxobutanoic acid (acetoacetic acid)	-	(Ivshina et al., 2019)
Diclofenac	15307-86-5	4,6,7-trioxooct-2-enedioic acid	-	(Ivshina et al., 2019)
Diclofenac	15307-86-5	4,6-dioxooct-2-trans-enedioic acid (fumarylacetoacetic acid)	-	(Ivshina et al., 2019)
Diclofenac	15307-86-5	5-amino-4,6-dichlorobenzene-1,2-diol	-	(Ivshina et al., 2019)
Diclofenac	15307-86-5	Phenylacetic acid	103-82-2	(Ivshina et al., 2019)
Diclofenac	15307-86-5	Fumaric acid	110-17-8	(Ivshina et al., 2019)
Diclofenac	15307-86-5	4-amino-3,5-dichlorophenol	26271-75-0	(Ivshina et al., 2019)
Diclofenac	15307-86-5	2,5-dihydroxyphenylacetic acid (homogentisic acid)	451-13-8	(Ivshina et al., 2019)
Diclofenac	15307-86-5	3-hydroxyphenylacetic acid	621-37-4	(Ivshina et al., 2019)
Diclofenac	15307-86-5	4HDQI	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 225	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 259	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 275	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 285	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 293a	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 293b	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 297	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 391a	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	TP 391b	-	(Jewell et al., 2016)
Diclofenac	15307-86-5	4-(2,6-dichlorophenylamino)-1,3-benzenedimethanol	-	(Marco-Urrea et al., 2010)
Diclofenac	15307-86-5	4-hydroxy diclofenac	64118-84-9	(Marco-Urrea et al., 2010)
Diclofenac	15307-86-5	DCF 10	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	DCF 11	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	DCF 12	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	DCF 3	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	DCF 4	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	DCF 5	-	(Moreira et al., 2018)

Diclofenac	15307-86-5	DCF 6	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	DCF 7	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	DCF 8	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	DCF 9	-	(Moreira et al., 2018)
Diclofenac	15307-86-5	Decarboxylated diclofenac	-	(Poirier-Larabie et al., 2016)
Diclofenac	15307-86-5	Nitroso diclofenac	-	(Poirier-Larabie et al., 2016)
Diclofenac	15307-86-5	TP241	-	(Poirier-Larabie et al., 2016)
Diclofenac	15307-86-5	TP259	-	(Poirier-Larabie et al., 2016)
Diclofenac	15307-86-5	5-hydroxy diclofenac	69002-84-2	(Poirier-Larabie et al., 2016)
Diclofenac	15307-86-5	TP1	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	TP11	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	TP12	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	TP2	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	TP4	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	TP5	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	TP6	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	TP7	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	TP9	-	(Roscher et al., 2016)
Diclofenac	15307-86-5	D1	-	(Salgado et al., 2013)
Diclofenac	15307-86-5	D2	-	(Salgado et al., 2013)
Diclofenac	15307-86-5	D3	-	(Salgado et al., 2013)
Diclofenac	15307-86-5	D4	-	(Salgado et al., 2013)
Diclofenac	15307-86-5	D5	-	(Salgado et al., 2013)
Diclofenac	15307-86-5	TP177	-	(Stylianou et al., 2018)
Diclofenac	15307-86-5	2-[2-(2,6-dichloroanilino)-5-nitrophenyl]acetic acid (TP341)	-	(Wu et al., 2019)
Diclofenac	15307-86-5	diclofenac-lactam	-	(Wu et al., 2019)
Diclofenac	15307-86-5	TP 298	-	(Wu et al., 2019)
Diclofenac	15307-86-5	TP 325	-	(Wu et al., 2019)
Diclofenac	15307-86-5	Diclofenac carboxylic acid	13625-57-5	(Wu et al., 2019)

Diclofenac	15307-86-5	MW 224	-	(Yu et al., 2013)
Diclofenac	15307-86-5	MW 261	-	(Yu et al., 2013)
Difloxacin	98105-99-8	Sarafloxacin	-	(Lamshöft et al.,2010)
Diphenhydramine	58-73-1	Diphenhydramine N-oxide	3922-74-5	(Topp et al., 2012)
Diphenhydramine	58-73-1	N-desmethyl-diphenhydramine	53499-40-4	(Wolfson et al., 2018)
d-Limonene	5989-27-5	(4R)-limonene-1,2-epoxyde	-	(Van der Werf et al., 1999)
d-Limonene	5989-27-5	Limonene-1,2-diol	1946-00-5	(Van der Werf et al., 1999)
d-Limonene	5989-27-5	1-hydroxy-2-oxolimonen	24047-73-2	(Van der Werf et al., 1999)
d-Limonene	5989-27-5	(3R)-3-isopropenyl-6-oxoheptanoate	4436-82-2	(Van der Werf et al., 1999)
Doxycycline	564-25-0	Metacycline	914-00-1	(Widyasari-Mehta et al., 2016)
Duloxetine	116539-59-4	TP 290	-	(Osawa et al., 2019a)
Duloxetine	116539-59-4	TP 312 -A	-	(Osawa et al., 2019a)
Duloxetine	116539-59-4	TP 312- B	-	(Osawa et al., 2019a)
Duloxetine	116539-59-4	TP 312-C	-	(Osawa et al., 2019a)
Duloxetine	116539-59-4	TP 328 - B	-	(Osawa et al., 2019a)
Duloxetine	116539-59-4	TP 330	-	(Osawa et al., 2019a)
Duloxetine	116539-59-4	TP 332	-	(Osawa et al., 2019a)
Duloxetine	116539-59-4	TP 348	-	(Osawa et al., 2019a)
Emtricitabine	143491-57-0	Carboxy-emtricitabine-S-oxide	-	(Funke et al., 2016)
Emtricitabine	143491-57-0	Emtricitabine carboxylate	1238210-10-0	(Funke et al., 2016)
Emtricitabine	143491-57-0	Emtricitabine-S-oxide	152128-77-3	(Funke et al., 2016)
Emtricitabine	143491-57-0	TP 129	-	(Prasse et al., 2015)
Emtricitabine	143491-57-0	TP 265	-	(Prasse et al., 2015)
Enrofloxacin	93106-60-6	Desethylene-enrofloxacin	-	(Parshikov et al., 2000)
Enrofloxacin	93106-60-6	Enrofloxacin N-oxide	-	(Parshikov et al., 2000)
Enrofloxacin	93106-60-6	N-acetylciprofloxacin	93594-20-8	(Parshikov et al., 2000)
Enrofloxacin	93106-60-6	ENR-A	-	(Sturini et al., 2012)
Enrofloxacin	93106-60-6	ENR-C	-	(Sturini et al., 2012)
Enrofloxacin	93106-60-6	ENR-D	-	(Sturini et al., 2012)

Enrofloxacin	93106-60-6	2',3'-dioxo-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	3-decarboxy-3-hydroxy-N-4′-deethyl-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	6-defluoro-6-hydroxy-trihydroxy-oxo-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	6-defluoro-N-4′-deethyl-dioxo-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	7-deethylpiperazino-7-amino-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Deethylene-EFL	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Deethylene-N-formyl-F-11	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Dehydro-hydroxy-EFL	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Dehydro-oxo-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Dihydro-trihydroxy-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Dihydroxy-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Dihydroxy-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Dihydroxy-F-11	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Dihydroxy-oxo-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Dioxo-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Enrofloxacin-N-4'oxide	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	F-16	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	F-20	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	F-3	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Hydroxy-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Hydroxy-F-3	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Hydroxy-F-4	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Hydroxy-oxo-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Hydroxy-oxo-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Hydroxy-oxo-F-3	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-1', N-4'-dioxide enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-4′-deethyl-F-4	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-4′-deethyl-hydroxy-F-11	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-4′-deethyl-hydroxy-oxo-enrofloxacin	-	(Wetzstein et al., 2006)

Enrofloxacin	93106-60-6	N-4′-deethyl-oxo-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-4′-deethyl-oxo-F-4	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-cyclopropyl-N-[5-(4-ethylpiperazine-1-yl)-4-fluoro-2-formylphenyl]-formamide	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-decyclopropyl-oxo-enrofloxacin	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-formyl-dihydroxy-F-11	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-formyl-F-11	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-formyl-hydroxy-F-11	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-formyl-trihydroxy-F-11	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-hydroxyethyl-F-9	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	N-hydroxyethyl-N-formyl-F-9	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	O-acetyl-dihydroxy-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	O-acetyl-trihydroxy-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Trihydroxy-F-1	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Trihydroxy-F-11	-	(Wetzstein et al., 2006)
Enrofloxacin	93106-60-6	Ciprofloxacin	85721-33-1	(Wetzstein et al., 2006)
Erythromycin	114-07-8	E-1	-	(Batchu et al., 2014)
Erythromycin	114-07-8	E-2	-	(Batchu et al., 2014)
Erythromycin	114-07-8	Erythralosamine	546-57-6	(Gómez-Ramos et al., 2011)
Erythromycin	114-07-8	Anhydroerythromycin	23893-13-2	(Schlüsener et al., 2006)
Erythromycin	114-07-8	Erythromycin enol ether	33396-29-1	(Senta et al., 2019)
Erythromycin	114-07-8	Erythromycin imino ether	99290-97-8	(Senta et al., 2019)
Erythromycin	114-07-8	EZY TP 419	-	(Terzic et al., 2018)
Erythromycin	114-07-8	EZY TP 576	-	(Terzic et al., 2018)
Erythromycin	114-07-8	EZY TP 720	-	(Terzic et al., 2018)
Erythromycin	114-07-8	EZY TP 750a	-	(Terzic et al., 2018)
Erythromycin	114-07-8	EZY TP 750b	-	(Terzic et al., 2018)
Erythromycin	114-07-8	EZY TP 814	-	(Terzic et al., 2018)
Estriol (E3)	50-27-1	16-hydroxyestrone	18186-49-7	(Ke et al., 2007)

Estrone (E1)	53-16-7	2-methoxy-estrone	362-08-3	(Goeppert et al., 2015)
Estrone (E1)	53-16-7	Estrone-3-sulfate	481-97-0	(Goeppert et al., 2015)
Estrone (E1)	53-16-7	2-hydroxyE1	-	(Wang et al., 2019)
Estrone (E1)	53-16-7	2-hydroxyE2	-	(Wang et al., 2019)
Estrone (E1)	53-16-7	2-methoxyestradiol	-	(Wang et al., 2019)
Estrone (E1)	53-16-7	TP254-1	-	(Wang et al., 2019)
Estrone (E1)	53-16-7	TP254-2	-	(Wang et al., 2019)
Estrone (E1)	53-16-7	TP268	-	(Wang et al., 2019)
Estrone (E1)	53-16-7	TP334	-	(Wang et al., 2019)
Estrone (E1)	53-16-7	Estriol	50-27-1	(Zheng et al., 2012)
Fenbendazole	43210-67-9	Oxfendazole	53716-50-0	(Kreuzig et al., 2007)
Fenbendazole	43210-67-9	Fenbendazole sulfone	54029-20-8	(Kreuzig et al., 2007)
Flumequine	42835-25-6	$C_{14}H_{13}FNO_2$ (F7)	-	(Čvančarová et al., 2013)
Flumequine	42835-25-6	$C_{14}H_{15}FNO_2$ (F6)	-	(Čvančarová et al., 2013)
Flumequine	42835-25-6	$C_{15}H_{15}FNO_3$ (F2)	-	(Čvančarová et al., 2013)
Flumequine	42835-25-6	$C_{15}H_{15}FNO_4$ (F3)	-	(Čvančarová et al., 2013)
Flumequine	42835-25-6	$C_{16}H_{17}FNO_3$ (F4)	-	(Čvančarová et al., 2013)
Flumequine	42835-25-6	$C_{16}H_{17}FNO_3$ (F5)	-	(Čvančarová et al., 2013)
Flumequine	42835-25-6	$C_{16}H_{19}FNO_2$ (F8)	-	(Čvančarová et al., 2013)
Flumequine	42835-25-6	Hydroxyflumequine (F1)	61293-22-9	(Čvančarová et al., 2013)
Flumequine	42835-25-6	P208	-	(Feng et al., 2016)
Flumequine	42835-25-6	P210	-	(Feng et al., 2016)
Flumequine	42835-25-6	P220	-	(Feng et al., 2016)
Flumequine	42835-25-6	P222	-	(Feng et al., 2016)
Flumequine	42835-25-6	P224	-	(Feng et al., 2016)
Flumequine	42835-25-6	P234	-	(Feng et al., 2016)
Flumequine	42835-25-6	P236	-	(Feng et al., 2016)
Flumequine	42835-25-6	P238	-	(Feng et al., 2016)
Flumequine	42835-25-6	P250	-	(Feng et al., 2016)

Flumequine	42835-25-6	P266	-	(Feng et al., 2016)
Flumequine	42835-25-6	P268	-	(Feng et al., 2016)
Flumequine	42835-25-6	P276	-	(Feng et al., 2016)
Flumequine	42835-25-6	P278B	-	(Feng et al., 2016)
Flumequine	42835-25-6	P294	-	(Feng et al., 2016)
Flumequine	42835-25-6	P296	-	(Feng et al., 2016)
Flumequine	42835-25-6	P312	-	(Feng et al., 2016)
Fluoxetine	54910-89-3	TP139	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP146	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP148	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP150	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP152	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP166	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP182a	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP182b	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP272	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP286a	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP286b	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP286c	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP326a	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP326b	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP326c	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP338	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP352	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP364	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TP366	-	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TFA	14477-72-6	(Tisler et al., 2019)
Fluoxetine	54910-89-3	TFMP	402-45-9	(Tisler et al., 2019)
Flurbiprofen	5104-49-4	4-(1-carboxyethyl)-2-fluorobenzoic acid	-	(Yanaç & Murdoch, 2019)

Furosemide	54-31-9	5-sulfamoylhydroxyanthranilic acid	-	(Jakimska et al., 2014)
Furosemide	54-31-9	N-furfuryl-5-sulfamoylhydroxyanthranilic acid	-	(Jakimska et al., 2014)
Furosemide	54-31-9	4-chloro-5-sulfamoylanthranilic acid	3086-91-7	(Jakimska et al., 2014)
Furosemide	54-31-9	5-sulfamoylanthranilic acid	3086-91-7	(Jakimska et al., 2014)
Furosemide	54-31-9	N-furfuryl-5-sulfamoylanthranilic acid	4818-85-3	(Jakimska et al., 2014)
Furosemide	54-31-9	Derivee pyrimidium furosemide	-	(Olvera-vargas et al., 2016)
Furosemide	54-31-9	Hydroxy-cetone furosemide	-	(Olvera-vargas et al., 2016)
Furosemide	54-31-9	Saluamine	3086-91-7	(Olvera-vargas et al., 2016)
Gabapentin	60142-96-3	TP 167a	-	(Henning et al., 2018)
Gabapentin	60142-96-3	TP 169b	-	(Henning et al., 2018)
Gabapentin	60142-96-3	TP 185a	-	(Henning et al., 2018)
Gabapentin	60142-96-3	TP 185c	-	(Henning et al., 2018)
Gabapentin	60142-96-3	TP 186	-	(Henning et al., 2018)
Gabapentin	60142-96-3	TP 187b	-	(Henning et al., 2018)
Gabapentin	60142-96-3	TP 213	-	(Henning et al., 2018)
Gabapentin	60142-96-3	Gabapentin lactam	64744-50-9	(Henning et al., 2018)
Gabapentin	60142-96-3	TP128	-	(Herrmann et al., 2015)
Gabapentin	60142-96-3	TP160a	-	(Herrmann et al., 2015)
Gabapentin	60142-96-3	TP160b	-	(Herrmann et al., 2015)
Gabapentin	60142-96-3	TP168	-	(Herrmann et al., 2015)
Gabapentin	60142-96-3	TP186-1	-	(Herrmann et al., 2015)
Gabapentin	60142-96-3	TP186-5	-	(Herrmann et al., 2015)
Gabapentin	60142-96-3	TP188	-	(Herrmann et al., 2015)
Gabapentin	60142-96-3	TP204a	-	(Herrmann et al., 2015)
Gabapentin	60142-96-3	TP204b	-	(Herrmann et al., 2015)
Galaxolide	1222-05-5	TP 1	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 10	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 11	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 12	-	(Herrera López et al., 2013)

Galaxolide	1222-05-5	TP 13	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 14	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 15	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 16	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 17	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 18	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 2	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 3	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 4	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 5	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 6	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 7	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 8	-	(Herrera López et al., 2013)
Galaxolide	1222-05-5	TP 9	-	(Herrera López et al., 2013)
Gemfibrozil	25812-30-0	FM1	-	(Kang et al., 2009)
Gemfibrozil	25812-30-0	FM2	-	(Kang et al., 2009)
Gemfibrozil	25812-30-0	FM3	-	(Kang et al., 2009)
Gemfibrozil	25812-30-0	FM4	-	(Kang et al., 2009)
Gemfibrozil	25812-30-0	FM6	-	(Kang et al., 2009)
Gemfibrozil	25812-30-0	FM6'	-	(Kang et al., 2009)
Gemfibrozil	25812-30-0	FM7	-	(Kang et al., 2009)
Gemfibrozil	25812-30-0	FM8	-	(Kang et al., 2009)
Gemfibrozil	25812-30-0	Photoproduit I	-	(Ma, Lv et al., 2016)
Gemfibrozil	25812-30-0	Photoproduit II	-	(Ma, Lv et al., 2016)
Gemfibrozil	25812-30-0	Photoproduit III	-	(Ma, Lv et al., 2016)
Gemfibrozil	25812-30-0	Photoproduit IV	-	(Ma, Lv et al., 2016)
Glibenclamide	10238-21-8	Glibenclamide B	-	(Markiewicz et al., 2017)
Glibenclamide	10238-21-8	m/z 169	-	(Radjenovic et al., 2008)
Glibenclamide	10238-21-8	m/z 395	-	(Radjenovic et al., 2008)

