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BTO report

Datamining in non-target chemical screening data

KWR Watercycle Research Institute

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BTO *Managementsamenvatting*

Suspect screening met verdere identificatie ondersteunt opsporing nieuwe antropogene stoffen in brede screeningsdata

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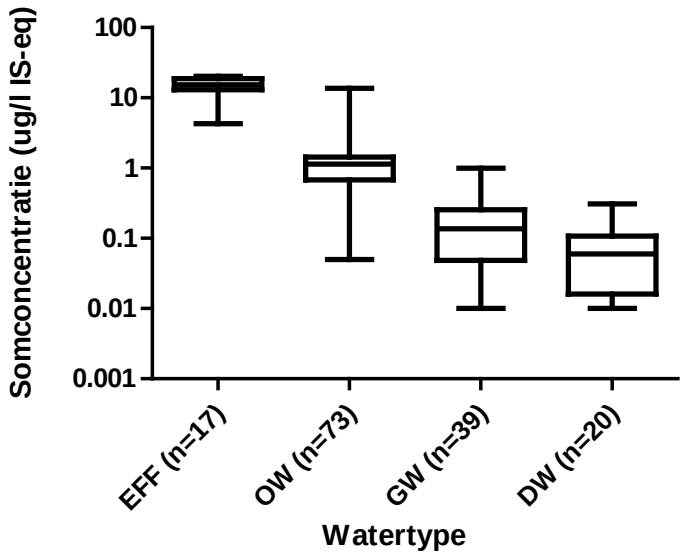
Suspect screening is in staat om betere toegang te verschaffen tot de omvangrijke databestanden met meerdere jaren aan LC-MS-gegevens over (voornamelijk onbekende) microverontreinigingen. Dat blijkt uit onderzoek naar snellere en effectievere verwerking van de bulk aan brede screeningsdata voor het ontsluiten van informatie over relevante antropogene stoffen. De aanpak biedt kansen voor toekomstig waterkwaliteitsonderzoek met behulp van brede screeningsmethoden. Daarnaast laat de dataset significante verschillen zien tussen de monsters van uiteenlopende watertypen: het aantal stoffen, de somconcentratie en de gemiddelde retentietijd bij chromatografische analyse. Met Principle Component Analysis en een statistische clusteringsmethode konden suspects naar chemische eigenschap worden gegroepeerd. De gebruikte methodiek bleek echter niet geschikt om uit de huidige dataset clusters te vinden die relateren aan watertype of het voorkomen in water. Voor verdere data-analyse wordt aanbevolen om de zekerheid van de stofidentiteit te verhogen en een kleinere set van typische chemische eigenschappen (expert- of data-gedreven) te selecteren.



De verschillen in somconcentratie van de stoffen per monster (in interne standaard equivalenten) tussen de verschillende watertypen. EFF = effluent, OW = oppervlaktewater, GW = grondwater, DW = drinkwater.

Belang: ontsluiten van brede screeningsdata

Brede screeningsanalyses die gedurende de afgelopen jaren zijn verzameld, bevatten een schat aan informatie. De gegevens zijn afkomstig van monsters van drinkwater, grondwater, oppervlaktewater en afvalwater effluenten. Het is echter niet makkelijk om uit al deze data de informatie en kennis te destilleren die erin ligt opgesloten (Hogenboom et al., 2009). Nieuwe software maakt het mogelijk om grote aantallen monsters onderling te vergelijken en om deze gelijktijdig te screenen op meerdere (on)bekende stoffen.

Aanpak: suspect screening en statistische analyse

De eerste fase van het onderzoek bestond uit het screenen van een grote hoeveelheid aan brede screeningsgegevens (151 monsters) bij een voorselectie van relevante antropogene stoffen op de Europese markt (5.200 stoffen). Vervolgens werden in een andere studie stoffen geprioriteerd (BTO 2015.003). In de tweede fase van het onderzoek lag de focus op het herkennen van patronen in de aanwezigheid van stoffen in verschillende watertypen. Met behulp van statistische methoden zijn de monsters onderling vergeleken. Zowel de grootschalige suspect screening als de gebruikte statistische methoden zijn nieuw voor data-analyse van breed screenend chemisch onderzoek.

Resultaten: 1.260 potentiële kandidaatstoffen

Suspect screening koppelt (onbekende) stoffen uit brede screeningdata aan potentiele kandidaten. Van de 5.200 ‘suspects’ werden 1.260 stoffen benoemd als potentiële kandidaatstoffen voor 700 gedetecteerde massa’s. Een massa kon worden gekoppeld aan meerdere kandidaatstoffen. De resultaten laten tussen de monsters van de uiteenlopende watertypen significante verschillen zien in het aantal stoffen, de somconcentratie en de gemiddelde retentietijd. Op grond van Principle Component Analysis (PCA) blijkt een hoge variabiliteit in chemische descriptoren van de suspects te bestaan, die niet te vatten is met twee nieuw gedefinieerde variabelen. Een statistische clusteringsmethode was bruikbaar om stoffen naar chemische eigenschap te groeperen. De gebruikte methodiek bleek echter niet geschikt om uit de huidige dataset clusters te vinden die relateren aan watertype of het voorkomen in water. Voor verdere data-analyse wordt aanbevolen om de zekerheid van de stofidentiteit te verhogen en een kleinere set van typische chemische eigenschappen (expert- of data-gedreven) te selecteren.

Implementatie: suspect screening als waardevolle methode bij het interpreteren van screeningsdata

Suspect screening blijkt een krachtige techniek te zijn voor het opsporen van nieuwe antropogene stoffen, mits verdere identificatie wordt uitgevoerd. Toepassing ervan is mogelijk als invulling van de doelstelling van het bestuderen van “overige antropogene stoffen” uit het Drinkwaterbesluit. Het identificeren van nieuwe stoffen geeft richting aan monitoring en het veilig houden van de waterkwaliteit.

Na identificatie van de suspects is het in principe mogelijk om op basis van chemische eigenschappen relaties tussen een specifiek watertype en het voorkomen van een stof te bepalen. Dergelijke relaties helpen bij het inschatten van het gedrag van niet-geanalyseerde stoffen in water.

Rapport

Dit onderzoek is beschreven in rapport *Datamining in non-target chemical screeningsdata* (BTO-2015.062) en verdure stofprioritering in *Data-driven prioritization of chemicals for various water types using suspect screening LC-HRMS* (BTO 2015.003).