Ibuprofen	15687-27-1	IbB3	-	(Boix et al., 2016).
Ibuprofen	15687-27-1	IbB4	-	(Boix et al., 2016).
Ibuprofen	15687-27-1	1-(4-ethylphenyl)2-methylpropn-1-ol	-	(Jakimska et al., 2014)
Ibuprofen	15687-27-1	1-ethyl-4-(2-methylprop-1-en-1-yl)benzene	-	(Jakimska et al., 2014)
Ibuprofen	15687-27-1	1-ethyl-4-(2-methylprop-2-en-1yl)benzene	-	(Jakimska et al., 2014)
Ibuprofen	15687-27-1	2-hydroxy-2-[4-(2-methylpropyl)]propanoic acid	-	(Jakimska et al., 2014)
Ibuprofen	15687-27-1	1-ethyl-4-isobutylbenzene	100319-40-2	(Jakimska et al., 2014)
Ibuprofen	15687-27-1	1-(4-isobutylphenyl)ethanol	40150-92-3	(Jakimska et al., 2014)
Ibuprofen	15687-27-1	1-isobutyl-4-vinylbenzene	63444-56-4	(Jakimska et al., 2014)
Ibuprofen	15687-27-1	1-(4-ethylphenyl)-2-methylpropan-2-ol	87077-46-1	(Jakimska et al., 2014)
Ibuprofen	15687-27-1	1,2-dihydroxy ibuprofen	-	(Marco-Urrea et al., 2009)
Ibuprofen	15687-27-1	Carboxyhydratropic acid	-	(Zwiener et al., 2002)
Ibuprofen	15687-27-1	2-hydroxyibuprofen	51146-55-5	(Zwiener et al., 2002)
Ibuprofen	15687-27-1	1-hydroxyibuprofen	53949-53-4	(Zwiener et al., 2002)
Indole	120-72-9	Anthranilic acid	118-92-3	(Johansen et al., 1997)
Indole	120-72-9	3-methyloxindole	1504-06-9	(Johansen et al., 1997)
Indole	120-72-9	7-methyloxindole	3680-28-2	(Johansen et al., 1997)
Indole	120-72-9	Isatoic acid	490-74-4	(Johansen et al., 1997)
Indole	120-72-9	Oxindole	59-48-3	(Johansen et al., 1997)
Indole	120-72-9	1-methylindole	603-76-9	(Johansen et al., 1997)
Indole	120-72-9	Isatin	91-56-5	(Johansen et al., 1997)
Indole	120-72-9	2-methylindole	95-20-5	(Johansen et al., 1997)
Indole	120-72-9	3-indoxyl	480-93-3	(Sadauskas et al., 2017)
Indole	120-72-9	Indigo	482-89-3	(Sadauskas et al., 2017)
Indole	120-72-9	4-(3-hydroxy-1-H-pyrrol-2-yl)-2-oxo-but-3-enoic acid	-	(Yang et al., 2017)
Indole	120-72-9	Pyrrole-2,3-dicarboxylic acid	1125-32-2	(Yang et al., 2017)
Indole	120-72-9	4,5-dihydroxyindole	412029-30-2	(Yang et al., 2017)
Indole	120-72-9	2,3-dihydroxyindole	5638-85-7	(Yang et al., 2017)
Indole	120-72-9	Salicylic acid	69-72-7	(Yang et al., 2017)

Indomethacin	53-86-1	CMBA	-	(Jiménez et al., 2017)
Indomethacin	53-86-1	DHINDO	-	(Jiménez et al., 2017)
Indomethacin	53-86-1	MMIA	-	(Jiménez et al., 2017)
Indomethacin	53-86-1	AMBA	38985-80-7	(Jiménez et al., 2017)
Indomethacin	53-86-1	MMIC	6260-86-2	(Jiménez et al., 2017)
Indomethacin	53-86-1	CBA	74-11-3	(Jiménez et al., 2017)
Iopromide	73334-07-3	TP 451	-	(Gros et al., 2014a).
Iopromide	73334-07-3	TP 465	-	(Gros et al., 2014a).
Iopromide	73334-07-3	TP 525 A	-	(Gros et al., 2014a).
Iopromide	73334-07-3	TP 525 B	-	(Gros et al., 2014a).
Iopromide	73334-07-3	TP 577	-	(Gros et al., 2014a).
Iopromide	73334-07-3	TP 651	-	(Gros et al., 2014a).
Iopromide	73334-07-3	TP 665	-	(Gros et al., 2014a).
Iopromide	73334-07-3	TP 643	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 701 A	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 701 B	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 729 A	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 731 A	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 731 B	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 759	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 787 A	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 805 A	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 805 B	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 817 A	-	(Schulz et al., 2008)
Iopromide	73334-07-3	TP 819	-	(Schulz et al., 2008)
Irbesartan	138402-11-6	IB3a	-	(Boix et al., 2016)
Irbesartan	138402-11-6	IB3b	-	(Boix et al., 2016)
Irbesartan	138402-11-6	IB4b	-	(Boix et al., 2016)
Irbesartan	138402-11-6	IB5	-	(Boix et al., 2016)

Irbesartan	138402-11-6	IB6	-	(Boix et al., 2016)
Irbesartan	138402-11-6	ISW1a	-	(Boix et al., 2016)
Irbesartan	138402-11-6	ISW1b	-	(Boix et al., 2016)
Irbesartan	138402-11-6	ISW2	-	(Boix et al., 2016)
Irbesartan	138402-11-6	IRB_444	-	(Letzel et al., 2015)
Ivermectin	70288-86-7	Ivermectin aglycone	123997-59-1	(Prasse et al., 2009)
Ivermectin	70288-86-7	Ivermectin monosaccharide	123997-64-8	(Prasse et al., 2009)
Ketoprofen	22071-15-4	3-(1-hydroperoxyethyl)benzophenone	-	(Illés et al., 2014)
Ketoprofen	22071-15-4	3-ethylbenzophenone	66067-43-4	(Illés et al., 2014)
Ketoprofen	22071-15-4	1-(3-benzoylphenyl)ethanone	66067-44-5	(Illés et al., 2014)
Ketoprofen	22071-15-4	3-(1-hydroxyethyl)benzophenone	67173-18-6	(Illés et al., 2014)
Ketoprofen	22071-15-4	2-[3-(1-hydroxy-2-methylpropyl)phenyl]propanoic acid	-	(Jakimska et al., 2014)
Ketoprofen	22071-15-4	3-acetylhydroxybenzophenone	-	(Jakimska et al., 2014)
Ketoprofen	22071-15-4	Hydroxybenzophenone	117-99-7	(Jakimska et al., 2014)
Ketoprofen	22071-15-4	4-hydroxy-2-oxovalerate	3318-73-8	(Lau et al., 1994)
Ketoprofen	22071-15-4	Pyruvate	57-60-3	(Lau et al., 1994)
Ketoprofen	22071-15-4	Acetaldehyde	75-07-0	(Lau et al., 1994)
Ketoprofen	22071-15-4	(2E,4Z)-7-[3-(1-carboxylatoethyl)phenyl]-2,7-dihydroxy-6-oxohepta-2,4-dienoate	-	(Quintana et al., 2005)
Ketoprofen	22071-15-4	2-[(3-hydroxy(phenyl)methyl)phenyl]-propanoate	-	(Quintana et al., 2005)
Ketoprofen	22071-15-4	2-[3-(carboxylatocarbonyl)phenyl]propanoate	-	(Quintana et al., 2005)
Ketoprofen	22071-15-4	2-{3-[(2,3-dihydroxyphenyl)(hydroxy)methyl]phenyl}propanoate	-	(Quintana et al., 2005)
Ketoprofen	22071-15-4	2-{3-[carboxylato(hydroxy)methyl]phenyl}propanoate	-	(Quintana et al., 2005)
Ketoprofen	22071-15-4	3-(hydroxy-carboxymethyl)hydratopic acid	-	(Quintana et al., 2005)
Ketoprofen	22071-15-4	3-(keto-carboxymethyl)hydratopic acid	-	(Quintana et al., 2005)
Ketoprofen	22071-15-4	cis-2-hydroxypenta-2,4-dienoate	159694-16-3	(Quintana et al., 2005)
Lamotrigine	84057-84-1	TP243	-	(Bollmann et al., 2016)
Lamotrigine	84057-84-1	TP260	-	(Bollmann et al., 2016)
Lamotrigine	84057-84-1	TP304	-	(Bollmann et al., 2016)

Lamotrigine	84057-84-1	Lamotrigine N2-oxide	136565-76-9	(Bollmann et al., 2016)
Levetiracetam	102767-28-2	Levetiracetam acid	103833-72-3	(Helbling et al., 2010)
Limonene	138-86-3	Perillyl aldehyde	2111-75-3	(Ballal et al., 1966)
Limonene	138-86-3	Alcool perillylique	536-59-4	(Ballal et al., 1966)
Limonene	138-86-3	Acide perillique	7694-45-3	(Dhavalikar et al., 1966)
Limonene	138-86-3	Isopiperitenone	529-01-1	(Kjonaas et al., 1985)
Limonene	138-86-3	α-terpineol	98-55-5	(Savithiry et al.,1997)
Limonene	138-86-3	Carvone	2244-16-8	(Savithiry et al., 1998)
Limonene	138-86-3	Carveol	99-48-9	(Savithiry et al., 1998)
Limonene	138-86-3	Dihydrocarvone	5524-05-0	(Van Der Werf & Boot, 2000)
Limonene	138-86-3	Isopiperitenol	491-05-4	(Van Der Werf & Boot, 2000)
Lincomycin	154-21-2	287	-	(Calza et al., 2012)
Lincomycin	154-21-2	359	-	(Calza et al., 2012)
Lincomycin	154-21-2	377	-	(Calza et al., 2012)
Lincomycin	154-21-2	343-A	-	(Calza et al., 2012)
Lincomycin	154-21-2	343-B	-	(Calza et al., 2012)
Lincomycin	154-21-2	343-C	-	(Calza et al., 2012)
Lincomycin	154-21-2	373-A	-	(Calza et al., 2012)
Lincomycin	154-21-2	373-B	-	(Calza et al., 2012)
Lincomycin	154-21-2	373-C	-	(Calza et al., 2012)
Lincomycin	154-21-2	375-A	-	(Calza et al., 2012)
Lincomycin	154-21-2	375-B	-	(Calza et al., 2012)
Lincomycin	154-21-2	405-A	-	(Calza et al., 2012)
Lincomycin	154-21-2	405-B	-	(Calza et al., 2012)
Lincomycin	154-21-2	423-A	-	(Calza et al., 2012)
Lincomycin	154-21-2	423-B	-	(Calza et al., 2012)
Lincomycin	154-21-2	423-C	-	(Calza et al., 2012)
Lincomycin	154-21-2	439-A,B	-	(Calza et al., 2012)
Lincomycin	154-21-2	439-C	-	(Calza et al., 2012)

Lincomycin	154-21-2	455-A	-	(Calza et al., 2012)
Lincomycin	154-21-2	455-C	-	(Calza et al., 2012)
Marbofloxacin	115550-35-1	C15H16N3O4F	-	(Sturini et al., 2010)
Marbofloxacin	115550-35-1	C30H29N6O8F2	-	(Sturini et al., 2010)
Mefenamic acid	61-68-7	P1	-	(Chen et al., 2016)
Mefenamic acid	61-68-7	P2	-	(Chen et al., 2016)
Mefenamic acid	61-68-7	P3	-	(Chen et al., 2016)
Mefenamic acid	61-68-7	P4	-	(Chen et al., 2016)
Methotrexate	59-05-2	M-1	-	(Calza et al., 2014)
Methotrexate	59-05-2	M-2	-	(Calza et al., 2014)
Methotrexate	59-05-2	M-7	-	(Calza et al., 2014)
Methotrexate	59-05-2	TP-152	-	(Kosjek et al., 2015)
Methotrexate	59-05-2	TP-191	-	(Kosjek et al., 2015)
Methotrexate	59-05-2	TP-206	-	(Kosjek et al., 2015)
Methotrexate	59-05-2	TP-207	-	(Kosjek et al., 2015)
Methotrexate	59-05-2	TP-312	-	(Kosjek et al., 2015)
Methotrexate	59-05-2	TP-325	-	(Kosjek et al., 2015)
Methotrexate	59-05-2	TP-326	-	(Kosjek et al., 2015)
Methotrexate	59-05-2	TP-342	-	(Kosjek et al., 2015)
Methotrexate	59-05-2	7-hydroxy methotrexate	5939-37-7	(Kosjek et al., 2015)
Methotrexate	59-05-2	TP179	-	(Lutterbeck et al., 2015)
Methotrexate	59-05-2	TP207	-	(Lutterbeck et al., 2015)
Methotrexate	59-05-2	TP209	-	(Lutterbeck et al., 2015)
Methotrexate	59-05-2	TP267	-	(Lutterbeck et al., 2015)
Methotrexate	59-05-2	TP281	-	(Lutterbeck et al., 2015)
Methotrexate	59-05-2	TP469	-	(Lutterbeck et al., 2015)
Methotrexate	59-05-2	TP471	-	(Lutterbeck et al., 2015)
Methylparaben	99-76-3	3,5-dichloro-methylparaben	-	(Mao et al., 2016)
Methylparaben	99-76-3	3-chloro-methylparaben	-	(Mao et al., 2016)

Methylparaben	99-76-3	4-hydroxybenzoic acid	99-96-7	(Wolfson et al., 2019)
Methylparaben	99-76-3	Phenol	108-95-2	(Wu et al., 2017)
Methylparaben	99-76-3	Benzoic acid	65-85-0	(Wu et al., 2017)
Metoprolol	37350-58-6	TP134	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP226A	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP226C	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP238	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP240	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP254	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP270	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP282A	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP282B	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP284	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP298	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP300	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	TP316	-	(Jaén-Gil et al., 2019)
Metoprolol	37350-58-6	α-ketometoprolol	-	(Li et al., 2014)
Metoprolol	37350-58-6	Met 210	-	(Li et al., 2014)
Metoprolol	37350-58-6	4-[2-hydroxy-3-(isopropylamino)propoxy]benzaldehyde (DMPLD)	-	(Lv et al., 2018)
Metoprolol	37350-58-6	4-[2-hydroxy-3-(isopropylamino)propoxy]benzoic acid (DMPLA)	-	(Lv et al., 2018)
Metoprolol	37350-58-6	Hydroxy{4-[2-hydroxy-3-(isopropylamino)propoxy]phenyl}acetic acid (alpha-HMPLA)	-	(Lv et al., 2018)
Metoprolol	37350-58-6	1-(4-(2-hydroxy-3-(isopropylamino)propoxy)phenyl)-2-methoxyethanone	-	(Rubirola et al., 2014)
Metoprolol	37350-58-6	Metoprolol acid	56392-14-4	(Rubirola et al., 2014)
Metoprolol	37350-58-6	α-Hydroxymetoprolol	56392-16-6	(Rubirola et al., 2014)
Metoprolol	37350-58-6	4-(2-hydroxy-3-(isopropylamino)propoxy)phenol	62340-37-8	(Rubirola et al., 2014)
Metoprolol	37350-58-6	O-demethylmetoprolol	62572-94-5	(Rubirola et al., 2014)
Metoprolol	37350-58-6	Deaminated metoprolol	-	(Svan et al., 2016)
Metoprolol	37350-58-6	N-dealkyl metoprolol	-	(Svan et al., 2016)

Monensin	17090-79-8	TP-MON	-	(Sun et al., 2014)
Morphine	57-27-2	14-hydroxymorphine	3371-56-0	(Long et al., 1995)
Morphine	57-27-2	14-hydroxymorphine-6-one	41135-98-2	(Long et al., 1995)
Morphine	57-27-2	Hydromorphone	466-99-9	(Long et al., 1995)
Morphine	57-27-2	Morphinone	467-02-7	(Long et al., 1995)
Morphine	57-27-2	Dihydromorphine 2	509-60-4	(Long et al., 1995)
Moxifloxacin	151096-09-2	Mox-A	-	(Maia et al., 2014)
Moxifloxacin	151096-09-2	Mox-B	-	(Maia et al., 2014)
Naproxen	22204-53-1	(1-(6-methoxynaphthalen-2-yl)ethanone)	-	(Marco-Urrea et al., 2010)
Naproxen	22204-53-1	7-hydroxynaproxen	-	(Marco-Urrea et al., 2010)
Naproxen	22204-53-1	NAP 1	-	(Śliwka-Kaszyńska et al., 2019)
Naproxen	22204-53-1	NAP 2b	-	(Śliwka-Kaszyńska et al., 2019)
Naproxen	22204-53-1	NAP 3	-	(Śliwka-Kaszyńska et al., 2019)
Naproxen	22204-53-1	NAP 4	-	(Śliwka-Kaszyńska et al., 2019)
Naproxen	22204-53-1	NAP 5	-	(Śliwka-Kaszyńska et al., 2019)
Naproxen	22204-53-1	NAP 6a	-	(Śliwka-Kaszyńska et al., 2019)
Naproxen	22204-53-1	NAP 6b	-	(Śliwka-Kaszyńska et al., 2019)
Naproxen	22204-53-1	Dihydroxynaproxen	-	(Wojcieszynska et al., 2014)
Naproxen	22204-53-1	Nap-Cliv-1	-	(Wojcieszynska et al., 2014)
Naproxen	22204-53-1	Nap-Cliv-2	-	(Wojcieszynska et al., 2014)
Naproxen	22204-53-1	Trihydroxynaproxen	-	(Wojcieszynska et al., 2014)
Naproxen	22204-53-1	6-O-desmethyl-naproxen	52079-10-4	(Wolfson et al., 2019)
Nitrofurantoin	67-20-9	N-1	-	(Biosic et al., 2017)
Nitrofurantoin	67-20-9	N-2	-	(Biosic et al., 2017)
Nitrofurantoin	67-20-9	N-3	-	(Biosic et al., 2017)
Nitrofurantoin	67-20-9	N-4	-	(Biosic et al., 2017)
Nitrofurantoin	67-20-9	N-5	-	(Biosic et al., 2017)
Nitrofurantoin	67-20-9	N-6	-	(Biosic et al., 2017)
Norfloxacin	70458-96-7	N-acetylnorfloxacin	-	(Adjei et al., 2006)

Norfloxacin	70458-96-7	N-nitrosonorfloxacin	-	(Adjei et al., 2006)
Norfloxacin	70458-96-7	NOR-C	-	(Amorim et al., 2014)
Norfloxacin	70458-96-7	Desethylene-N-acetylnorfloxacine (N3)	-	(Čvančarová et al., 2015)
Norfloxacin	70458-96-7	N-formylnorfloxacine (N4)	70459-04-0	(Čvančarová et al., 2015)
Norfloxacin	70458-96-7	N-acetylnorfloxacine (N5)	74011-56-6	(Čvančarová et al., 2015)
Norfloxacin	70458-96-7	7-amino-1-ethyl-6-fluoro-4-oxo- 1, 4-dihydroquinoline-3-carboxylic acid (N2) (75001-63-7)	75001-63-7	(Čvančarová et al., 2015)
Norfloxacin	70458-96-7	Desethylene norfloxacine (N1)	78295-91-7	(Čvančarová et al., 2015)
Norfloxacin	70458-96-7	6-defluoro-6-hydroxynorfloxacin	-	(Kim et al., 2011)
Norfloxacin	70458-96-7	8-hydroxynorfloxacine	-	(Kim et al., 2011)
Norfloxacin	70458-96-7	C16H20N3O4	-	(Maia et al., 2014)
Nortriptyline	72-69-5	m/z 251.3	-	(Chen et al., 2016)
Nortriptyline	72-69-5	m/z 261.4	-	(Chen et al., 2016)
Nortriptyline	72-69-5	m/z 280.6-1	-	(Chen et al., 2016)
Nortriptyline	72-69-5	m/z 280.6-2	-	(Chen et al., 2016)
Nortriptyline	72-69-5	2-OH-hydroxynortriptyline	-	(Li et al., 2013)
Nortriptyline	72-69-5	10-hydroxynortriptyline	1156-99-6	(Li et al., 2013)
O-Cresol	95-48-7	cis,cis-2-hydroxy-6-oxohept-2,4-dienoate	7244-95-3	(Kukor & Olsen, 1991)
O-Cresol	95-48-7	Pyruvate	127-17-3	(Lau et al., 1994)
O-Cresol	95-48-7	4-hydroxy-2-oxovalerate	3318-73-8	(Lau et al., 1994)
O-Cresol	95-48-7	Acetaldehyde	75-07-0	(Lau et al., 1994)
O-Cresol	95-48-7	cis-2-hydroxypenta-2,4-dienoate	159694-16-3	(Menn, Zylstra, & Gibson, 1991)
O-Cresol	95-48-7	Acetate	64-19-7	(Menn et al., 1991)
O-Cresol	95-48-7	3-methycatechol	488-17-5	(Shields et al.,1995)
Ofloxacin	82419-36-1	OFL-B	-	(Amorim et al., 2014)
Ofloxacin	82419-36-1	10-(4-acetylpiperazin-1-yl)-9- fluoro-3-methyl-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quin- oline-6-carboxylic acid (O6)	-	(Čvančarová et al., 2015)
Ofloxacin	82419-36-1	10-[(2-acetamidoethyl)amino]-9-fluoro-3-methyl- 7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (O4)	-	(Čvančarová et al., 2015)
Ofloxacin	82419-36-1	10-amino-9-fluoro-3-methyl-7-oxo-2,3-dihydro-7H-[1,4] oxazino[2,3,4-ij]quinoline-6-carboxylic acid (O5)	-	(Čvančarová et al., 2015)

Ofloxacin	82419-36-1	9-fluoro- 10-(4-formylpiperazin-1-yl)-3-methyl-7-oxo-2,3-dihydro-7H-[1,4] oxazino[2,3,4-ij]quinoline-6-carboxylic acid (O2)	-	(Čvančarová et al., 2015)
Ofloxacin	82419-36-1	9-fluoro-10- [(2-formamidoethyl)amino]-3-methyl-7-oxo-2,3-dihydro-7H-[1,4] oxazino[2,3,4-ij]quinoline-6-carboxylic acid (O1)	-	(Čvančarová et al., 2015)
Ofloxacin	82419-36-1	Desethylene-N-ofloxacine (O3)	-	(Čvančarová et al., 2015)
Ofloxacin	82419-36-1	Desmethyl ofloxacin	82419-46-3	(Čvančarová et al., 2015)
Ofloxacin	82419-36-1	TP 375	-	(Gros et al., 2014b)
Ofloxacin	82419-36-1	TP 389	-	(Gros et al., 2014b)
Ofloxacin	82419-36-1	TP10	-	(Vasquez et al., 2013)
Ofloxacin	82419-36-1	TP2	-	(Vasquez et al., 2013)
Ofloxacin	82419-36-1	TP3	-	(Vasquez et al., 2013)
Ofloxacin	82419-36-1	TP4	-	(Vasquez et al., 2013)
Ofloxacin	82419-36-1	TP6	-	(Vasquez et al., 2013)
Ofloxacin	82419-36-1	TP7	-	(Vasquez et al., 2013)
Ofloxacin	82419-36-1	TP8	-	(Vasquez et al., 2013)
Ofloxacin	82419-36-1	TP9	-	(Vasquez et al., 2013)
Omeprazole	73590-58-6	6-(hydroxymethyl)-4-methoxy-3,5-dimethylpyridin-2-ol	-	(Kosma et al., 2017)
Omeprazole	73590-58-6	6-methoxy-1H-benzo[d]imidazole	-	(Kosma et al., 2017)
Omeprazole	73590-58-6	6-methoxy-2-(((4-methoxy-3,5-dimethylpyridin-2-yl)methyl)thio)-1H-benzo[d]imidazole	-	(Kosma et al., 2017)
Omeprazole	73590-58-6	6-methoxy-2-((4-methoxy-3,5-dimethylpyridin-2-yl)methyl)-1H-benzo[d]imidazole	-	(Kosma et al., 2017)
Omeprazole	73590-58-6	4-methoxy-3,5-dimethylpicolinic acid	138569-60-5	(Kosma et al., 2017)
Omeprazole	73590-58-6	(4-methoxy-3,5-dimethylpyridin-2-yl)methanol	86604-78-6	(Kosma et al., 2017)
Oxazepam	604-75-1	TP-271	-	(Kosjek et al., 2012)
Oxazepam	604-75-1	(6-chloro-4-phenyl-1,2-dihydroquinazolin-2-yl)methanol	-	(West & Rowland, 2012)
Oxazepam	604-75-1	4--phenyl-2(1H)-quinazolinone	-	(West & Rowland, 2012)
Oxazepam	604-75-1	6-chloro-4-phenyl-1,2-dihydroquinazoline-2-carbadehyde	-	(West & Rowland, 2012)
Oxazepam	604-75-1	6-chloro-4-phenylquinazolinone	-	(West & Rowland, 2012)
Oxazepam	604-75-1	6-chloro-4-phenyl-2(1H)-quinazolinone	4797-43-7	(West & Rowland, 2012)
Oxazepam	604-75-1	2-amino-5-chlorobenzophenone	719-59-5	(West & Rowland, 2012)

Oxazepam	604-75-1	4-chloro-10-H-acridin-9-one	7497-52-1	(West & Rowland, 2012)
Oxazepam	604-75-1	P232	-	(Yang et al., 2018)
Oxazepam	604-75-1	P241	-	(Yang et al., 2018)
Oxazepam	604-75-1	P257	-	(Yang et al., 2018)
Oxazepam	604-75-1	P260	-	(Yang et al., 2018)
Oxazepam	604-75-1	P273	-	(Yang et al., 2018)
Oxazepam	604-75-1	P291	-	(Yang et al., 2018)
Oxazepam	604-75-1	P294	-	(Yang et al., 2018)
Oxazepam	604-75-1	P301b	-	(Yang et al., 2018)
Oxcarbazepine	28721-07-5	TP 195	-	(Kaiser et al., 2014)
Oxcarbazepine	28721-07-5	TP 223A	-	(Kaiser et al., 2014)
Oxcarbazepine	28721-07-5	TP 239	-	(Kaiser et al., 2014)
Oxcarbazepine	28721-07-5	TP 266	-	(Kaiser et al., 2014)
Oxcarbazepine	28721-07-5	TP 268	-	(Kaiser et al., 2014)
Oxcarbazepine	28721-07-5	TP 282	-	(Kaiser et al., 2014)
Oxcarbazepine	28721-07-5	TP 300	-	(Kaiser et al., 2014)
Oxcarbazepine	28721-07-5	TP207	-	(Kaiser et al., 2014)
Oxymorphone	76-41-5	Oxymorphol	2183-56-4	(Long et al., 1995)
Oxytetracycline	79-57-2	4-epi-oxytetracycline	14206-58-7	(Halling-Sørensen et al., 2002)
Oxytetracycline	79-57-2	β-apo-oxytetracycline	18695-01-7	(Halling-Sørensen et al., 2002)
Oxytetracycline	79-57-2	α-apo-oxytetracycline	18751-99-0	(Halling-Sørensen et al., 2002)
Oxytetracycline	79-57-2	Terrinolide	569-33-5	(Halling-Sørensen et al., 2002)
Oxytetracycline	79-57-2	m/z 415	-	(Liu et al., 2016)
Oxytetracycline	79-57-2	m/z 429	-	(Liu et al., 2016)
Oxytetracycline	79-57-2	m/z 431	-	(Liu et al., 2016)
Oxytetracycline	79-57-2	m/z 433	-	(Liu et al., 2016)
Oxytetracycline	79-57-2	m/z 443	-	(Liu et al., 2016)
Oxytetracycline	79-57-2	m/z 447	-	(Liu et al., 2016)
Oxytetracycline	79-57-2	m/z 449	-	(Liu et al., 2016)

Oxytetracycline	79-57-2	m/z 475	-	(Liu et al., 2016)
Oxytetracycline	79-57-2	m/z 477	-	(Liu et al., 2016)
Oxytetracycline	79-57-2	m/z 491	-	(Liu et al., 2016)
Para-cresol	106-44-5	4-hydroxybenzoate	456-23-5	(Bossert et al., 1989)
Para-cresol	106-44-5	2-hydroxy-cis,cis-muconate semialdehyde	3270-98-2	(Cerdan et al., 1994)
Para-cresol	106-44-5	p-benzoquinone	106-51-4	(Chauhan et al., 2000)
Para-cresol	106-44-5	2-hydroxy-1,4-benzoquinone	2474-72-8	(Chauhan et al., 2000)
Para-cresol	106-44-5	Hydroquinone	123-31-9	(Eppink et al., 1997)
Para-cresol	106-44-5	1,2,4-benzenetriol	533-73-3	(Eppink et al., 2000)
Para-cresol	106-44-5	Catechol	120-80-9	(Grant & Patel, 1969)
Para-cresol	106-44-5	Maleylacetate	24740-88-3	(Jain et al., 1994)
Para-cresol	106-44-5	2-pyrone-4,6-dicarboxylate	72698-24-9	(Kasai et al., 2005)
Para-cresol	106-44-5	3-oxoadipate	689-31-6	(Kaschabek & Reineke, 1995)
Para-cresol	106-44-5	3,4-dihydroxybenzoate	99-50-3	(Lah et al., 1994)
Para-cresol	106-44-5	Carbon dioxide	124-38-9	(Lamzin et al., 1992)
Para-cresol	106-44-5	Pyruvate	127-17-3	(Lau et al., 1994)
Para-cresol	106-44-5	4-hydroxy-2-oxovalerate	3318-73-8	(Lau et al., 1994)
Para-cresol	106-44-5	Acetaldehyde	75-07-0	(Lau et al., 1994)
Para-cresol	106-44-5	4-oxalomesaconate	85179-60-8	(Masai et al., 1999)
Para-cresol	106-44-5	4-hydroxybenzaldehyde	123-08-0	(McIntire et al., 1987)
Para-cresol	106-44-5	Cis-2-hydroxypenta-2,4-dienoate	159694-16-3	(Nishino & Spain, 1995)
Para-cresol	106-44-5	Formate	64-18-6	(Nishino & Spain, 1995)
Para-cresol	106-44-5	2-hydroxy-4-carboxymuconate semialdehyde	28345-81-5	(Noda et al., 1990)
Para-cresol	106-44-5	3-carboxy-cis,cis-muconate	1116-26-3	(Ohlendorf et al., 1988)
Para-cresol	106-44-5	cis,cis-4-hydroxymuconic semialdehyde	-	(Spain & Gibson, 1991)
Paroxetine	61869-08-7	Photoproduit I	-	(Kwon & Armbrust, 2004)
Paroxetine	61869-08-7	Photoproduit III	-	(Kwon & Armbrust, 2004)
Propanolol	525-66-6	Pro 176	-	(Li et al., 2014)
Propranolol	525-66-6	1-naphtol	90-15-3	(Li et al., 2014)

Propranolol	525-66-6	P2	-	(Xie et al., 2019)
Propranolol	525-66-6	P5	-	(Xie et al., 2019)
Propranolol	525-66-6	P7	-	(Xie et al., 2019)
Propranolol	525-66-6	P8	-	(Xie et al., 2019)
Propranolol	525-66-6	P9	-	(Xie et al., 2019)
Propylparaben	94-13-3	3,5-dichloro-propylparaben	-	(Mao et al., 2016)
Propylparaben	94-13-3	3-chloro-propylparaben	-	(Mao et al., 2016)
Propylparaben	94-13-3	Phenol	108-95-2	(Wu et al., 2017)
Propylparaben	94-13-3	Benzoic acid	65-85-0	(Wu et al., 2017)
Quetiapine	111974-69-7	BTP 356	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	BTP 398	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	BTP 400	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	BTP 414	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	PTP 251	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	PTP 296	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	PTP 358	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	PTP 400-1	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	PTP 400-2	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	PTP 400-3	-	(Herrmann et al., 2016)
Quetiapine	111974-69-7	PTP 414	-	(Herrmann et al., 2016)
Ranitidine	66357-35-5	TP 1	-	(Elias et al., 2019)
Ranitidine	66357-35-5	TP 10	-	(Elias et al., 2019)
Ranitidine	66357-35-5	TP 2	-	(Elias et al., 2019)
Ranitidine	66357-35-5	TP 3	-	(Elias et al., 2019)
Ranitidine	66357-35-5	TP 5	-	(Elias et al., 2019)
Ranitidine	66357-35-5	TP 6	-	(Elias et al., 2019)
Ranitidine	66357-35-5	TP 7	-	(Elias et al., 2019)
Ranitidine	66357-35-5	TP 8	-	(Elias et al., 2019)
Ranitidine	66357-35-5	TP 9	-	(Elias et al., 2019)

Ranitidine	66357-35-5	TP11	-	(Elias et al., 2019)
Roxithromycin	80214-83-1	Phosphoryle roxythromycin	-	(Terzic et al., 2011b)
Salicylic acid	69-72-7	2-hydroxy-cis,cis-muconate semialdehyde	3270-98-2	(Cerdan et al., 1994)
Salicylic acid	69-72-7	cis,cis-muconate	1119-72-8	(Hartnett et al., 1990)
Salicylic acid	69-72-7	Maleic acid	110-16-7	(Hu et al., 2016)
Salicylic acid	69-72-7	Fumaric acid	110-17-8	(Hu et al., 2016)
Salicylic acid	69-72-7	2,3-dihydroxybenzoic acid	303-38-8	(Hu et al., 2016)
Salicylic acid	69-72-7	Acrylic acid	79-10-7	(Hu et al., 2016)
Salicylic acid	69-72-7	Carbon dioxide	124-38-9	(Lamzin et al., 1992)
Salicylic acid	69-72-7	Pyruvate	127-17-3	(Lau et al., 1994)
Salicylic acid	69-72-7	4-hydroxy-2-oxovalerate	3318-73-8	(Lau et al., 1994)
Salicylic acid	69-72-7	Acetaldehyde	75-07-0	(Lau et al., 1994)
Salicylic acid	69-72-7	cis-2-hydroxypenta-2,4-dienoate	159694-16-3	(Nishino & Spain, 1995)
Salicylic acid	69-72-7	Formate	64-18-6	(Nishino & Spain, 1995)
Salicylic acid	69-72-7	Catechol	120-80-9	(Suzuki et al., 1991)
Salicylic acid	69-72-7	Gentisate	490-79-9	(Zhou et al., 2002)
Sertraline	79617-96-2	N-hydroxysertraline	124345-07-9	(Li et al., 2013)
Sertraline	79617-96-2	Norsertraline / Desmethyl sertraline	87857-41-8	(Li et al., 2013)
Sildenafil	139755-83-2	TP 391	-	(Eichhorn et al., 2012)
Sildenafil	139755-83-2	TP 392	-	(Eichhorn et al., 2012)
Sildenafil	139755-83-2	TP 434	-	(Eichhorn et al., 2012)
Sildenafil	139755-83-2	TP 448-A	-	(Eichhorn et al., 2012)
Sildenafil	139755-83-2	TP 460	-	(Eichhorn et al., 2012)
Sildenafil	139755-83-2	TP 462	-	(Eichhorn et al., 2012)
Sildenafil	139755-83-2	TP 488-C	-	(Eichhorn et al., 2012)
Sildenafil	139755-83-2	TP 449	-	(Herbert et al., 2015)
Sildenafil	139755-83-2	TP 463	-	(Herbert et al., 2015)
Sildenafil	139755-83-2	TP 477	-	(Herbert et al., 2015)
Simvastatin	79902-63-9	6-exomethylene simvastatin	121624-18-8	(Sulaiman et al., 2015)

Simvastatin	79902-63-9	Hydroxysimvastatatin	126313-98-2	(Sulaiman et al., 2015)
Simvastatin	79902-63-9	3,5-dihydrodiol simvastatin	159143-77-8	(Sulaiman et al., 2015)
Sotalol	3930-20-9	SOT-254	-	(Khalit & Tay, 2017)
Sotalol	3930-20-9	SOT-306	-	(Khalit & Tay, 2017)
Sotalol	3930-20-9	SOT-340	-	(Khalit & Tay, 2017)
Sotalol	3930-20-9	TP1	-	(Stadlmair et al., 2018)
Sulfachloropyridazine	80-32-0	TP186	-	(Ge et al., 2019)
Sulfachloropyridazine	80-32-0	TP220	-	(Ge et al., 2019)
Sulfachloropyridazine	80-32-0	TP255	-	(Ge et al., 2019)
Sulfachloropyridazine	80-32-0	TP300 b	-	(Ge et al., 2019)
Sulfachloropyridazine	80-32-0	TP300a	-	(Ge et al., 2019)
Sulfachloropyridazine	80-32-0	TP316	-	(Ge et al., 2019)
Sulfachloropyridazine	80-32-0	m/z 130	-	(Liu et al., 2018)
Sulfachloropyridazine	80-32-0	m/z 146	-	(Liu et al., 2018)
Sulfachloropyridazine	80-32-0	m/z 162	-	(Liu et al., 2018)
Sulfachloropyridazine	80-32-0	m/z 201.5	-	(Liu et al., 2018)
Sulfadiazine	68-35-9	2-amino-4-hydroxypyrimidine	108-53-2	(Tappe et al., 2013)
Sulfadiazine	68-35-9	2-aminopyrimidine	109-12-6	(Tappe et al., 2013)
Sulfadiazine	68-35-9	Phenol	108-95-2	(Zhang et al., 2017)
Sulfadiazine	68-35-9	Aniline	62-53-3	(Zhang et al., 2017)
Sulfadiazine	68-35-9	4-aminobenzenesulfonamide	63-74-1	(Zhang et al., 2017)
Sulfadiazine	68-35-9	4-hydroxybenzenesulfonic acid	98-67-9	(Zhang et al., 2017)
Sulfadimethoxine	122-11-2	peak 16	-	(Guerard et al., 2009)
Sulfadimethoxine	122-11-2	peak 2	-	(Guerard et al., 2009)
Sulfadimethoxine	122-11-2	peak 26	-	(Guerard et al., 2009)
Sulfadimethoxine	122-11-2	peak 3	-	(Guerard et al., 2009)
Sulfadimethoxine	122-11-2	peak 4	-	(Guerard et al., 2009)
Sulfadimethoxine	122-11-2	peak 6	-	(Guerard et al., 2009)
Sulfadimethoxine	122-11-2	peak 9	-	(Guerard et al., 2009)