Contents

1 Introduction

1.1 Introduction

In the last 10 years non-target chemical screening data of water samples have been collected at KWR. The liquid chromatography-high resolution mass spectrometry (LC-HRMS) analysis is a more comprehensive method for broad screening water quality than the commonly used target analysis (Ter Laak., 2010) and provides qualitative information on a broad spectrum of chemicals present in the water samples. However, the identification and quantification of all observed compounds remains challenging.

The collected large set of water quality monitoring data contains much information on the presence of chemicals. In the last years, over 150 samples were analysed of waste water effluent, surface water, groundwater and drinking water samples all over The Netherlands. Besides the presence of chemicals, this large dataset contains information on the occurrence of chemicals related to geographical setting, hydrology and land use. However, uncertainties on identification and quantification of compounds make it hard to distil relevant information and obtain knowledge on water quality (Hogenboom et al., 2009).

Therefore, in this study we extract information from the derived data in non-target chemical screening. The study is divided in two phases. The first phase deals with the selection of potential candidates for identification of chemicals using suspect screening. The second phase links the occurrence of compounds to different water types.

In the first phase we extract most relevant information from the non-target screening LC-HRMS dataset. Therefore we use software to study the presence of compounds in the samples through the years. The identification of the compounds is based on ‘suspect screening’, a recently developed tool to link peaks of an exact mass in chromatograms to known molecular formulas of suspect chemicals. The size of the suspects screening makes this study unique; the study is performed with 5219 suspects, represented by chemicals on the European market, and LC-HRMS screening data of 151 water samples. This tool focusses on the presence of anthropogenic compounds and has the advantage to make a selection of potential relevant compounds being produced at large scale or containing toxic properties.

The second phase focusses on the relation between the presence or absence of (groups of) compounds and the water types. First it is studied if the water types (waste water effluent, surface, groundwater and drinking water) show different characteristics for chromatographical parameters (retention time, total concentration). Second, multivariate statistical methods are used to obtain information on the chemical properties of compounds present in different water types. This last method can be considered as a try-out for the application of multivariate statistics in suspect screening results.

2 Suspect screening of LC-HRMS screening data

2.1 Introduction

In recent years liquid chromatography-high resolution mass spectrometry (LC-HRMS) is increasingly used for analysis of the presence of chemicals in water (Hogenboom et al. 2009, Krauss et al. 2010). The accuracy allows for a broader overview on the chemicals that are present in the environment than target analytical approaches do (Ter Laak et al. 2012, Schymanski et al. 2014a, Chiaia-Hernandez et al. in press). Given the sensitivity and selectivity it is possible to detect a large amount of chemicals at the same time, on the condition that they are isolated, separated, ionized and detected during the analytical process. In suspect screening approaches, LC-HRMS data is screened for a (large) list of chemicals or 'suspects' (Moschet et al. 2013, Hug et al. 2014, Schymanski et al. 2014b), or for a specific group of chemicals such as pharmaceuticals or pesticides (Moschet et al. 2014, Vergeynst et al. 2014). Identities of the chemicals might be confirmed by reference standards, using libraries or MS2 data; various levels of confidence can be discerned (Schymanski et al. 2014a, Zedda and Zwiener 2012).

Here, we used a large scale study on suspect screening to find potential candidates for identification relevant for (drinking) water. We based the suspect list on 5219 chemicals authorized on the European market via various regulations, including hardly studied chemicals. This list was applied to 151 Dutch water samples, including effluents, surface waters, ground waters and drinking waters.

2.2 Material and methods

2.2.1 Selection of suspects

The suspect list is composed based on chemicals authorized on the market via various European regulatory frameworks (Attachment I). Included are chemicals applied in industry in volumes above 1000, or from 100 to 1000, tons per year in Europe, as registered under the REACH legislation (Registration, Evaluation, Authorization and restriction of Chemicals, Regulation EC 1907/2006, data obtained via the European Chemical Agency ECHA (2015)). In addition substances of very high concern (SVHC) as defined under REACH for their carcinogenicity, mutagenicity, reproductive toxicity, persistency or bioaccumulative properties are included (CMR and PBT). CMR compounds as defined under the CLP Regulation on classification, labelling and packaging of substances and mixtures (1272/2008) are included, completed by Dutch legislation on CMR compounds. Furthermore included are chemicals authorized on the Dutch market under the Plant Protection Product Regulation (1107/2009/EC) and Biocidal Product Regulation (528/2012/EC), for which data were obtained via the Dutch Board for the Authorization of Plant Protection Products and Biocides. Finally, pharmaceuticals and veterinary pharmaceuticals as authorized under the EU Directives 2001/83/EC and 2001/82/EC and listed in previous research (Ter Laak, 2011) are included.

Mixtures, inorganic chemicals, metalloids and non-ionisable chemicals are excluded from the suspect list. Only compounds are considered containing at least one hetero-atom (e.g. N, S,

O, and P) and practically ionisable with ESI. For each chemical, the structural formula, CAS number and accurate molecular mass were collected.

For comparison, all chemicals regulated via the EU Drinking Water Directive and EU Water Framework Directive, including the Priority Substances Directive, are included in the suspect list, as are chemicals listed as potentially relevant for ecosystem health by the Norman network (Brack et al., 2012) and for drinking water by IAWR/RIWA (Hin and Bannink, 2013a, b).

2.2.2 Water sampling and LC-HRMS analysis

The water sampling and LC-HRMS analysis was performed as described in Hogenboom et al. (2009). Waters were sampled in the Netherlands in the period 2007-2014. The 151 samples are distributed over the Netherlands (Figure 1), and comprise 20 drinking waters (DW), 39 ground waters (GW), 73 surface waters (SW) and 19 industrial and STP effluents (EFF).

STP effluents are 24h flow corrected samples, other water samples are grab samples. All samples were stored in the dark at 1-5˚C and pretreated within one week after sampling, or (incidentally) directly frozen at -25˚C before pretreatment. Samples were isolated using Solid Phase Extraction (SPE) on OASIS HLB columns (Waters, Milford, MA, USA), 200 mL for effluents and 1 L for other waters. Water samples were acidified to pH 2.3 before SPE. After loading the SPE cartridges were washed, dried using nitrogen and eluted with acetonitrile. The eluate is evaporated to 500 µL. As internal standards atrazine-d5, bentazone-d6, chloroxuron, benzotriazole-d4, fenuron and neburon were added to each sample at a concentration level of 0.5 µg/L. The internal standards for quantification purposes (atrazine-d5 and bentazone-d6) were selected due to the stable ionization response in different sample matrices. The other internal standards are used for retention time alignment.