Sulfadimethoxine	122-11-2	4-(2-iminopyr-imidin-1(2H)-yl)aniline	-	(Schwarz et al., 2010)
Sulfadimethoxine	122-11-2	TP1	-	(Spielmeyer et al., 2016)
Sulfadimethoxine	122-11-2	TP2	-	(Spielmeyer et al., 2016)
Sulfamethazine	57-68-1	Desulfo-sulfamethazine	-	(García-Galán et al., 2011)
Sulfamethazine	57-68-1	N4-hydroxy-sulfamethazine	-	(García-Galán et al., 2011)
Sulfamethazine	57-68-1	N-hydroxy-sulfamethazine	-	(García-Galán et al., 2011)
Sulfamethazine	57-68-1	Desaminosulfamethazine	6149-31-1	(García-Galán et al., 2011)
Sulfamethazine	57-68-1	P1-139	-	(Li et al.,2017)
Sulfamethazine	57-68-1	P3-230-A	-	(Li et al.,2017)
Sulfamethazine	57-68-1	P3-230-B	-	(Li et al.,2017)
Sulfamethazine	57-68-1	P4-214	-	(Li et al.,2017)
Sulfamethazine	57-68-1	P5-294	-	(Li et al.,2017)
Sulfamethazine	57-68-1	P6-294	-	(Li et al.,2017)
Sulfamethazine	57-68-1	2-amino-4,6-dimethylpyrimidine	767-15-7	(Martin-Laurent et al., 2019)
Sulfamethazine	57-68-1	TP 1	-	(Oliveira et al., 2019)
Sulfamethazine	57-68-1	TP 4	-	(Oliveira et al., 2019)
Sulfamethazine	57-68-1	TP 6	-	(Oliveira et al., 2019)
Sulfamethazine	57-68-1	TP 7	-	(Oliveira et al., 2019)
Sulfamethazine	57-68-1	P1	-	(Xiong et al., 2019)
Sulfamethazine	57-68-1	P2	-	(Xiong et al., 2019)
Sulfamethazine	57-68-1	P3	-	(Xiong et al., 2019)
Sulfamethazine	57-68-1	P4	-	(Xiong et al., 2019)
Sulfamethazine	57-68-1	P5	-	(Xiong et al., 2019)
Sulfamethazine	57-68-1	P6	-	(Xiong et al., 2019)
Sulfamethazine	57-68-1	S1	-	(Zhu et al., 2019)
Sulfamethazine	57-68-1	S5	-	(Zhu et al., 2019)
Sulfamethoxazole	723-46-6	3-amino-5-methylisoxazole	1072-67-9	(Eibes et al., 2011)
Sulfamethoxazole	723-46-6	Hydroxy-N-(5-methyl-1,2-oxazol-3-yl)benzene-1-sulfonamide	-	(Gauthier et al., 2010)
Sulfamethoxazole	723-46-6	3-hydroxylamine-amino-5-carboxyl	-	(Martin-Laurent et al., 2019)

Sulfamethoxazole	723-46-6	4-hydroxy-N-(5-methyl-3-isoxazole)benzene-1-sulfonamide	-	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	N-hydroxyacetyl-sulfamethoxazole	-	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	N-hydroxymethyl-sulfamethoxazole	-	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	3-amino-5-methylisoxazole	1072-67-9	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	4-aminothiophenol	1193-02-8	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	4-aminobenzenesulfonic acid	121-57-3	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	4-aminophenol	123-30-8	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	Hydroquinone	123-31-9	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	1,2,4-trihydroxybenzene	533-73-3	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	Aniline	62-53-3	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	4-aminobenzenesulfonamide	63-74-1	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	4-hydroxybenzenesulfonic acid	98-67-9	(Martin-Laurent et al., 2019)
Sulfamethoxazole	723-46-6	N-hydroxy sulfamethoxazole	114438-33-4	(Poirier-Larabie et al., 2016)
Sulfamethoxazole	723-46-6	TP177	-	(Su et al., 2016)
Sulfamethoxazole	723-46-6	TP254	-	(Su et al., 2016)
Sulfamethoxazole	723-46-6	TP270	-	(Su et al., 2016)
Sulfamethoxazole	723-46-6	P1	-	(Xiong et al., 2019)
Sulfamethoxazole	723-46-6	P2	-	(Xiong et al., 2019)
Sulfamethoxazole	723-46-6	P3	-	(Xiong et al., 2019)
Sulfamethoxazole	723-46-6	P4	-	(Xiong et al., 2019)
Sulfamethoxazole	723-46-6	P6	-	(Xiong et al., 2019)
Sulfamethoxazole	723-46-6	4-nitroso sulfamethoxazole	131549-85-4	(Xiong et al., 2019)
Sulfamethoxazole	723-46-6	C10H11N3O6S	-	(Zhang et al., 2017)
Sulfamethoxazole	723-46-6	C10H12N4O8S2	-	(Zhang et al., 2017)
Sulfamethoxazole	723-46-6	C14H18N4O5S	-	(Zhang et al., 2017)
Sulfamethoxazole	723-46-6	C16H16N2O7S2	-	(Zhang et al., 2017)
Sulfamethoxazole	723-46-6	S2	-	(Zhu et al., 2019)
Sulfamethoxazole	723-46-6	S3	-	(Zhu et al., 2019)
Sulfamethoxazole	723-46-6	S4	-	(Zhu et al., 2019)

Sulfamethoxazole	723-46-6	S5	-	(Zhu et al., 2019)
Sulfapyridine	144-83-2	N4-acetyl-sulfapyridine	-	(Aymerich et al., 2016)
Sulfapyridine	144-83-2	peak 1	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 10	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 2	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 3	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 4a	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 4b	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 6	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 7	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 8	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	peak 9	-	(García-Galán et al., 2012)
Sulfapyridine	144-83-2	C11H12N3 (P4)	-	(Rodríguez, 2012)
Sulfapyridine	144-83-2	C7H11N2O4S (P1)	-	(Rodríguez, 2012)
Sulfapyridine	144-83-2	Formyl sulfapyridine (P7)	-	(Rodríguez, 2012)
Sulfapyridine	144-83-2	P2	-	(Rodríguez, 2012)
Sulfapyridine	144-83-2	P3	-	(Rodríguez, 2012)
Sulfapyridine	144-83-2	P5	-	(Rodríguez, 2012)
Sulfapyridine	144-83-2	P6	-	(Rodríguez, 2012)
Sulfathiazole	72-14-0	C7H8N203S	-	(Rodríguez, 2012)
Sulfathiazole	72-14-0	C9H10N3S	-	(Rodríguez, 2012)
Sulfathiazole	72-14-0	C9H8N2OS	-	(Rodríguez, 2012)
Sulfathiazole	72-14-0	N-formyl sulfathiazole	786-25-4	(Rodríguez, 2012)
Sulfathiazole	72-14-0	S1	-	(Zhu et al., 2019)
Sulfathiazole	72-14-0	S2	-	(Zhu et al., 2019)
Sulfathiazole	72-14-0	S3	-	(Zhu et al., 2019)
Sulfathiazole	72-14-0	S4	-	(Zhu et al., 2019)
Sulfathiazole	72-14-0	S5	-	(Zhu et al., 2019)
Sulfathiazole	72-14-0	S7	-	(Zhu et al., 2019)

Sulpiride	23672-07-3	Sulpiride N-oxide	-	(Bollmann et al., 2016)
Temazepam	846-50-4	{4-chloro-2-[imino(phenyl)methyl]phenyl}methyl carbamic acid	-	(West & Rowland, 2012)
Temazepam	846-50-4	4-chloro-10-methylacridin-9-one	-	(West & Rowland, 2012)
Temazepam	846-50-4	6-chloro-4-phenyl-1,2-dihydriquinolin-2-ol	-	(West & Rowland, 2012)
Temazepam	846-50-4	6-chloro-4-phenylquinolin-2-ol	-	(West & Rowland, 2012)
Temazepam	846-50-4	5-chloro-2-(methylamino)benzophenone	1022-13-5	(West & Rowland, 2012)
Temazepam	846-50-4	2-methylaminobenzophenone	1859-76-3	(West & Rowland, 2012)
Temazepam	846-50-4	2-aminobenzophenone	2835-77-0	(West & Rowland, 2012)
Temazepam	846-50-4	2-amino-5-chlorobenzophenone	719-59-5	(West & Rowland, 2012)
Temazepam	846-50-4	4-chloro-10-H-acridin-9-one	7497-52-1	(West & Rowland, 2012)
Tetrabromobisphenol A	79-94-7	P10	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P11	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P12	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P13	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P14	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P15	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P16	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P17	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P18	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P19	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P2	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P20	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P21	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P23	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P24	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P25	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P26	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P27	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P28	-	(Liu et al., 2018)

Tetrabromobisphenol A	79-94-7	P29	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P3	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P31	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P33	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P34	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P35	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P36	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P37	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P38	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P39	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P40	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P41	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P42	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P43	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P44	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P45	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P46	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P47	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P48	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P51	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P52	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P53	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P54	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P55	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P56	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P57	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P6	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P61	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P62	-	(Liu et al., 2018)

Tetrabromobisphenol A	79-94-7	P63	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P64	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P67	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P68	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P69	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P7	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P70	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P71	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P72	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P73	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P74	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P76	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P77	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P78	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P79	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P80	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P81	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P82	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P83	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P84	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P85	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P86	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P87	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P88	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P89	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P90	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P91	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P92	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P93	-	(Liu et al., 2018)

Tetrabromobisphenol A	79-94-7	P95	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P96	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	P97	-	(Liu et al., 2018)
Tetrabromobisphenol A	79-94-7	3,3'-dibromobisphenol A	29426-78-6	(Ronen & Abeliovich, 2000)
Tetrabromobisphenol A	79-94-7	3-monobromobisphenol A	6073-11-6	(Ronen & Abeliovich, 2000)
Tetrabromobisphenol A	79-94-7	3,3',5-tribromobisphenol A	6386-73-8	(Ronen & Abeliovich, 2000)
Tetrabromobisphenol A	79-94-7	Bisphenol A	80-05-7	(Ronen & Abeliovich, 2000)
Tetracycline	60-54-8	4-epi-anhydro-tetracycline hydrochloride (EATC)	-	(Halling-Sørensen et al., 2002)
Tetracycline	60-54-8	5a,6-anhydrotetracycline hydrochloride (ATC)	1665-56-1	(Halling-Sørensen et al., 2002)
Tetracycline	60-54-8	ETC 445	-	(Leng et al., 2016)
Tetracycline	60-54-8	ISO-TC 445	-	(Leng et al., 2016)
Tetracycline	60-54-8	ISO-TP 387	-	(Leng et al., 2016)
Tetracycline	60-54-8	ISO-TP 415	-	(Leng et al., 2016)
Tetracycline	60-54-8	TP 370	-	(Leng et al., 2016)
Tetracycline	60-54-8	TP 387	-	(Leng et al., 2016)
Tetracycline	60-54-8	TP 415	-	(Leng et al., 2016)
Tetracycline	60-54-8	TP 431	-	(Leng et al., 2016)
Tetracycline	60-54-8	12-deshydrotetracycline	-	(Śliwka-Kaszyńska et al., 2019)
Tetracycline	60-54-8	TC3	-	(Śliwka-Kaszyńska et al., 2019)
Tetracycline	60-54-8	TC4	-	(Śliwka-Kaszyńska et al., 2019)
Tetracycline	60-54-8	TC6	-	(Śliwka-Kaszyńska et al., 2019)
Tetracycline	60-54-8	N-desmethyltetracycline	267244-12-2	(Śliwka-Kaszyńska et al., 2019)
Thiabendazole	148-79-8	Catechol	120-80-9	(Perruchon et al., 2017)
Thiabendazole	148-79-8	Catechol	120-80-9	(Perruchon et al., 2017)
Thioridazine	50-52-2	TP 245	-	(Wilde et al., 2016)
Thioridazine	50-52-2	TP 339	-	(Wilde et al., 2016)
Thioridazine	50-52-2	TP 355	-	(Wilde et al., 2016)
Thioridazine	50-52-2	TP 369	-	(Wilde et al., 2016)
Thioridazine	50-52-2	TP 385	-	(Wilde et al., 2016)

Thioridazine	50-52-2	TP 401	-	(Wilde et al., 2016)
Thioridazine	50-52-2	TP 419-I	-	(Wilde et al., 2016)
Thioridazine	50-52-2	TP 419-II	-	(Wilde et al., 2016)
Thioridazine	50-52-2	TP357	-	(Wilde et al., 2016)
Tramadol	27203-92-5	N,N-didesmethyltramadol	-	(Kostanjevecki et al., 2019)
Tramadol	27203-92-5	N-desmethyltramadol	73806-55-0	(Kostanjevecki et al., 2019)
Tramadol	27203-92-5	OP 235	-	(Zimmermann et al., 2012)
Tramadol	27203-92-5	OP 249	-	(Zimmermann et al., 2012)
Tramadol	27203-92-5	OP 278	-	(Zimmermann et al., 2012)
Triclocarban	101-20-2	4-chloroaniline	106-47-8	(Armstrong et al.,2017)
Triclocarban	101-20-2	3,4-dichloroaniline	95-76-1	(Armstrong et al.,2017)
Triclocarban	101-20-2	5-chloro-2-hydroxymuconic acid semialdehyde	-	(Miller et al., 2010)
Triclocarban	101-20-2	4-chlorocatechol	2138-22-9	(Miller et al., 2010)
Triclocarban	101-20-2	3-chloro-cis,cis-muconic acid	22752-96-1	(Miller et al., 2010)
Triclocarban	101-20-2	Carbanilide	102-07-8	(Miller et al., 2010)
Triclocarban	101-20-2	Dichlorocarbanilide	13208-32-7	(Miller et al., 2010)
Triclocarban	101-20-2	Chlorocarbanilide	2008-71-1	(Miller et al., 2010)
Triclocarban	101-20-2	Aniline	62-53-3	(Yun et al., 2016)
Triclosan	3380-34-5	Triclosan-o-sulfate	-	(Armstrong et al., 2017)
Triclosan	3380-34-5	Methyl triclosan	4640-01-1	(Armstrong et al., 2017)
Triclosan	3380-34-5	(4-chloro-2-hydroxyphenoxy)methanediol	-	(Ding et al., 2018)
Triclosan	3380-34-5	1-(4-chloro-2-(dihydroxymethoxy)phenoxy)ethane-1,2-diol	-	(Ding et al., 2018)
Triclosan	3380-34-5	2-(3-chlorophenoxy)ethane-1,1,2-triol	-	(Ding et al., 2018)
Triclosan	3380-34-5	3-chlorophenyl 2-amino-3-methylbutanoate	-	(Ding et al., 2018)
Triclosan	3380-34-5	3-chlorophenyl 2-oxoacetate	-	(Ding et al., 2018)
Triclosan	3380-34-5	4-chloro-2-methoxyphenyl 3,4,5,6-tetrahydroxytetrahydro-2H-pyran-2-carboxylate	-	(Ding et al., 2018)
Triclosan	3380-34-5	5-chloro-2-(2,4-dichlorophenoxy)phenyl 2,4,4-trihydroxybutanoate	-	(Ding et al., 2018)
Triclosan	3380-34-5	5-chloro-2-(2,4-dichlorophenoxy)phenyl 2-hydroxyacetate	-	(Ding et al., 2018)

Triclosan	3380-34-5	5-chloro-2-methoxyphenoxy(pyrrolidin-2-ylidene)methanol	-	(Ding et al., 2018)
Triclosan	3380-34-5	3-chloro-4-(5,7-dichloro-3-oxo-2,3-dihydrobenzo[1,4]dioxin-2-yl)-2-oxobut-3-enal	-	(Lee et al., 2012)
Triclosan	3380-34-5	6-chloro-3-(2,4-dichlorophenoxy)-4-hydroxycyclohexa-3,5-diene-1,2-dione	-	(Lee et al., 2012)
Triclosan	3380-34-5	Monohydroxy-triclosan	-	(Lee et al., 2012)
Triclosan	3380-34-5	3,5-dichloro-4,6-dihydroxycyclohexa-3,5-diene-1,2-dione	144400-58-8	(Lee et al., 2012)
Triclosan	3380-34-5	Dichlorohydroxydiphenyl ether	-	(Sanchez-Prado et al., 2006)
Triclosan	3380-34-5	Monochlorohydroxydiphenyl ether	-	(Sanchez-Prado et al., 2006)
Triclosan	3380-34-5	Monochlorophenol	106-48-9	(Sanchez-Prado et al., 2006)
Triclosan	3380-34-5	2,8-dichlorodibenzo-p-dioxin	38964-22-6	(Sanchez-Prado et al., 2006)
Triclosan	3380-34-5	Hydroquinone	123-31-9	(Tian, Ma, Li, & Wang, 2018)
Triclosan	3380-34-5	2-chlorohydroquinone	615-67-8	(Tian et al., 2018)
Triclosan	3380-34-5	Phenol	108-95-2	(Gangadharan Puthiya Veetil et al., 2012)
Triclosan	3380-34-5	Catechol	120-80-9	(Gangadharan Puthiya Veetil et al., 2012)
Triclosan	3380-34-5	2,4-dichlorophenol	120-83-2	(Gangadharan Puthiya Veetil et al., 2012)
Triclosan	3380-34-5	m/z 137	-	(Wang et al., 2018)
Triclosan	3380-34-5	m/z 159	-	(Wang et al., 2018)
Triclosan	3380-34-5	m/z 195	-	(Wang et al., 2018)
Triclosan	3380-34-5	m/z 215	-	(Wang et al., 2018)
Triclosan	3380-34-5	m/z 225	-	(Wang et al., 2018)
Triclosan	3380-34-5	m/z 273	-	(Wang et al., 2018)
Trimethoprim	738-70-5	4-demethyltrimethoprim	21253-58-7	(Gonzalez-Gil et al., 2018)
Trimethoprim	738-70-5	DAPC	-	(Jewell et al., 2016)
Trimethoprim	738-70-5	TP 290	-	(Jewell et al., 2016)
Trimethoprim	738-70-5	TP 292	-	(Jewell et al., 2016)
Trimethoprim	738-70-5	TP 306	-	(Jewell et al., 2016)
Trimethoprim	738-70-5	TP 324	-	(Jewell et al., 2016)
Trimethoprim	738-70-5	α-hydroxytrimethoprim	29606-06-2	(Koba et al., 2017)
Trimethoprim	738-70-5	OP 140	-	(Kuang et al., 2013)