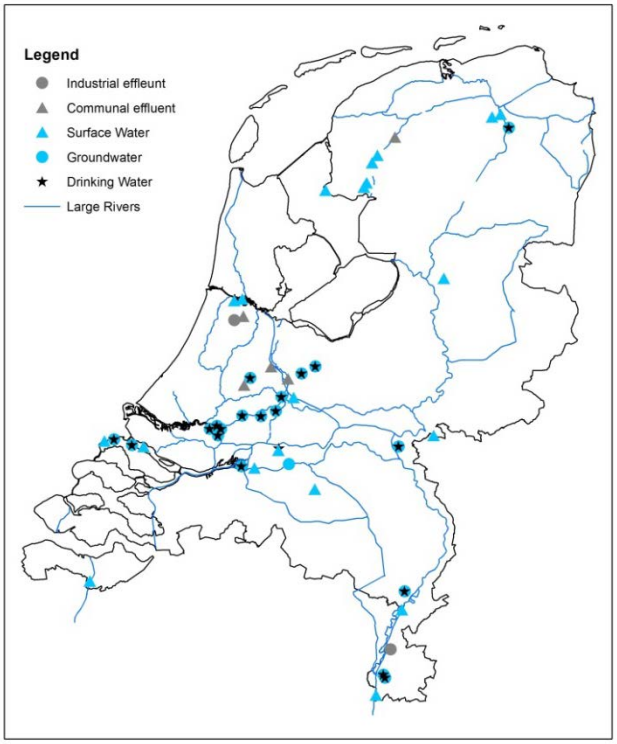


Figure 2-1 Overview on the sample origin for drinking waters, ground waters, surface waters and effluents.

The resulting sample extracts were analysed using Liquid Chromatography coupled to a Linear Ion Trap (LTQ) Orbitrap High Resolution Mass Spectrometer (Thermo Fisher Scientific, Bremen, Germany), in the positive and negative ionization mode.

Full scan accurate mass spectra were recorded from 50 to 1300 Da at a resolution of 60,000 – 100,000 FWHM (at m/z 400). Data dependant MS2 spectra were acquired at low resolution without the need to specify parent masses, only the most intense ions were analysed by MS2. The product ions were generated in the LTQ trap at a normalized collision energy setting of 35% and using an isolation width of 2 Da.

Electrospray ionization (ESI) source conditions were: capillary voltage 4.0 kV (positive-ion measurements), 2.5 kV (negative-ion measurements), heated capillary temperature 300 ºC, capillary voltage 24 V, tube lens 70 V.

The LC system consisted of an Accela UHPLC system and an Accela autosampler (Thermo Fisher Scientific). The chromatographic separation was performed on an Omnisphere C18 column (150 mm × 2.0 mm i.d., 3 µm, Varian-Chrompack, Middelburg, the Netherlands). The precolumn used was a C18 Guard column (4.0 mm × 3.0 mm i.d., Phenomenex). The columns were maintained at 21ºC with a column thermostat. A linear gradient was used at a flow of 0.3 mL/min, starting at 5% acetonitrile/95% water/0.05% formic acid (v/v/v) increasing to 100% acetonitrile with 0.05% formic acid in 40 min. The analytical column was re-equilibrated at starting conditions between consecutive runs for 15 min.

For the blank procedure, a sample consisted of ultra-pure water (Millipore) with the same treatment and analysis as the samples was included in each analytical run. Additionally, for quantification purposes, a set of 67 regularly in water detected compounds were analysed also within each analytical run (Table S.1 and S.2).

2.2.3 Data interpretation

The recorded chromatograms were screened for the chemicals on the suspect list, using the MsXelerator software (MsMetrix Maarssen, The Netherlands) (Jacobs et al., 2013). The suspect screening was performed by screening for the accurate molecular ions [M+H]+ and [M-H]- with a mass window of ±5 ppm for the positive and negative ionization mode, respectively. The mass spectra of the detected masses were manually checked on possible adduct ions (sodium and ammonium).

As chromatograms obtained in the period 2007 to 2014 are used in the present study, replacement or adjustment of the instrumental parts of the LC-HRMS system -such as columns, tubing or valves – might have led to minor changes in chromatography and retention time. MSXelarator software was used to align the chromatograms based on internal standards, to improve the comparability between samples. The chromatograms were compared from 2 - 40 minutes and retention time clustering is used, with a window of 5 min. As no suitable internal standards were used prior to 2010, data in the negative ionization mode were only obtained after 2010, i.e. 9 drinking waters, 14 ground waters, 29 surface waters and 14 effluents.

Peaks with a sample to blank ratio higher than 10 were considered for further analysis. Per sample, peaks were matched with the exact masses of the suspect list, with a maximum deviation of 5 ppm without a retention time restriction. The concentration of the matching detected masses was expressed in terms of atrazine-d5 or bentazone-d6 equivalents (IS-eq) for all chemicals detected in the positive or negative ionization mode respectively, with a detection limit of 0.01 µg/L IS-eq.

The selection of priority compounds was carried out in another study (BTO 2015.003).

2.3 Results

The suspects screening resulted 1591 potential candidates for identification of 721 compounds. The larger number of potential candidates is a consequence of the linking based on accurate mass. One compound can be coupled to multiple potential candidates with a similar mass (Figure 2-2). In addition, different detected peaks can have a similar mass (with different retention times); one suspect can thus be linked to different peaks. The compounds have identity confidence level 5 (Schymanski et al, 2014: the identity of the compound to be the potential suspect is only confirmed by a similar mass. In a different study, the detected suspects have been prioritized based on their response (BTO 2015.003). Currently, out of 158 prioritized compounds, 45 compouds were false positives (28%), 21 compounds have a confirmed structure (13%) (see Attachment II) and 92 of the prioritized compounds have a confirmed molecular formula (58%) (Sjerps et al., in prep). In a future project the identity of the 92 compounds will be confirmed or rejected (BTO project 2016 “Bevestiging identiteit geprioriteerde stiffen”).

Table 2-1 Results of the suspect screening.

Number of peaks	721	484 positive mode and 237 in negative mode
Number of suspects	1260	
Number of unique suspects	899	

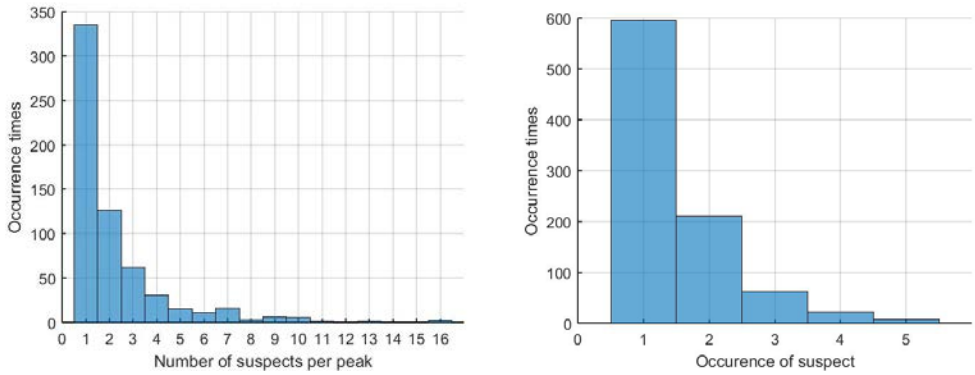


Figure 2-2 Left: Distribution of the occurrence times that one or multiple suspects are linked to a detected peak. Right: Distribution of the occurrence times that one suspects is linked to multiple detected peaks.

2.4 Discussion

The suspect screening approach shows to be a fast and usable tool to screen for the presence of a large set of antropogenic chemicals in (big) non-target data containing natural and unknown compounds. The large scale of the performed suspect screening is novel in the field of chemical screening. The approach shows to be complementary to target-based approaches. The suspect screening can be used as a filter mechanism to select the potential relevant candidates for future prioritization, monitoring and risk assessment studies. However, potential relevant transformation products of these parent compounds are not taken into account in the approach followed.

However, suspect screening alone still holds identity uncertainties. Suspect screening itself only links potential candidates to detected peaks in chromatograms. For further analysis and risk assessment these potential candidates should be confirmed with MS data and preferably

with a pure reference standard. This activity will be performed for only the prioritized compounds (BTO 2015.003) in the BTO study ‘Bevestiging identiteit geprioriteerde stoffen’ (2016). Currently, 28% of the prioritized compounds were false positives (Sjerps et al., in prep)

3 Multivariate analysis of LC-HRMS screening data

3.1 Introduction

The LC-HRMS dataset contains abundant information on the occurrence of compounds in the different water types. This chapter describes the method and the results of the multivariate statistics of the LC-HRMS dataset collected at KWR. The analysis focusses on the link between chemicals and their presence in different water types. The results of the suspect screening (phase one, Chapter 3) is the starting dataset for the analysis. The results contain the presence of more than 700 compounds detected in four different water types.

The aim is to explore the potential of statistical techniques to the large dataset of the LC-HRMS non-target screening data to extract information and obtain knowledge on water quality. The statistical analysis includes principle component analysis and clustering analysis. Principle component analysis helps to obtain a simplified description of the dataset composed of numerous variables. Clustering analysis helps to organise and structure compounds based on their similarity. Regression analysis links certain variables to other variables. With these methods the dataset is processed in order to find relevant information regarding the presence of compounds in certain water types and the exploratory value of chemical properties.

Three research questions are distinguished:

1. *Characteristics of different water types:* To what extent do the samples of the different water types differentiate or resemble?

2. *Clustering and dimensionality reduction of compound property data*
   - *Presence or absence of compounds in water*
     Can we observe clusters of compound properties that relate to compounds that are present or absent in water matrices?
   - *Compounds related to water type*
     Can we observe clusters of compound properties that relate to the occurrence of compounds in the different water types?

3. *Analysis of chemical descriptors:* What do these compounds have in common? Which set of chemical descriptors can describe/explain the presence of a compound in a certain water type**?**

Finally, we test if the results obtained by clustering analysis are reproducible, discuss the relevance of the approach and future possibilities for data handling and machine learning techniques.

3.2 Material and methods

3.2.1 Characteristics of different water types

To answer the question regarding the characteristics of the different water types, the difference between the water types is expressed by the total concentrations and the average retention time per sample. The samples are specified by their total concentration equivalents (µg/L IS-eq) and the average retention time. The sample characteristics are based on the compounds present in the sample in concentrations above 0.01 µg/L internal standard equivalents (IS-eq) to remove signal noise from the suspect screening results. The average retention time per sample is calculated by averaging the retention times of the compounds present corrected for the concentration (IS-eq). The variables are plotted per water type using Graphpad.

$$\bar{t_R} = \frac{\sum_{i=1}^{n} t_{Ri} \cdot c_i}{\sum_{i=1}^{n} c_i} \qquad \text{eq 1}$$

$\bar{t_R}$ = Average retention time per sample

t_{Ri} = Retention time of compound

c_i = Concentration of compound

3.2.2 Clustering and dimensionality reduction of compound property data

To answer the main questions 2 and 3, multivariate statistics was applied on compound property data and occurrence of compounds. Each potential candidate is described by a set of chemical descriptors that are measured or calculated. Measured descriptors are the chemical mass and retention time in the LC RP column. Besides these measured properties, chemical descriptors were calculated using the open source Pharmaceutical Data Exploration Laboratory (PaDEL)-Descriptor software. From the software we obtained 1444 1D and 2D descriptors for the potential candidates. These descriptors contain for example logP and the number of specific atoms (see Figure 3-1). It should be noted that a large part of the descriptors cover similar properties, such as the chemical descriptors for autocorrelation (346 descriptors), atom type electrotopological state (489 descriptors). The used descriptors are listed in Attachment III.

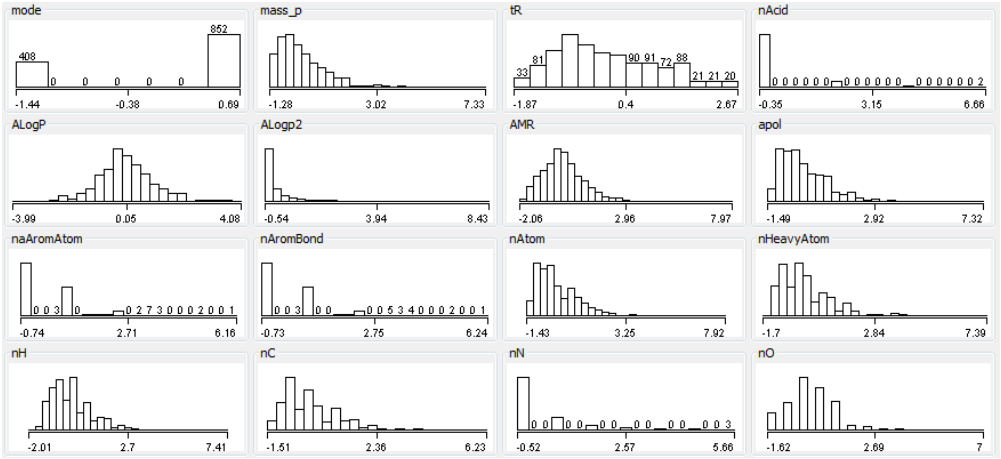


Figure 3-1 Examples of chemical descriptors in the dataset (normalized values).mode = ionisation mode. Mass = molecular mass, tR = retention time, NAcid = number of acidic groups, AlogP = Ghose-Crippen LogKow, AMR = Molar refractivity, apol = Sum of the atomic polarizabilities (including implicit hydrogens, naAromAtom = Number of aromatic atoms.