Trimipramine	739-71-9	134	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	196	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	210	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	212	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	250	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	268	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	311	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	313	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	327	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	329	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	405	-	(Khaleel, et al., 2017)
Trimipramine	739-71-9	309a	-	(Khaleel, et al., 2017)
Tylosin	1401-69-0	Dehydroxy-tylonolide	-	(Angenent et al., 2008)
Tylosin	1401-69-0	Isotylosin A alcohol	-	(Hu et al., 2008)
Tylosin	1401-69-0	Isotylosin A aldol	-	(Hu et al., 2008)
Tylosin	1401-69-0	Tylosin A aldol	-	(Hu et al., 2008)
Tylosin	1401-69-0	Tylosin D	-	(Ingerslev & Halling-Sørensen, 2001)
Tylosin	1401-69-0	Tylosin C (macrosin)	11049-15-3	(Ingerslev & Halling-Sørensen, 2001)
Tylosin	1401-69-0	23-O-desmycinosyltylosin	79592-92-0	(Ingerslev & Halling-Sørensen, 2001)
Valsartan	137862-53-4	VAL 252	-	(Helbling et al., 2010)
Valsartan	137862-53-4	VAL 267	-	(Helbling et al., 2010)
Valsartan	137862-53-4	VAL 336	-	(Helbling et al., 2010)
Venlafaxine	93413-69-5	V2	-	(Boix et al., 2016)
Venlafaxine	93413-69-5	VB2	-	(Boix et al., 2016)
Venlafaxine	93413-69-5	VB3	-	(Boix et al., 2016)
Venlafaxine	93413-69-5	VB4	-	(Boix et al., 2016)
Venlafaxine	93413-69-5	N,N-didesmethyl venlafaxine	-	(Llorca et al., 2019)
Venlafaxine	93413-69-5	N,O-didesmethyl venlafaxine	135308-74-6	(Llorca et al., 2019)
Venlafaxine	93413-69-5	N-desmethyl venlafaxine	149289-30-5	(Llorca et al., 2019)

Venlafaxine	93413-69-5	O-desmethyl-venlafaxin	93413-62-8	(Llorca et al., 2019)

TPNNN(m) where NNN is the molar mass and m for the isomer.
TPNNN-m where NNN is the molar mass and m for the isomer.
NNN where NNN is the molar mass.
In red: Articles not in Web of Science, data from EAWAG-BDD.

Table S2. List of 83 PPCPs with information on human transformation pathways or without information.

4-tert-octylphenol	Cashmeran	Diltiazem	Flunixin	MDMA	Olaquindox	Propafenone	Tonalide
Acetylcedrene	Celestolide	Dosulepin	Flurazepam	Meclofenamic acid	Oleandomycin	Propoxyphene	Torsemide
Aciclovir	Clobazam	Doxepin	Hydrochlorothiazide	Mepivacaine	Olmesartan	Pyrimethamine	Valproic acid
Aliskiren	Clofibrate	Enalapril	Imipramine	Mestranol	Orlistat	Ramiprilat	Verapamil
Alprazolam	Clomipramine	Ephedrine	Kanamycin	Metamizol	Oxolinicacid	Risperidone	Warfarin
Amphetamine	Clonazepam	Famotidine	Ketamine	Methadone	Oxycodone	Sitagliptin	Xipamide
Aspirin	Clopidogrel	Fenofibrate	Levalbuterol	Metrodinazole	Pantoprazole	Stigmastanol	
Bromazepam	Clozapine	Fentanyl	Levamisole	Mirtazapine	Pentobarbital	Sulfamethoxine	
Buprenorphine	Desipramine	Flecainide	Lidocaine	Nevirapine	Phenobarbital	Sulfasalazine	
Bupropion	Dihydrocodeine	Fluconazole	Loratadine	Nimesulide	Pravastatin	Tamoxifen	
Candesartan	Dilantin/Phenytoin	Flunitrazepam	Losartan	Olanzapine	Primidone	Telmisartan	

Table S3. Confidence level scale of transformation products (TPs) according to the analytical methods of used for their identification

Confidence level	**Analytical method of identification**	**Number of TP**
Very Good	MS/MS	621
Good	MS + references or MS + other methods (NMR, X-ray, IR spectra, MRM…)	676
Intermediate	Methods other than MS (UV, NMR, IR spectra…)	32
Low	Without information	42

Table S4. Molecular descriptors of the 116 PPCP molecules (see Section 3).

The details of the 153 molecular descriptors and their values are provided in the xlsx S4 spreadsheet.

Table S5. Composition of the clusters obtained by the statistical analysis (see Section 4).

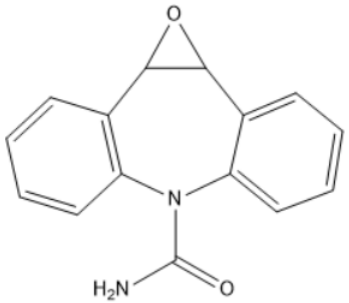
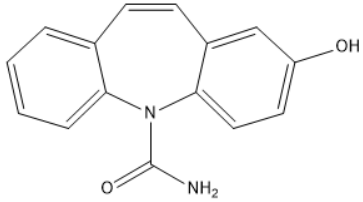
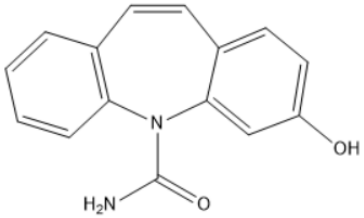
Cluster 1	**Cluster 2**	**Cluster 3**	**Cluster 4**	**Cluster 5**	**Cluster 6**	**Cluster 7**	**Cluster 8**	**Cluster 9**
4-Nonylphenol (NP)	Acetyl-sulfamethoxazole	Caffeine	Amitriptyline	Amisulpride	Ciprofloxacin	17b-estradiol (E2)	Chlortetracycline	Azithromycin
Acetaminophen	Sulfachloropyridazine	Camphor	Atorvastatin	Amoxicillin	Danofloxacin	17-Ethinylestradiol (EE2)	Doxycycline	Clarithromycin
Acetophenone	Sulfadiazine	Cimetidine	Bezafibrate	Ampicillin	Difloxacin	Cholesterol	Oxytetracycline	Erythromycin
Acid clofibric	Sulfadimethoxine	Cotinine	Bisphenol A	Ceftiofur	Enrofloxacin	Clindamycin	Tetracycline	Ivermectin
Atenolol	Sulfamethazine	d-Limonene	Carbamazepine	Furosemide	Flumequine	Codeine		Monensin
Benzotriazole	Sulfamethoxazole	Emtricitabine	Cetirizine	Glibenclamide	Marbofloxacin	Estriol (E3)		Roxithromycin
Gemfibrozil	Sulfapyridine	Gabapentin	Citalopram	Iopromide	Moxifloxacin	Estrone (E1)		Tylosin
Ibuprofen	Sulfathiazole	Levetiracetam	Diazepam	Methotrexate	Norfloxacin	Galaxolide		
Indole		Limonene	Diclofenac	Sildenafil	Ofloxacin	Lincomycin		
Lamotrigine		Nitrofurantoin	Diphenhydramine	Sulpiride		Morphine		
Methylparaben		Ranitidine	Duloxetine	Trimethoprim		Oxymorphone		
Metoprolol			Fenbendazole			Simvastatin		
O-Cresol			Fluoxetine			Tramadol		
Para-cresol			Flurbiprofen			Venlafaxine		
Propylparaben			Indomethacin					
Salicylic acid			Irbesartan					
Sotalol			Ketoprofen					
Thiabendazole			Mefenamic acid					
			Naproxen					
			Nortriptyline					
			Omeprazole					
			Oxazepam					
			Oxcarbazepine					
			Paroxetine					
			Propranolol/Propanolol					
			Quetiapine					
			Sertraline					
			Temazepam					
			Tetrabromobisphenol A					

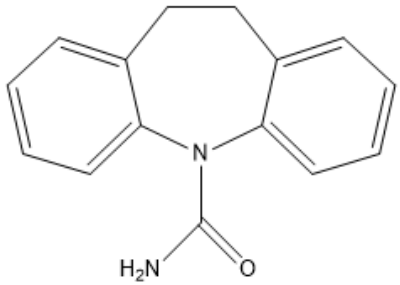
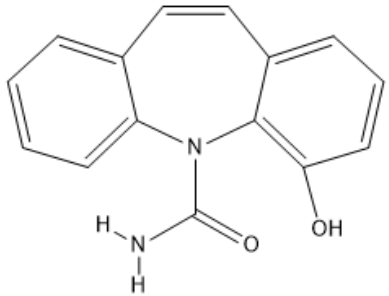
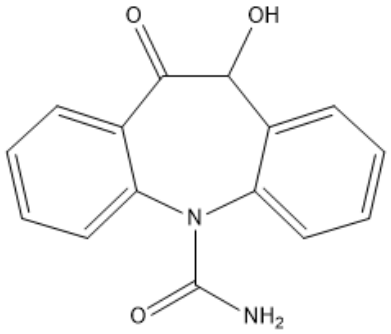
			Thioridazine					
			Triclocarban					
			Triclosan					
			Trimipramine					
			Valsartan					

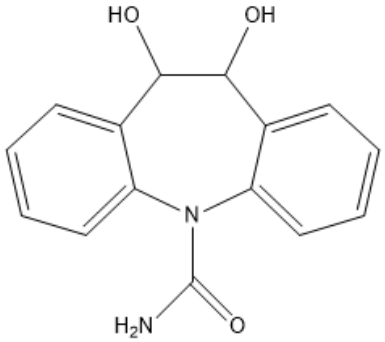
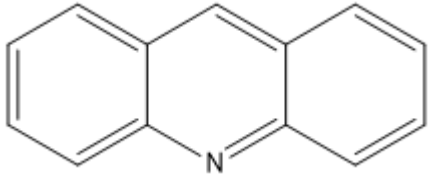
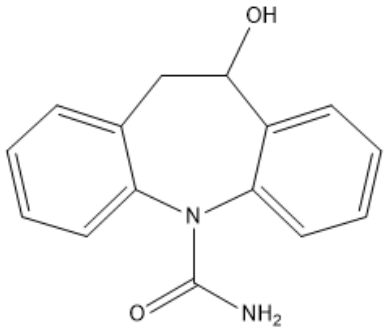
Table S6. Main reactions types involved in the transformation of PPCPs in decreasing order of importance (X for halogen, R for alkyl group).

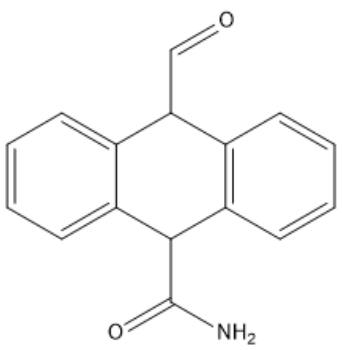
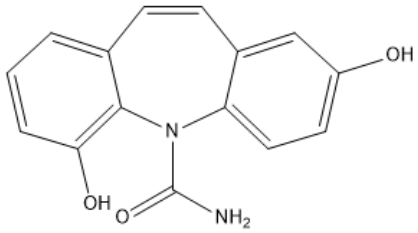
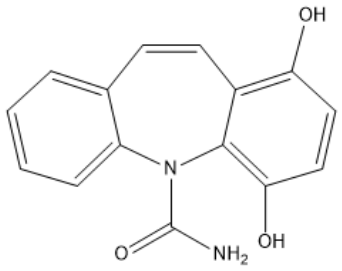
Reaction	**Chemical transformation (+ for gain of atom and - for loss of atom)**
Hydroxylation	+ OH
Dehydrogenation	- H_2
Cleavage	C-C bond break
Other eliminations	- Functional group (- COOH, - CO, - COH, - O)
Hydrolysis	C-C bond break with H_2O
Other substitutions	+ Functional group (+ R, + Cl, + NH_2, + COOH, + CO, + COH)
Dealkylation	- R
Oxygenation	+ O
Addition	Hydrogenation (+ H_2), conjugaison
Dehalogenation	- X
Rearrangement	Structure modification (ring contraction, benzylic rearrangement, α-ketol rearrangement…)

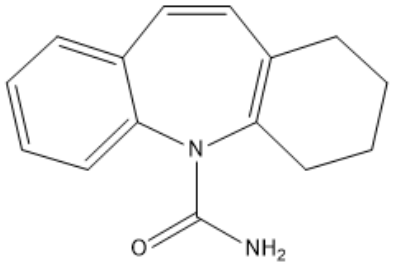
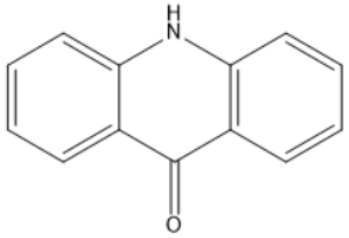
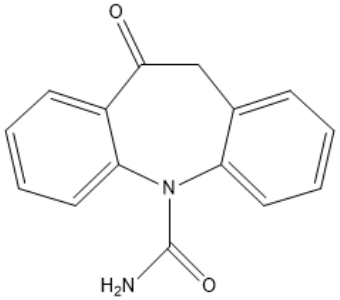
Table S7. Carbamazepine transformation products (TPs). ATP: Abiotic transformation product. BTP: Biotic transformation product. TP: Transformation product; Bold: TPs from oxcarbazepine.

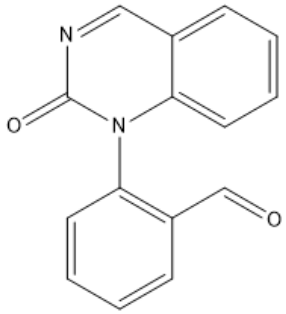
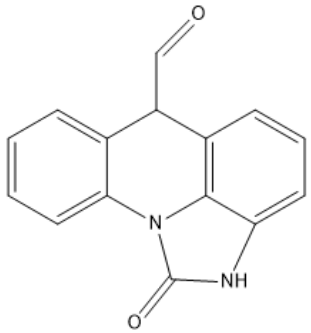
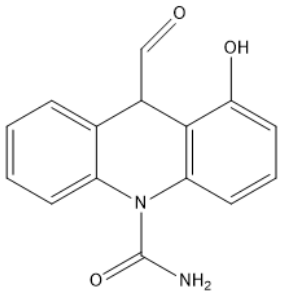
TP name (CAS number into brackets)	Transformation pathway	2D structure	TP types	Matrix	References
Carbamazepine 10,11-epoxide (36507-30-9)	Oxygenation		BTP	Synthetic media	(Jelic et al., 2012)
			BTP	Synthetic media	(Kang et al., 2008)
			TP	Soils	(Koba et al., 2016)
			BTP	Sediments	(Li et al., 2014)
			TP	Natural waters	(Lopez-Serna et al., 2012)
			ATP	Synthetic media	(Vogna et al., 2004)
2-hydroxycarbamazepine (68011-66-5)	Hydroxylation		BTP	Synthetic media	(Kang et al., 2008)
			TP	Natural waters	(Lopez-Serna et al., 2012)
			ATP	Synthetic media	(Calza et al., 2012)
3-hydroxycarbamazepine (68011-67-6)	Hydroxylation		BTP	Synthetic media	(Kang et al., 2008)
			TP	Natural waters	(Lopez-Serna et al., 2012)
			ATP	Synthetic media	(Calza et al., 2012)
	Hydrogenation		TP	Soils	(Koba et al., 2016)

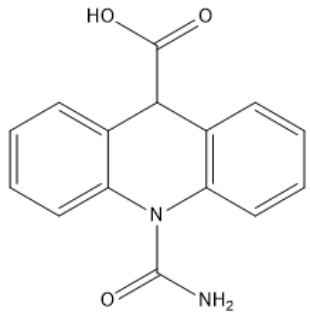
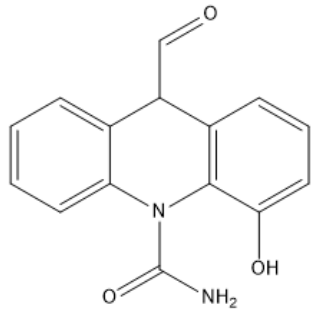
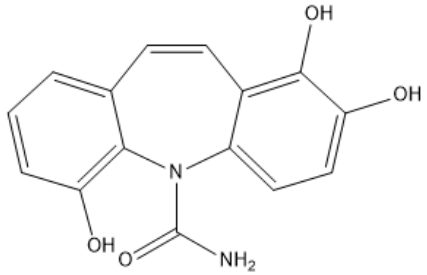
10,11-dihydrocarbamazepine (3564-73-6)				Synthetic media	(König et al., 2016)
1-hydroxycarbamazepine /253-D	Hydroxylation		BTP	Synthetic media	(Kang et al., 2008)
			ATP	Synthetic media	(Calza et al., 2012)
TP 268[a]	Hydroxylation		TP	Solid waste	(Kaiser et al., 2014)
			BTP	Synthetic media	(Jelic et al., 2012)

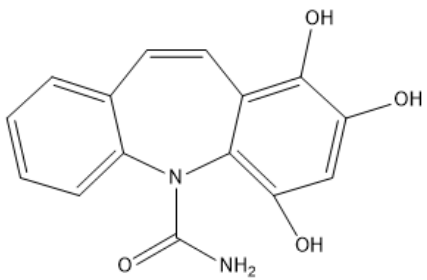
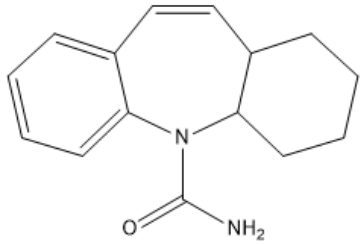
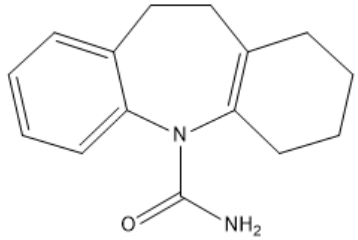
10,11-dihydroxy carbamazepine (35079-97-1)	Oxygenation + Hydroxylation		TP	Soils	(Koba et al., 2016)
Acridine (260-94-6)	Other Eliminations + Rearrangement		BTP	Synthetic media	(Jelic et al., 2012)
			TP	Soils	(Koba et al., 2016)
			BTP	Synthetic media	(Kang et al., 2008)
			TP	Natural waters	(Lopez-Serna et al., 2012)
			ATP	Synthetic media	(Vogna et al., 2004)
10-hydroxycarbamazepine (29331-92-8)	Hydrogenation + Hydroxylation		TP	Solid waste	(Kaiser et al., 2014)

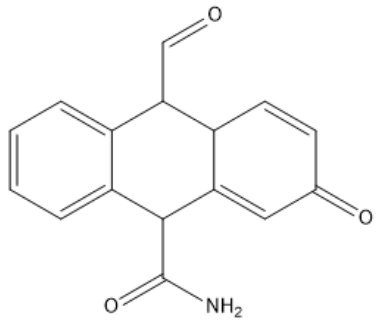
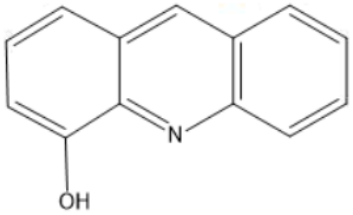
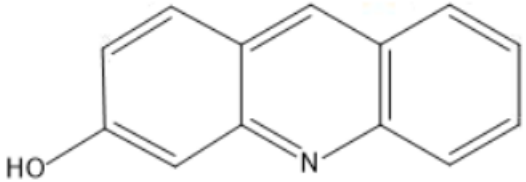
253-A[b]	Hydroxylation + rearrangement		ATP	Synthetic media	(Calza et al., 2012)
269-C[b]	Hydroxylation + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)
269-G[b]	Hydroxylation + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)

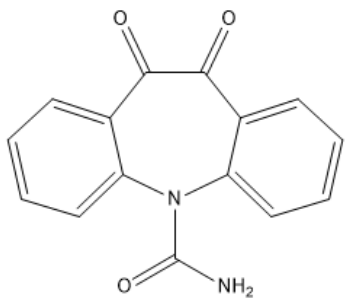
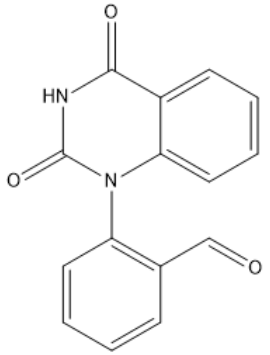
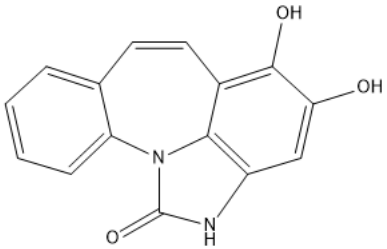
(4H)-carbamazepine	Hydrogenation + Hydrogenation		ATP	Synthetic media	(König et al., 2016)
Acridone/C1[c] (578-95-0)	Other Eliminations + Rearrangement + Oxygenation		BTP	Synthetic media	(Jelic et al., 2012)
			TP	Natural waters	(Lopez-Serna et al., 2012)
				Soils	(Koba et al., 2016)
Oxcarbazepine (28721-07-5)	Hydrogenation + Hydroxylation + Dehydrogenation		TP	Soils	(Koba et al., 2016)
			TP	Solid waste	(Kaiser et al., 2014)

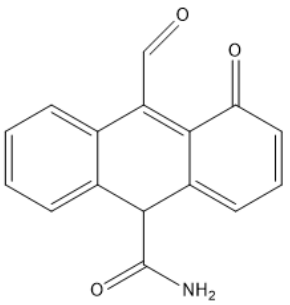
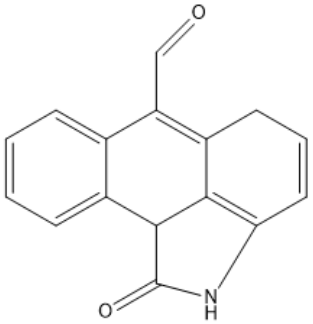
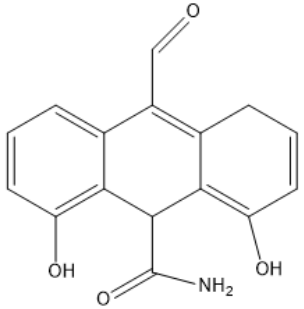
BQM 1-(2-benzaldehyde)-4-hydro-(1H, 3H)- quinazoline-2-one	Cleavage + Rearrangement + Hydratation		ATP	Natural waters	(McDowell et al., 2005)
251[b]	Hydroxylation + Rearrangement + Rearrangement		ATP	Synthetic media	(Calza et al., 2012)
269-A[b]	Hydroxylation + Rearrangement + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)

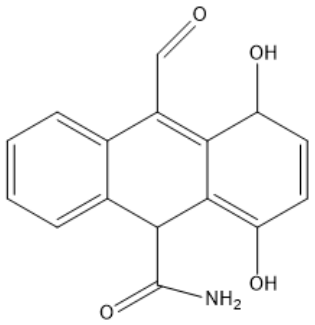
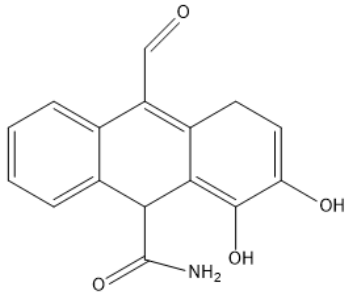
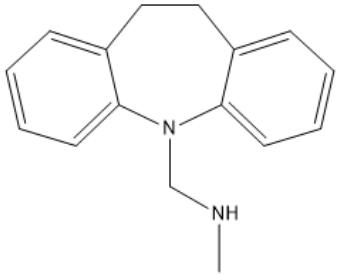
269-B[b]	Hydroxylation + Rearrangement + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)
269-H[b]	Hydroxylation + Rearrangement + hydroxylation		ATP	Synthetic media	(Calza et al., 2012)
285-D[b]	Hydroxylation + Hydroxylation + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)

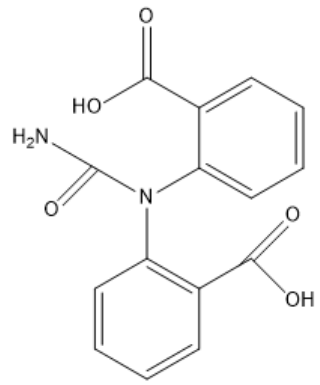
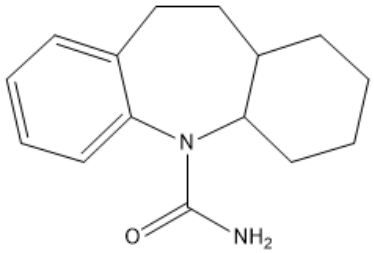
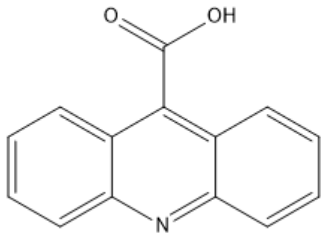
285-E[b]	Hydroxylation + Hydroxylation + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)
(6H)-carbamazepine a	Hydrogenation + Hydrogenation + Hydrogenation		ATP	Synthetic media	(König et al., 2016)
(6H)-carbamazepine b	Hydrogenation + Hydrogenation + Hydrogenation		ATP	Synthetic media	(König et al., 2016)

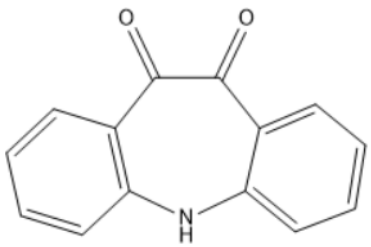
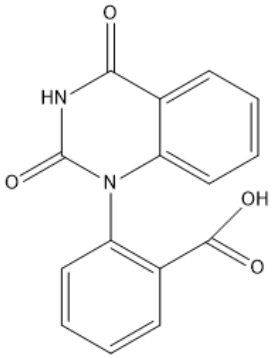
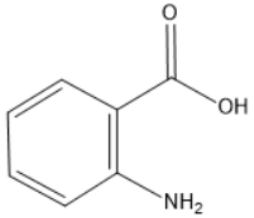
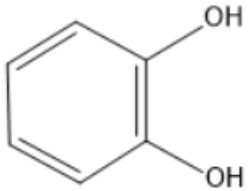
267-D[b]	Hydroxylation + Rearrangement + Hydroxylation + Dehydrogenation		ATP	Synthetic media	(Calza et al., 2012)
1-OH-Acridine	Oxygenation + Rearrangement + Other eliminations + Hydroxylation		ATP	Synthetic media	(Vogna et al., 2004)
2-OH-Acridine	Oxygenation + Rearrangement + Other eliminations + Hydroxylation		ATP	Synthetic media	(Vogna et al., 2004)

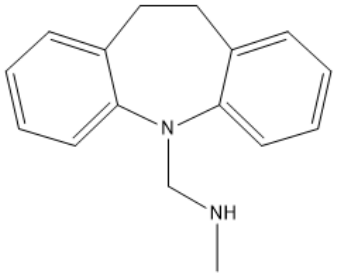
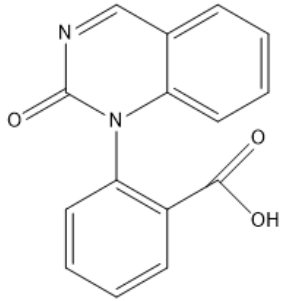
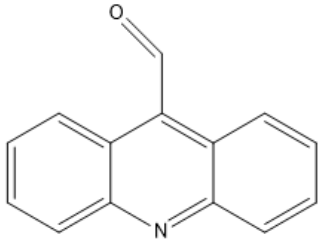
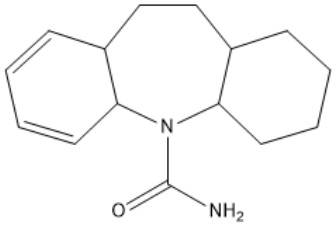
C3[c]	Addition + Hydroxylation + Hydroxylation + Dehydrogenation		TP	Soils	(Koba et al., 2016)
BQD 1-(2-benzaldehyde)-(1H, 3H)-quinazoline- 2,4-dione	Cleavage + Rearrangement + Addition + Oxygenation		ATP	Natural waters	(McDowell et al., 2005)
267-A[b]	Hydroxylation + Hydroxylation + Hydroxylation + Rearrangement		ATP	Synthetic media	(Calza et al., 2012)

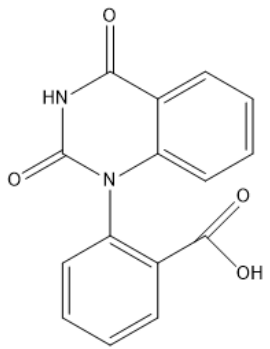
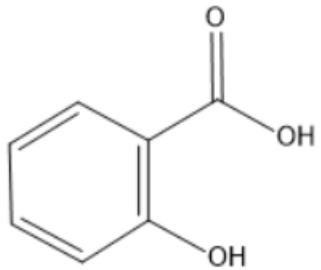
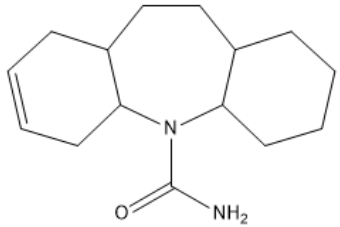
267-B[b]	Hydroxylation + Rearrangement + Hydroxylation + Dehydrogenation		ATP	Synthetic media	(Calza et al., 2012)
267-C[b]	Hydroxylation + Rearrangement + Hydroxylation + Dehydrogenation		ATP	Synthetic media	(Calza et al., 2012)
285-A[b]	Hydroxylation + Rearrangement + Hydroxylation + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)

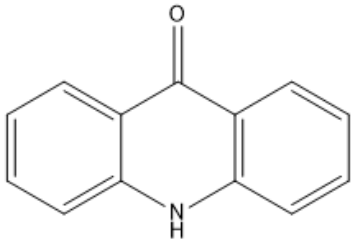
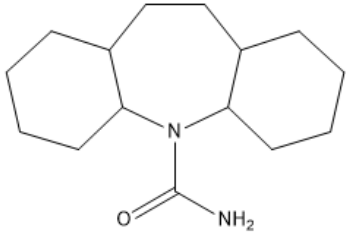
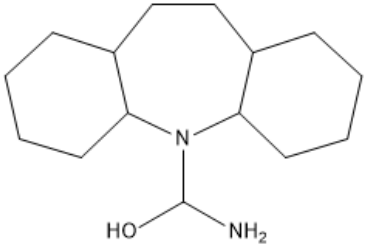
285-B[b]	Hydroxylation + Rearrangement + Hydroxylation + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)
285-C[b]	Hydroxylation + Rearrangement + Hydroxylation + Hydroxylation		ATP	Synthetic media	(Calza et al., 2012)
TP 239[d]	Dehydrogenation + Dehydrogenation + Other elimination + Other substitutions		BTP	Synthetic media	(König et al., 2016)

TP 300[a]	Hydroxylation + Cleavage + Oxygenation + Oxygenation		TP	Solid waste	(Kaiser et al., 2014)
(8H)-carbamazepine	Addtion + Addition + Addition + Addition		ATP	Synthetic media	(König et al., 2016)
9-carboxylic acid-acridine/ TP223B[a] (5336-90-3)	Hydroxylation + Dehydrogenation + Other eliminations + Rearrangement + Other eliminations		TP	Solid waste	(Kaiser et al., 2014)
			TP	Natural waters	(Lopez-Serna et al., 2012)
			ATP	Synthetic media	(Vogna et al., 2004)
C2* / TP223A[c]			TP	Soils	(Koba et al. 2016)

	Hydrogenation + Hydroxylation + Hydroxylation + Dehydrogenation + Other eliminations			Solid waste	(Kaiser et al., 2014)
BaQD 1-(2-benzoic acid)-(1H,3H)-quinazoline-2,4- dione	Cleavage + Rearrangement + Addition + Oxygenation + Oxygenation		ATP	Natural waters	(McDowell et al., 2005)
2-aminobenzoic acid (118-92-3)	Oxygenation + Rearrangement + Other substitutions + cleavage + Other substitutions		ATP	Synthetic media	(Vogna et al., 2004)
Catechol (120-80-9)	Oxygenation + Rearrangement + Other substitutions + Cleavage + Hydroxylation		ATP	Synthetic media	(Vogna et al., 2004)

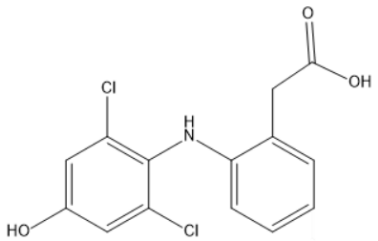
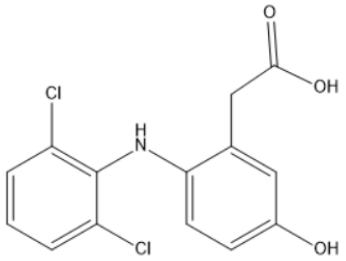
TP 239[a]	Hydroxylation + Other eliminations + Rearrangement + Other eliminations + Hydroxylation		TP	Solid waste	(Kaiser et al., 2014)
TP 266[a]	Hydroxylation + Cleavage + Oxygenation + Rearrangement + Other eliminations		TP	Solid waste	(Kaiser et al., 2014)
TP 207[a]	Hydroxylation + Other eliminations + Rearrangement + Rearrangement + Other eliminations		TP	Solid waste	(Kaiser et al., 2014)
(10H)-carbamazepine	Addition + Addition + Addition + Addition + Addition		ATP	Synthetic media	(König et al., 2016)

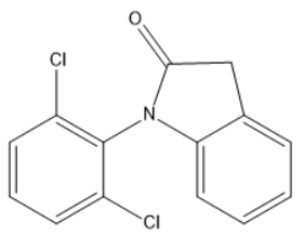
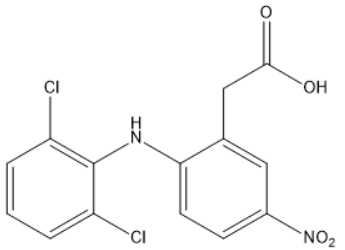
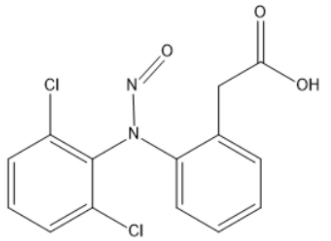
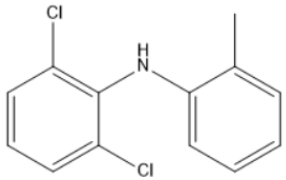
TP 282[a]	Hydroxylation + Cleavage + Oxygenation + Rearrangement + Other eliminations + Oxygenation		TP	Solid waste	(Kaiser et al., 2014)
Salicylic acid (69-72-7)	Oxygenation + Rearrangement + Other substitutions + Cleavage + Other substitutions + Hydroxylation		ATP	Synthetic media	(Vogna et al., 2004)
(12H)-carbamazepine	Addition + Addition + Addition + Hydrogenation + Addition + Addition		ATP	Synthetic media	(König et al., 2016)

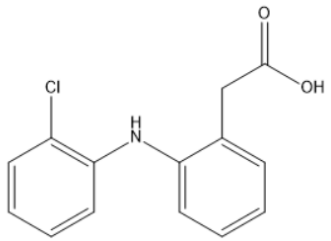
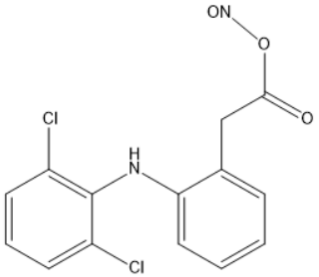
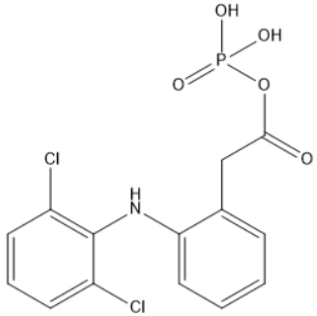
TP 195[a]	Hydroxylation + Dehydrogenation + Rearrangement + Other eliminations + Other eliminations + Hydroxylation + Oxygenation		TP	Solid waste	(Kaiser et al., 2014)
(14H)-carbamazepine	Addition + Addition + Addition + Addition + Addition + Addition + Addition		ATP	Synthetic media	(König et al., 2016)
(16H)-carbamazepine	Addition + Addition + Addition + Addition + Addition + Addition + Addition		ATP	Synthetic media	(König et al., 2016)

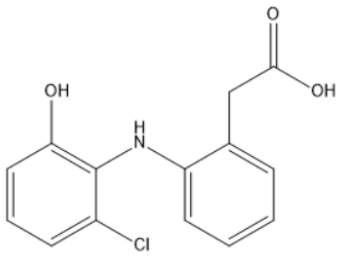
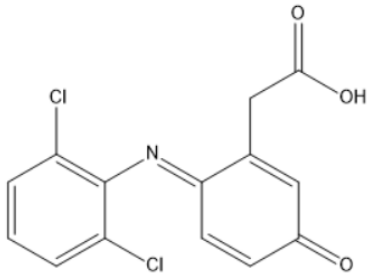
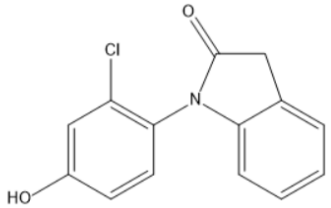
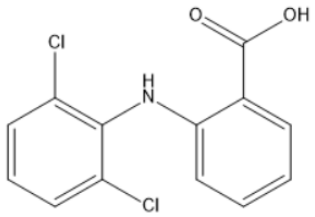
[a] From Kaiser et al. (2014) meaning TP NNNm where NNN is the molar mass and m for the isomer.
[b] From Calza et al. (2012) meaning TP NNN-m where NNN is the molar mass and m for the isomer.
[c] From Koba et al. (2016) meaning Carbamazepine-1 (C1), Carbamazepine-2 (C2) and Carbamazepine-3 (C3).
[d] From König et al. (2016) meaning TP NNN where NNN is the molar mass.