The statistical analysis comprises of Principle Component Analysis (PCA) and clustering analysis. PCA and clustering analysis were performed in the numerical computing environment Matlab version R2015a. PCA can be used as a tool for exploring and analysing the dataset due to the way PCA handles the data. The method seeks for a component in the variable space explaining as much variation of the data as possible. Consequently, few components may be able to describe a large part (say 95%) of the variance. These components may then be used to provide an informative view on how the data can be represented by these few components. Clustering divides data into clusters according to a distance metric (dissimilarity), hence in this case it assigns different clusters of alike chemicals. Our hypothesis is that clusters are assigned in such a way that similar compounds can be grouped and related to their presence in different water types. Former to clustering, the suspects were organised using a Self-Organizing Map (SOM). A SOM is a type of artificial neural network that is trained using an unsupervised learning technique. With unsupervised learning, there is no need to structure or label the data prior to using the learning technique. A SOM can be considered as a nonlinear generalisation of PCA (with two components) since it produces a two-dimensional representation (a map) of the input parameters – in this case the descriptor space. Training of the SOM is achieved by connecting an amount of nodes (or neurons) to the input data points as good as possible. The procedure for placing a data point onto the map is to find the node with the closest (smallest distance metric) weight vector to the data space vector. The map structures compounds of alike properties. The U-matrix is a representation of the SOM which visualises the distances between the neurons. The SOM-toolbox is a freely available software package. The resulting map is then used to cluster nodes by the k-means algorithm. With k-means clustering, each observation is assigned to the cluster whose mean yields the least within-cluster sum of squares – hence 'nearest' mean.

In short, statistics are used to structure the data in such a way which increases the suitability to find chemical descriptors that can explain the presence of compounds in certain water types.

3.2.2.1 Analysis of chemical descriptors

After the data is distributed into clusters, the clusters are analyzed. Per cluster it is studied if a certain set of chemical descriptors has a relation to the presence in water in general or certain water types. Second, for a specific set of descriptors that could influence environmental fate, the variation of the distribution of values is studied for the different water types.

3.3 Results

This chapter presents the results of the statistical analysis. First, the difference in the characteristics between water types is shown. Second, the relation between the presence of chemicals in the different water types is studied using multivariate statistics. Finally, the selection of chemical descriptors that could have a relation to different water types is studied in more detail.

3.3.1 Characteristics of different water types

Data

Table 3-1 and 3-2 present the detected compounds per water type for the positive and negative ionisation mode, respectively. Combining the compounds detected in positive and negative ionisation mode, on average less than ten compounds are detected per drinking water or groundwater sample. In surface water on average 50 compounds are detected, while in waste water effluent on average more than 200 compounds are detected.

Table 3-1 Number of compounds detected (>0.01 µg/L IS-eq) in the positive mode for each water type.

Positive mode	Number of samples	Average number of compounds per sample (>0.01 µg/L IS-eq)	Standard deviation of the average number of compounds per sample	Minimum number of compounds per sample	Maximum number of compounds per sample
Drinking water	20	3	2	0	6
Groundwater	39	6	6	0	25
Surface water	73	32	21	2	140
Effluent	19	152	62	52	298

Table 3-2 Number of compounds detected (>0.01 µg/L IS-eq) in the negative mode for each water type.

Negative mode	Number of samples	Average number of compounds per sample (>0.01 µg/L IS-eq)	Standard deviation of the average number of compounds per sample	Minimum number of compounds per sample	Maximum number of compounds per sample
Drinking water	9	8	7	1	23
Groundwater	14	2	2	0	6
Surface water	29	24	29	3	115
Effluent	16	118	14	85	192

Totals of detected compounds

In total, i.e. after summation of positive and negative mode data, 520, 372, 65 and 44 compounds have been detected in effluent, surface water, groundwater and drinking water, respectively. Further downstream in this water treatment chain the number of compounds reduces. 59% of the compounds detected in effluent are found in surface water, 13% of the compounds detected in surface water are found in groundwater. 35% of the compounds present in groundwater and 11% of the compounds present in surface water are detected in drinking water. An overview is given in Table 3-3. Note that these numbers can be biased due to different population sizes and undetected occurrence of compounds, due to detection limits or chemical properties needed for detection (eg. response to ionization). The decrease of occurrence of detected compounds further downstream the treatment chain is as expected based on dilution, environmental removal processes and water treatment. The less advanced treatment methods for the production of drinking water from groundwater shows that a larger fraction of the compounds in groundwater end up in drinking water (35%) compared to drinking water produced from surface water (11%).

Table 3-3 Total number of compounds detected in the water types with the overlapping part between brackets.

Source	Effluent	Surface water	Groundwater	Drinking water
Effluent	520	309 (58.9%)	56 (10.8%)	36 (6.9%)
Surface water	-	372	53 (13.0%)	36 (10.5%)
Groundwater	-	-	65	22 (34.8%)
Drinking water	-	-	-	44

Total concentration

The water quality of the sample varies between samples. Figure 3-2 shows the summed response of all suspects detected in the water sample. The total concentration expressed in µg/L IS-eq is to be considered a generic semi-quantitative parameter, as some suspects will have a higher response after ionization than others (Chalcraft et al. 2009, Gosetti et al. 2010, Bergman et al. 2014, Kruve et al. 2014).

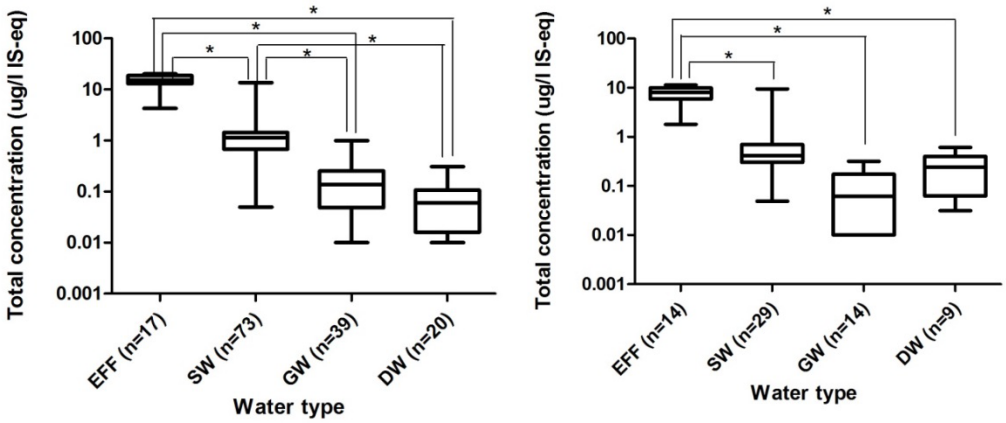


Figure 3-2 Distribution of the total concentration equivalents (IS-eq) of the compounds detected in the positive mode (left) and in negative mode (right) for the different water types. The box represents the median and the 25% and 75% percentile values. The whiskers extend to the minimum and maximum values. Combinations with significant different means are indicated with an asterisk (*).