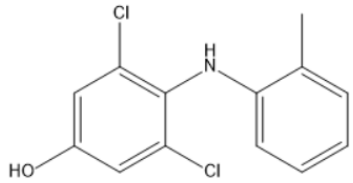
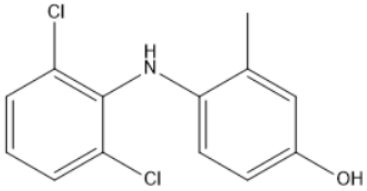
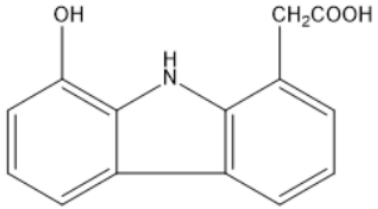
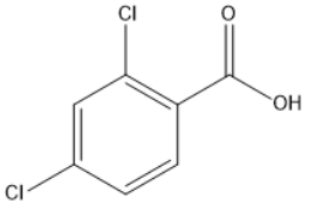
Table S8. Diclofenac transformation products (TPs). ATP: Abiotic transformation product, BTP: Biotic transformation product, TP: Transformation product.

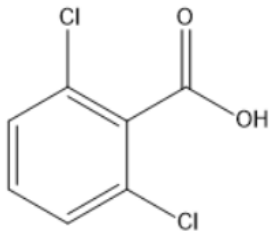
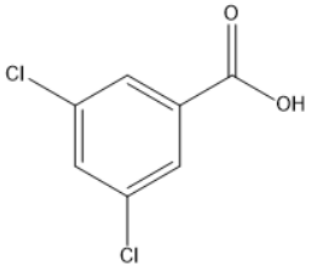
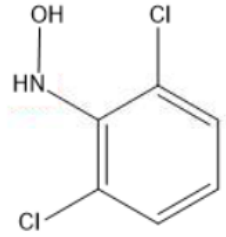
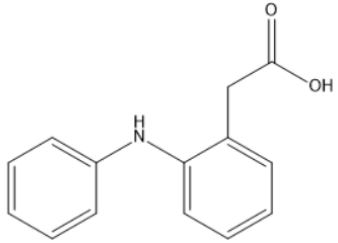
TP name (CAS number into brackets)	Transformation pathway	2D Structure	TP types	Matrix	References
4'-hydroxy diclofenac (64118-84-9)	Hydroxylation		BTP	Synthetic media	(Ivshina et al., 2019)
			TP	Solid waste	(Jewell et al., 2016)
			BTP	Synthetic media	(Marco-Urrea et al., 2010)
			BTP	Synthetic media	(Moreira et al., 2018)
			ATP	Synthetic media	(Webster et al., 1998)
			TP	Solid waste	(Wu et al., 2019)
			BTP	Sediment	(Groening et al., 2007)
5-hydroxy diclofenac (69002-84-2)	Hydroxylation		TP	Soils	(Dodgen et al., 2014)
			BTP	Sediment	(Groening et al., 2007)
			BTP	Synthetic media	(Ivshina et al., 2019)
			TP	Solid waste	(Jewell et al., 2016)
			TP	Solid waste	(Kosjek et al., 2008)
			BTP	Synthetic media	(Marco-Urrea et al., 2010)
			BTP	Synthetic media	(Moreira et al., 2018)
			BTP	Synthetic media	(Poirier-Larabie et al., 2016)
			ATP	Synthetic media	(Webster et al., 1998)
			TP	Solid waste	(Wu et al., 2019)
			BTP	Synthetic media	(Stylianou et al., 2018)
Diclofenac-lactam	Rearrangement		TP	Solid waste	(Jewell et al., 2016)
			TP	Solid waste	(Wu et al., 2019)

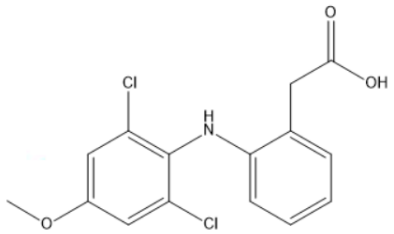
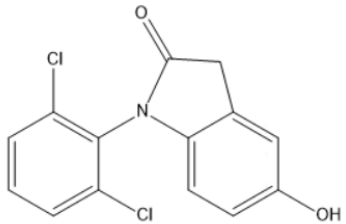
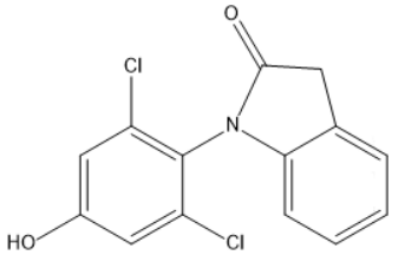
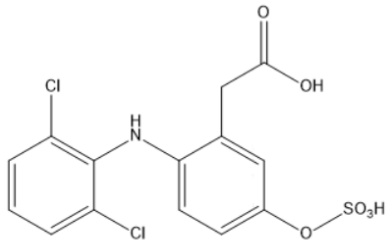
			BTP	Synthetic media	(Stylianou et al., 2018)
TP 341[a]	Other substitutions		TP	Solid waste	(Wu et al., 2019)
TP 325[a]	Other substitutions		TP	Solid waste	(Wu et al., 2019)
TPGG2-2019[i]	Other eliminations		BTP	Solid waste	(Gonzalo-Gil et al., 2019)

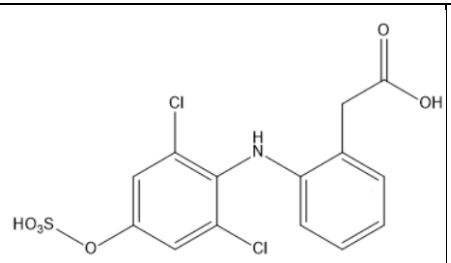
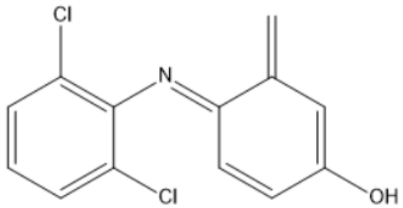
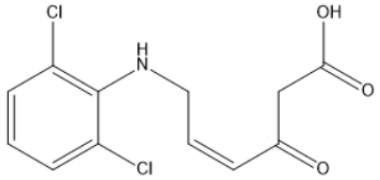
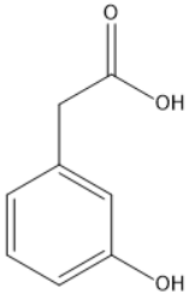
MW 261[c]	Other eliminations		ATP	Synthetic media	(Yu et al., 2013)
Nitroso diclofenac	Other substitutions		BTP	Synthetic media	(Poirier-Larabie et al., 2016)
TPGG1-2019[i]	Other substitutions		BTP	Solid waste	(Gonzalo-Gil et al., 2019)

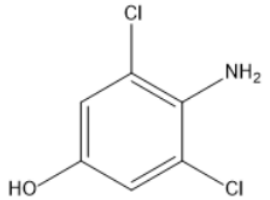
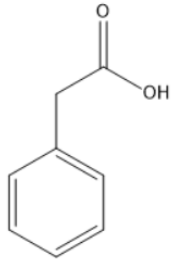
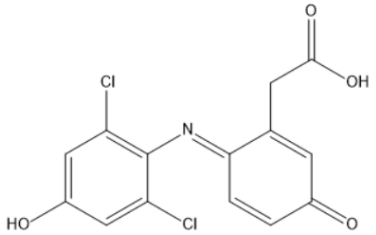
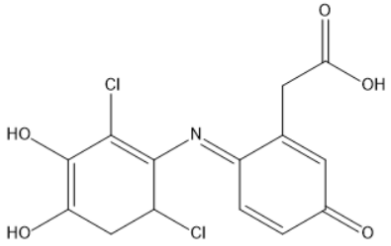
DCF 3[f] – 277 g.mol^{-1}	Other substitutions		BTP	Synthetic media	(Moreira et al., 2018)
5-hydroxydiclofenac quinone imine	Hydroxylation + Dehydrogenation		BTP	Sediment	(Groening et al., 2007)
			BTP	Synthetic media	(Ivshina et al., 2019)
			TP	Solid waste	(Jewell et al., 2016)
			TP	Solid waste	(Kosjek et al., 2008)
			BTP	Synthetic media	(Moreira et al., 2018)
			TP	Solid waste	(Wu et al., 2019)
			BTP	Synthetic media	(Stylianou et al., 2018)
TP259[b] / MW 259[c] / TP8[h] / D6[f] – 259 g.mol^{-1}	Other eliminations + Rearrangement		ATP	Synthetic media	(Poirier-Larabie et al., 2016)
			ATP	Synthetic media	(Yu et al., 2013)
			ATP	Synthetic media	(Roscher et al., 2016)
			ATP	Synthetic media	(Salgado et al., 2013)
Diclofenac carboxylic acid (13625-57-5)	Other eliminations + Other substitutions		TP	Solid waste	(Jewell et al., 2016)
			TP	Solid waste	(Wu et al., 2019)

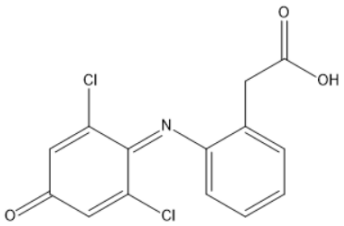
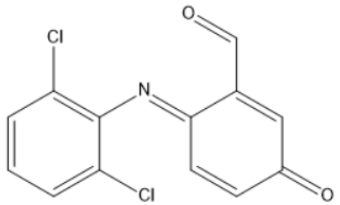
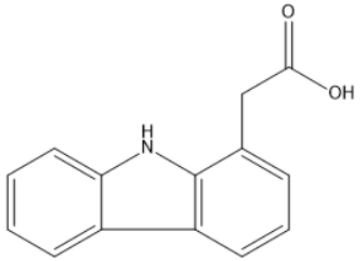
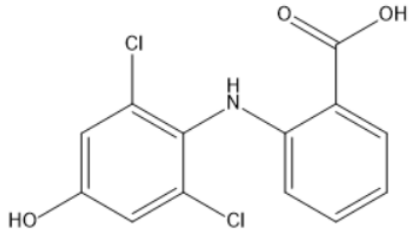
DCF 5[f] – 267 g.mol^{-1}	Hydroxylation + Other eliminations		BTP	Synthetic media	(Moreira et al., 2018)
TP 268[a]	Hydroxylation + Other eliminations		TP	Solid waste	(Wu et al., 2019)
TP241[b]	Other eliminations + Hydroxylation		ATP	Synthetic media	(Poirier-Larabie et al., 2016)
2,4-dichlorobenzoic acid (50-84-0)	Cleavage + Other substitutions		TP	Soils	(Dodgen et al., 2014)

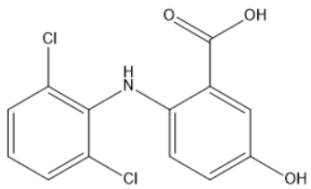
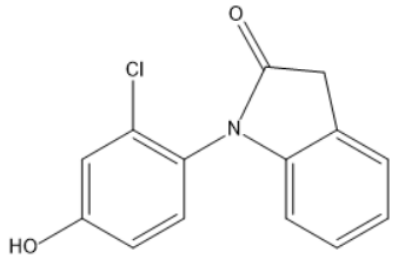
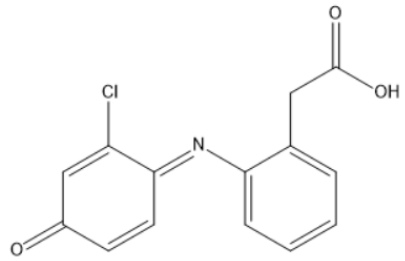
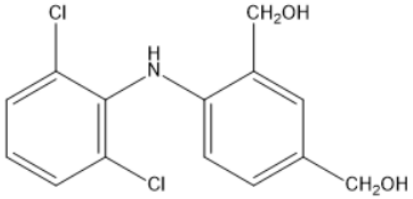
2,6-dichlorobenzoic acid (50-30-6)	Cleavage + Other substitutions		TP	Soils	(Dodgen et al., 2014)
3,5-dichlorobenzoic acid (51-36-5)	Cleavage + Other substitutions		TP	Soils	(Dodgen et al., 2014)
TP177[e]	Cleavage + Hydroxylation		BTP	Synthetic media	(Stylianou et al., 2018)
D5[f] 2-[2-(phenylamino]phenyl) acetic acid	Other eliminations + Other eliminations		ATP	Synthetic media	(Salgado et al., 2013)

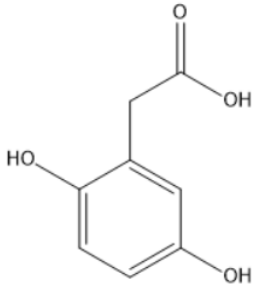
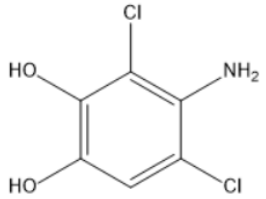
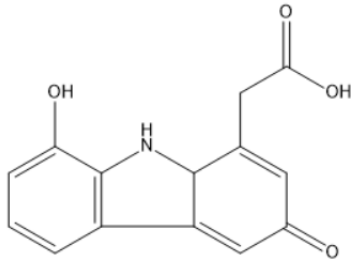
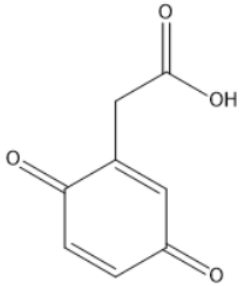
DCF 4[g] – 325 g.mol^{-1}	Hydroxylation + Addition		BTP	Synthetic media	(Moreira et al., 2018)
TP 293a[d]	Hydroxylation + Rearrangement		TP	Solid waste	(Jewell et al., 2016)
TP 293b[d]	Hydroxylation + Rearrangement		TP	Solid waste	(Jewell et al., 2016)
TP 391a[d]	Hydroxylation + Addition		TP	Solid waste	(Jewell et al., 2016)

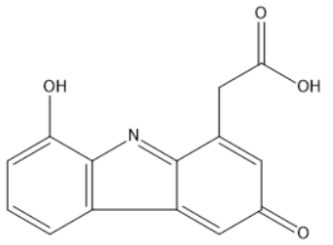
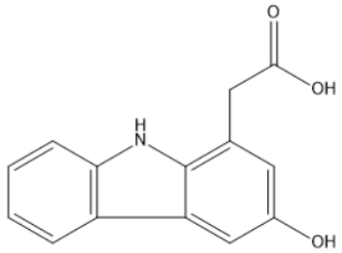
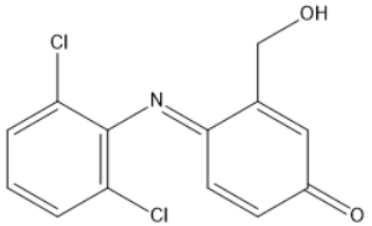
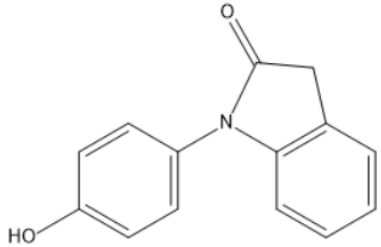
TP 391b[d]	Hydroxylation + Addition		TP	Solid waste	(Jewell et al., 2016)
TP 265[b]	Hydroxylation + Dehydrogenation + Other eliminations		BTP	Synthetic media	(Poirier-Larabie et al., 2016)
TP 285[d]	Hydroxylation + Cleavage		TP	Solid waste	(Jewell et al., 2016)
3-hydroxyphenylacetic acid (9)[e] (621-37-4)	Hydroxylation + Cleavage		BTP	Synthetic media	(Ivshina et al., 2019)

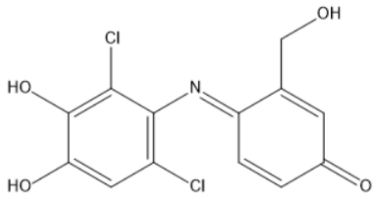
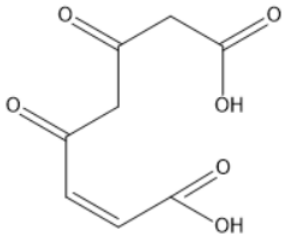
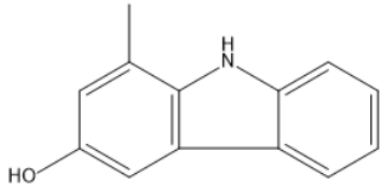
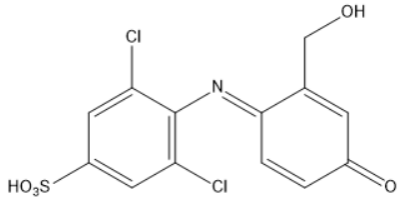
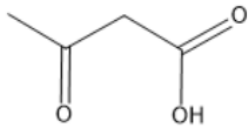
4-amino-3,5-dichlorophenol (6)[e] (26271-75-0)	Hydroxylation + Cleavage		BTP	Synthetic media	(Ivshina et al., 2019)
Phenylacetic acid (7)[e] (103-82-2)	Hydroxylation + Cleavage		BTP	Synthetic media	(Ivshina et al., 2019)
D4[f] – 325 g.mol^{-1}	Hydroxylation + Dehydrogenation		ATP	Synthetic media	(Salgado et al., 2013)
DCF 7[g] / 2-[1-(5-oxocyclohexa-1,3-dienyl-2-(3′,4′-dihydroxy-2′,6′-dichlorophenyl)imino]acetic acid 4-(2,6-D)-1,3B (16)[e]	Hydroxylation + Dehydrogenation + Hydroxylation		BTP	Synthetic media	(Moreira et al., 2018)
			BTP	Synthetic media	(Ivshina et al., 2019)