The total concentration (IS-eq) in effluent samples (10-20 µg/L IS-eq) is approximately 10 times higher than the total concentration in surface water samples (±1 µg/L IS-eq). Groundwater and drinking water show the lowest total concentrations (±0.1 µg/L IS-eq). The total concentration exceeds the sum TTCs for non-genotoxic compounds (Mons et al. 2013) in effluent and surface water. The total concentration exceeds the sum TTCs for genotoxic or endocrine disruptors (Mons et al. 2013) for all matrices. So, adverse effects of the mixture cannot be waived without a more thorough risk assessment of the mixture after confirmation of the identity of the observed suspects.

The total concentration in positive ionization mode in the different water types differs significantly (ANOVA, $p \leq 0.0001$) for effluent (14.75±1.16 µg/L IS-eq.) - surface water (1.55±0.25 µg/L IS-eq) – ground water (0.19±0.03 µg/L IS-eq) and drinking water (0.08±0.02 µg/L IS-eq). The total concentration in groundwater does not significantly differ from that in drinking water. Within a water matrix obviously there are differences between individual samples, for example the total concentration in two contaminated small rivers (11.57±2.03 µg/L IS-eq) significantly differs from other surface waters (1.27±0.14 µg/L IS-eq) ($p<0.0001$).

The total concentration in the negative ionisation mode is somewhat different to the positive mode. Only effluent (16.85±6.45 µg/L IS-eq) differs significantly from surface water (1.03±0.38 µg/L IS-eq), ground water (0.10±0.03 µg/L IS-eq) and drinking water (0.25±0.07 µg/L IS-eq) ($p<0.0001$).

The total concentration in groundwater and drinking water reported in the current suspect screening study are in the same range as average values reported earlier in a non-target screening study of 0.08 µg/L IS-eq for confined groundwater, 0.32 µg/L IS-eq for phreatic groundwater and 0.03 µg/L IS-eq for drinking water (ter Laak et al. 2012). Slight differences

are explained by differences in the sample set, here we only include suspects in concentrations >0.01 µg/L IS-eq and do not include all ionizing chemicals but only the predefined suspects in the total concentration. The ratio between the compounds with a potential candidate or suspect to the total number of compounds detected in the water sample will be studied in the BTO project 'Hoe breed is brede screening?'.

The total concentration expressed in µg/L IS-eq is to be considered a generic semi-quantitative parameter, due to differences in the isolation recovery (SPE) and the ionization efficiency. Each analytical series was accompanied with procedure controls including drinking water fortified with 67 reference compounds: 53 in the positive ionisation mode and 14 in the negative ionisation mode. The absolute response of the 53 reference compounds in the positive ionisation mode, influenced by isolation recovery and ionisation efficiency, is given in Figure 3-3. In the positive ionization mode, the response varies within 4 orders of magnitude, however for 80% of these standards the variation remains within 2 orders of magnitude (Figure 3-3). The 53 reference compounds are most likely a good representation of all detected compounds, as they were selected for their relevance for surface water quality.

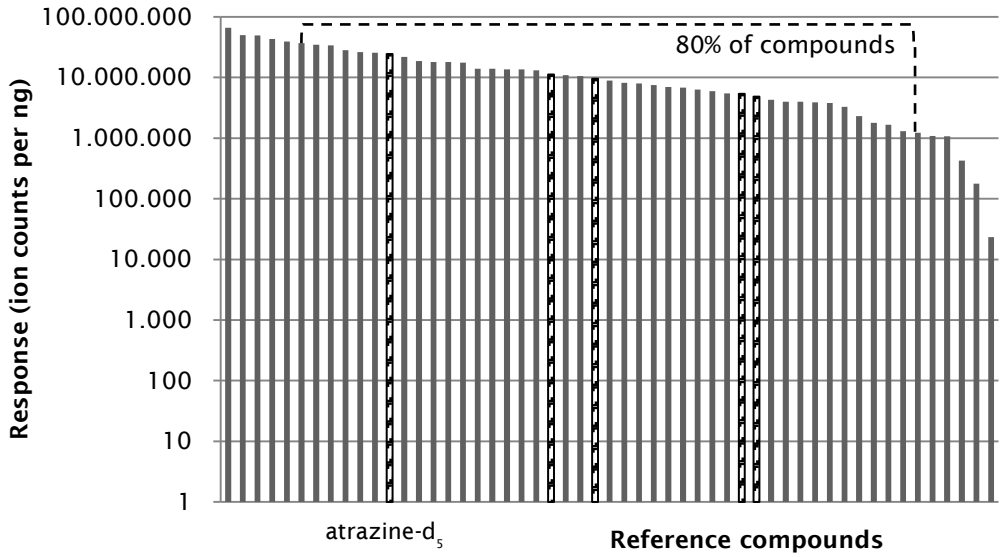


Figure 3-3 Response of 53 reference compounds in the positive ionization mode, including atrazine-d5 and four other internal standards indicated by the striped columns (from left to right: atrazine-d5, neburon, chloroxuron, 1H-benzotriazole and fenuron).

While the internal standard for negative ionization, bentazone-d6, has an average response compared to the other reference compounds (not shown), the internal standard for positive ionization, atrazine-d5, shows relatively high responses (Figure 3-3). Therefore the (total) concentrations expressed as in atrazine-d5-eq will generally be underestimated, and more suspects might be prioritized according to chosen thresholds, based on analytical standards.

Retention time

The retention time through the LC column reflects the hydrophobicity of a chemical (Casoni et al., 2009; Bade et al., 2015). The average retention time, weighted for peak intensity, is plotted per water type (Figure 3-4). A significant decrease in retention time is observed from effluent towards drinking water (for effluent – surface water - groundwater $p<0.0001$, for

groundwater – drinking water p=0.0418). This confirms that the more polar chemicals occur and might be problematic in drinking water (Wode et al., 2015), as hydrophobic chemicals are more easily removed from the water phase during environmental loss processes such as sorption and during water treatment. The fact that the REACH legislation by using the PBT criterion gives an impetus to produce more polar chemicals, has obvious environmental benefits by preventing bioaccumulation and biomagnification of chemicals within the ecological food-chain (Kelly et al., 2004) but at the same time poses challenges to drinking water utilities to remove the more polar chemicals.