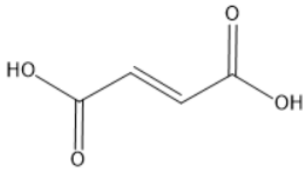
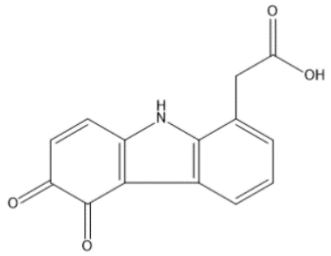
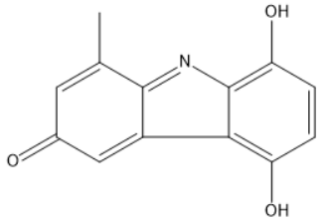
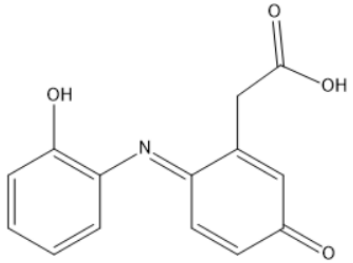
4-hydroxydiclofenac quinone imine	Rearrangement + Hydrolysis + Dehydrogenation		TP	Solid waste	(Jewell et al., 2016)
D2[f] – 279 g.mol^{-1}	Other eliminations + Hydroxylation + Dehydrogenation		ATP	Synthetic media	(Salgado et al., 2013)
MW 224[c] /TP6[h] – 224 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations		ATP	Synthetic media	(Yu et al., 2013) (Roscher et al., 2016)
TP 297[d]	Other eliminations + Hydroxylation + Dehydrogenation		TP	Solid waste	(Jewell et al., 2016)

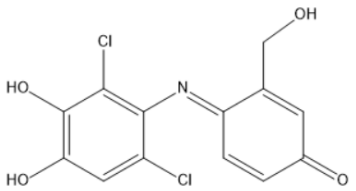
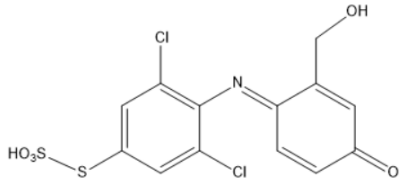
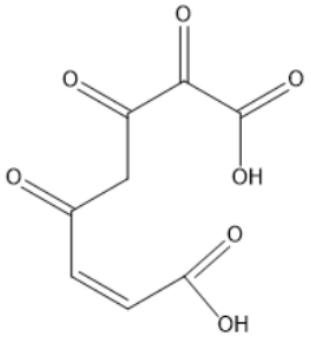
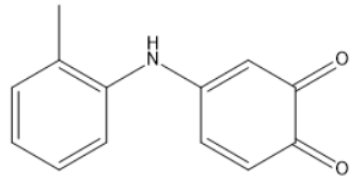
TP298[a]	Hydroxylation + Other eliminations + Other substitutions		TP	Solid waste	(Wu et al., 2019)
TP 259[d]	Hydroxylation + Other eliminations + Rearrangement		TP	Solid waste	(Jewell et al., 2016)
TP 275[d]	Hydroxylation + Other eliminations + Dehydrogenation		TP	Solid waste	(Jewell et al., 2016)
4-(2,6-dichlorophenylamino)-1,3-benzenedimethanol	Other eliminations + Other substitutions + Hydroxylation		BTP	Synthetic media	(Marco-Urrea et al., 2010)

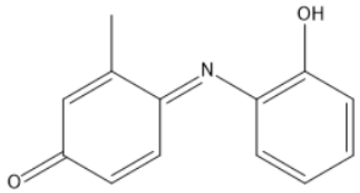
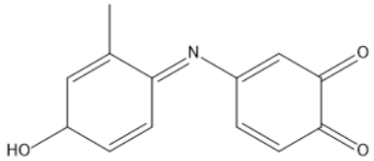
2,5-dihydroxyphenylacetic acid (homogentisic acid) (10)[e] 451-13-8	Hydroxylation + Cleavage + Hydroxylation		BTP	Synthetic media	(Ivshina et al., 2019)
5-amino-4,6-dichlorobenzene-1,2-diol (8)[e]	Hydroxylation + Cleavage + Hydroxylation		BTP	Synthetic media	(Ivshina et al., 2019)
D3[f] – 256 g.mol^{-1}	Other eliminations + Hydroxylation + Oxygenation		ATP	Synthetic media	(Salgado et al., 2013)
2-(p-benzoquinone-2)acetic acid (11)[e]	Hydroxylation + Dehydrogenation + Hydroxylation + Hydrolysis		BTP	Synthetic media	(Ivshina et al., 2019)

D1[f] – 255 g.mol^{-1}	Other eliminations + Hydroxylation + Rearrangement + Dehydrogenation		ATP	Synthetic media	(Salgado et al., 2013)
TP12[h] – 241 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations + Hydroxylation		ATP	Synthetic media	(Roscher et al., 2016)
DCF 8[g] / TP282[e]	Hydroxylation + Dehydrogenation + Other eliminations + Hydroxylation		BTP	Synthetic media	(Moreira et al., 2018)
			BTP	Synthetic media	(Stylianou et al., 2018)
TP 225[d]	Hydroxylation + Other eliminations + Rearrangement + Other eliminations		TP	Solid waste	(Jewell et al., 2016)

DCF 9[g] – 297 g.mol^{-1}	Hydroxylation + Dehydrogenation + Other eliminations + Hydroxylation + Hydroxylation		BTP	Synthetic media	(Moreira et al., 2018)
4,6-dioxooct-2-trans-enedioic acid (fumarylacetoacetic acid) (12)[e]	Hydroxylation + Cleavage + Hydroxylation + Dehydrogenation + Cleavage		BTP	Synthetic media	(Ivshina et al., 2019)
TP11[h] – 196 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations + Hydroxylation + Other eliminations		ATP	Synthetic media	(Roscher et al., 2016)
DCF 11[g] – 360 g.mol^{-1}	Hydroxylation + Dehydrogenation + Other eliminations + Hydroxylation + Other substitutions		BTP	Synthetic media	(Moreira et al., 2018)
3-oxobutanoic acid (acetoacetic acid) (13)[e]	Hydroxylation + Cleavage + Hydroxylation + Dehydrogenation + Cleavage + Hydrolyse		BTP	Synthetic media	(Ivshina et al., 2019)

Fumaric acid (14)[e] 110-17-8	Hydroxylation + Cleavage + Hydroxylation + Dehydrogenation + Cleavage + Hydrolyse		BTP	Synthetic media	(Ivshina et al., 2019)
TP1[h] – 254 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations + Oxygenation + Oxygenation + Dehydrogenation		ATP	Synthetic media	(Roscher et al., 2016)
TP4[h] – 226 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations + Hydroxylation + Other eliminations + Hydroxylation		ATP	Synthetic media	(Roscher et al., 2016)
TP2[h] – 254 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations + Hydroxylation + Hydroxylation + Dehydrogenation		ATP	Synthetic media	(Roscher et al., 2016)

DCF 10[g] – 313 g.mol^{-1}	Hydroxylation + Dehydrogenation + Other eliminations + Hydroxylation + Hydroxylation + Hydroxylation		BTP	Synthetic media	(Moreira et al., 2018)
DCF 12[g] – 393 g.mol^{-1}	Hydroxylation + Dehydrogenation + Other eliminations + Hydroxylation + Other substitutions + Oxygenation		BTP	Synthetic media	(Moreira et al., 2018)
4,6,7-trioxooct-2-enedioic acid (15)[e]	Hydroxylation + Cleavage + Hydroxylation + Dehydrogenation + Cleavage + Hydroxylation + Dehydrogenation		BTP	Synthetic media	(Ivshina et al., 2019)
TP7[h] – 210 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations + Oxygenation + Oxygenation + Dehydrogenation + Other eliminations		ATP	Synthetic media	(Roscher et al., 2016)

TP9[h] – 210 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations + Hydroxylation + Hydroxylation + Dehydrogenation + Other eliminations		ATP	Synthetic media	(Roscher et al., 2016)
TP5[h] – 226 g.mol^{-1}	Other eliminations + Rearrangement + Other eliminations + Hydroxylation + Other eliminations + Hydroxylation + Dehydrogenation		ATP	Synthetic media	(Roscher et al., 2016)

[a] From Wu et al. (2019) meaning TP NNN where NNN is the molar mass.
[b] From Poirier-Larabie et al. (2016) meaning TP NNN where NNN is the molar mass.
[c] From Yu, Nie et al. (2013) meaning MW NNN where NNN is the molar mass.
[d] From Jewell et al. (2016) meaning TPNNNm where NNN is the molar mass from analytical analyze and m the letter for isomer.
[e] Number in brackets from Ivshina et al. (2019) are the number used in the article.
[f] From Salgado et al. (2013) meaning DN where D means Diclofenac and N the number of TP.
[g] From Moreira et al. (2018) meaning DCFN where DCF means Diclofenac and N the number of TP.
[h] From Roscher et al. (2016) meaning TPN where TP means Transformation Product and N the number of TP.
[i] From Gonzalo-Gil et al. (2019) meaning TPGGN-2019 where TP means Transformation Product, N the number of TP, GG 2019.

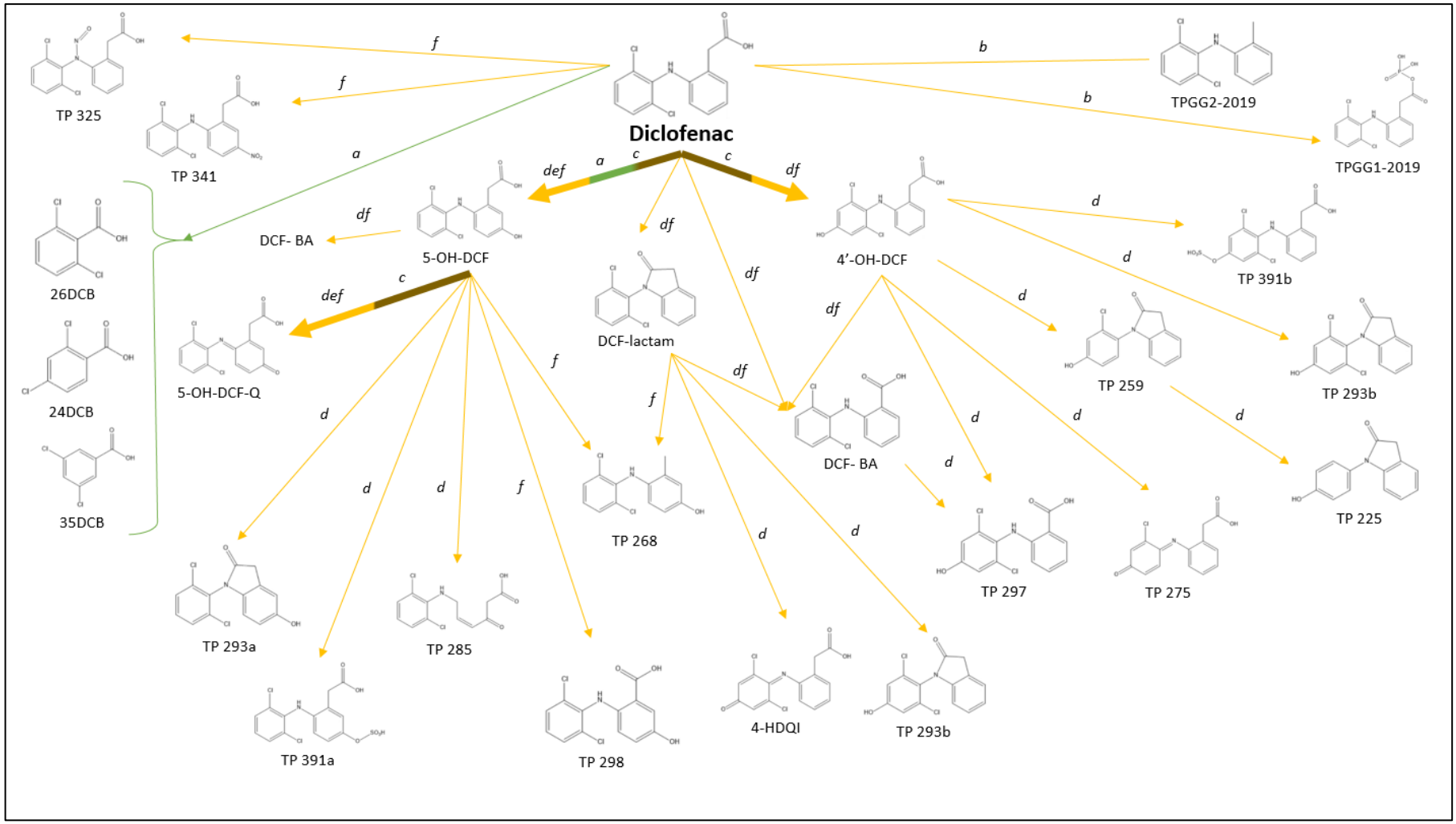


Figure S1. Transformation pathways of diclofenac in non-synthetic matrices. Arrow in bold: reactions evidenced in two matrices or more; yellow arrow: solid waste; green arrow: soils; brown arrow: sediments. (a) Dodgen et al. (2014); (b) Gonzalez-Gil et al. (2019); (c) Gröning et al. (2007); (d) Jewell et al. (2016); (e) Kosjek et al. (2008); (f) Wu et al. (2019).

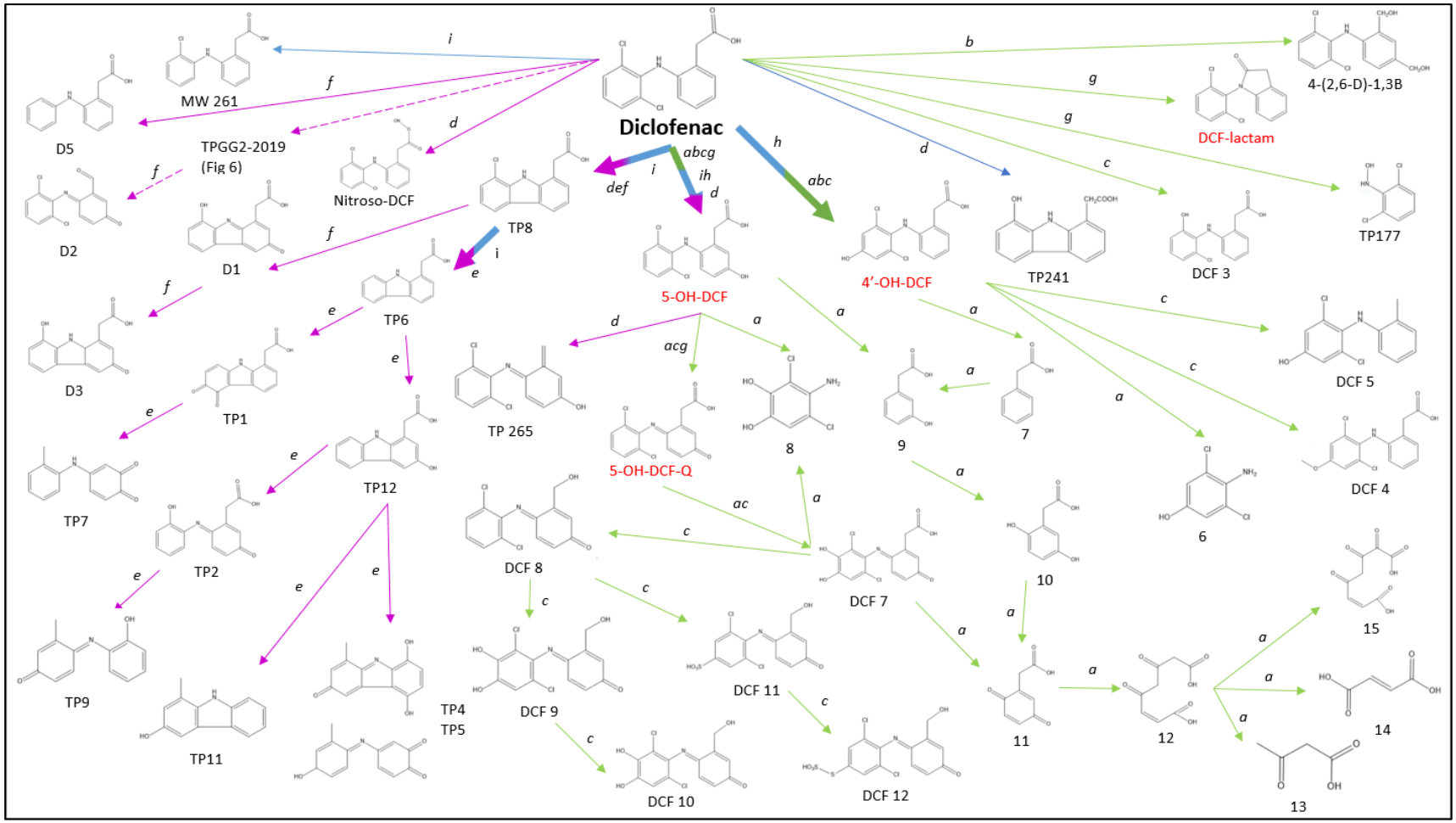


Figure S2. Transformation pathways of diclofenac in synthetic matrices. In red: transformation products observed in both synthetic and non-synthetic matrices; arrow in bold: reactions evidenced in biotic and abiotic conditions; purple arrow: photodegradation; green arrow: biotic transformation; blue arrow: abiotic transformation except photodegradation (i.e ozonation, catalysis…); dotted arrow: putative pathway. (a) Ivshina et al. (2019); (b) Marco-Urrea et al. (2010); (c) Moreira et al. (2018); (d) Poirier-Larabie et al. (2016); (e) Roscher et al. (2016); (f) Salgado et al. (2013); (g) Stylianou et al. (2018); (h) Webster et al. (1998); (i) Yu et al. (2013).

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