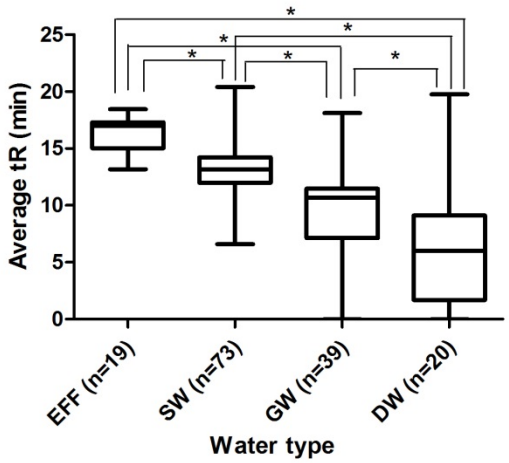


Figure 3-4 Distribution of the retention time (tR) (min) of the compounds detected >0.01 µg/L weighted for the peak intensity, in the positive mode for the different water types. The means of the water types are all significantly different, indicated with an asterisk (*).

3.3.2 Clustering analysis

The aim of the cluster analysis is to structure the data in relation to the water type. The data is enriched with (calculated) chemical properties of the detected suspects. This is applied for two datasets, first all suspects from the suspect list and second the retrieved suspects in the various water types.

3.3.2.1 Presence or absence of compounds in water

The suspect screening started with a suspect list of 5219 compounds present on the EU market. From the 5219 compounds, 1068 suspects are the potential identity of one of the 721 detected peaks the LC-HRMS data. Each suspect is described by 1444 chemical descriptors, of which 1220 show variance between the suspects. With Principle Component Analysis (PCA), one can show how many degrees of freedom (components) are needed to explain a large, specified part of the data set variance. Figure 3-5, left panel, represents the data projected on the first two components. The right panel shows that these two components only explain about 30% of the total variance of the data set and that 10 components cover approximately 58% of the total variance of the data set.

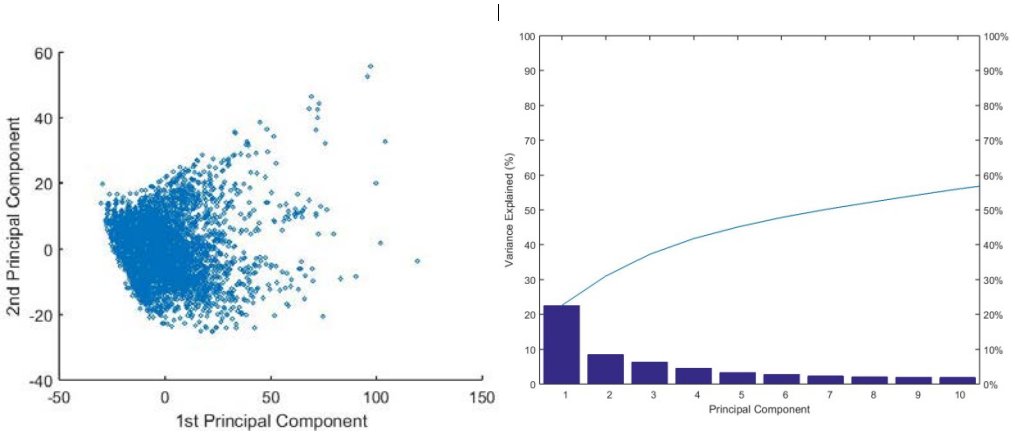


Figure 3-5 Result of the PCA of the chemical properties of all suspects from the suspect list (5219).

Results obtained with PCA show that there is high variability of chemical properties in the set of suspects and that is not feasible to catch all these compounds with two newly defined variables (the two first principle components).

Another method to use a clustering technique with the aim is to assign groups (clusters) of data points that have similar properties, which could be absent or present in water samples. Clustering is performed on a Self-Organising Map (SOM). Advantage of using a SOM before clustering is the straightforward and homogeneous selection of data points for validation and visualisation in two dimensions. The disadvantage is that the SOM is not a unique (lower dimensional) representation of the data set and could be subject to changes, e.g. removal of chemical descriptors or suspects from the total data set. The resulting SOM and found clusters are shown in Figure 3-6 3-6, in the left and right panel respectively. The figure on the left hand side shows the U-matrix (unified distance matrix). This matrix represents the SOM where the distance between the node weight vectors and its neighbours is visualised in greyscale. The darker the distance, the more differences there are between the chemical descriptor values of the suspect. The input data is plotted on the U-matrix in a pie diagram made of suspects present in water (red) and absent in water (green). The clustering analysis by k-means (see 3.2.2) resulted in 7 clusters shown in the figure on the right hand side (Figure 3-6).

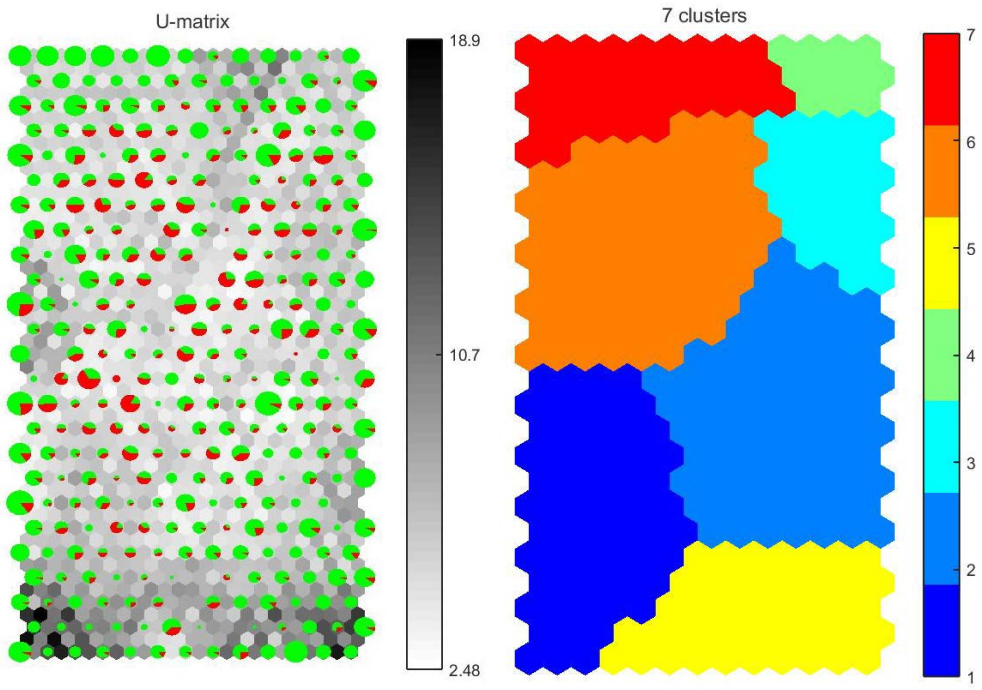


Figure 3-6 Result of the clustering on a Self-Organising Map (SOM). Left: The U-matrix (unified distance matrix) of the SOM with data 'hits' plotted on the nodes compounds present in water (red) and absent in water (green). Right: Results of the clustering on the SOM by k-means.

Within each cluster, the descriptors of the chemicals and the presence of the chemicals in water were studied. Of the 7 found clusters, two clusters (cluster 1, 3 and 7) contain a small part, i.e. approximately 5-10% of the compounds that are retrieved in water. In cluster 6, about 40% of the compounds are found in water. In the clusters 2, 4 and 5, the part of the compounds that is found in water varies from 20 to 25%.

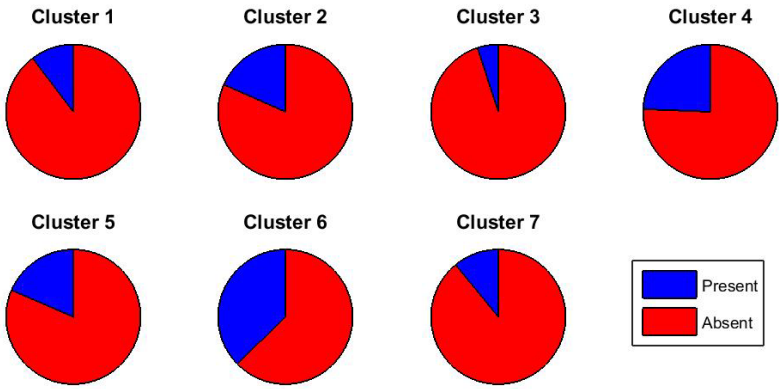


Figure 3-7 Distribution of compounds present or absent in different clusters.

Whether the chemical descriptors are distinct for each cluster was studied by calculating the median of the z-score of chemical descriptor values, see Figure 3-13). The z-score is a normalised value (dimensionless) obtained by subtracting the mean from each individual value and divided the difference by the standard deviation. The z-score provides a measure for the distribution of values within a cluster and the clusters can be compared using the

median z-score. For most descriptors the median z-scores do seem distinct across different clusters, indicating that the clustering procedure searches for clusters with maximal separation in chemical properties. However several descriptors seem to differ between clusters one to seven. The chemicals descriptors that show distinct values between the clusters are: the number of atoms and the Broto-Moreau autocorrelation [1-80], the Barysz Matrix Descriptors [370-480], the Burden Modified Eigenvalues Descriptors [480-580], the Ring Count Descriptor [1110-1135], the PaDEL Weight Descriptor and the PaDEL Weighted Path Descriptor [1210-1220]. All unique descriptors are shown in Attachment III.

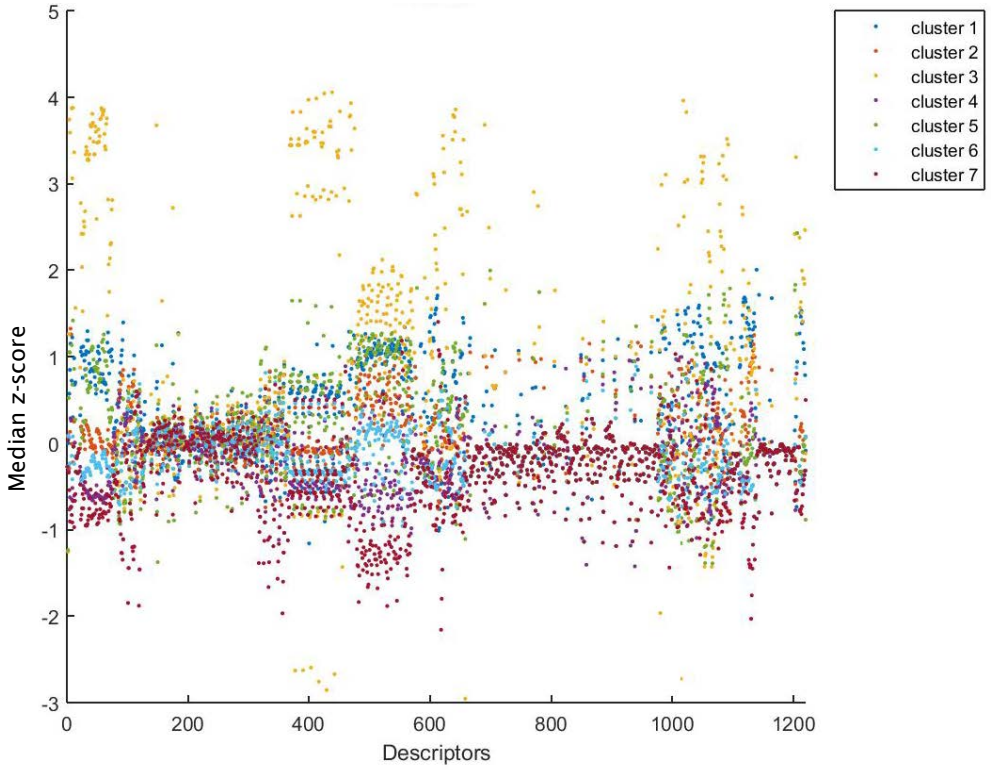


Figure 3-8 Median of the z-score of the descriptor values per cluster.

3.3.2.2 Compounds related to water types

The analysis of the second dataset encompasses the same statistical methods described as in the previous paragraph. The aim here is to study whether there are clusters of compounds with similar chemical descriptor values that relate to their presence in a water type: effluent, surface -, ground- and drinking water. The data set comprises of all detected peaks and their potential suspects.

In Figure 3-9 all detected peaks (721) are plotted for their accurate mass and their retention time. Peak values show a spread in both mass and retention time. Each peak is then coupled to potential suspects (see Chapter 3). The potential suspects and their chemical characteristics are studied using PCA. Each suspect is described by (again) 1444 chemical descriptors, of which 1220 show variance between the suspects. The results of the PCA of the dataset are shown in Figure 3-10.

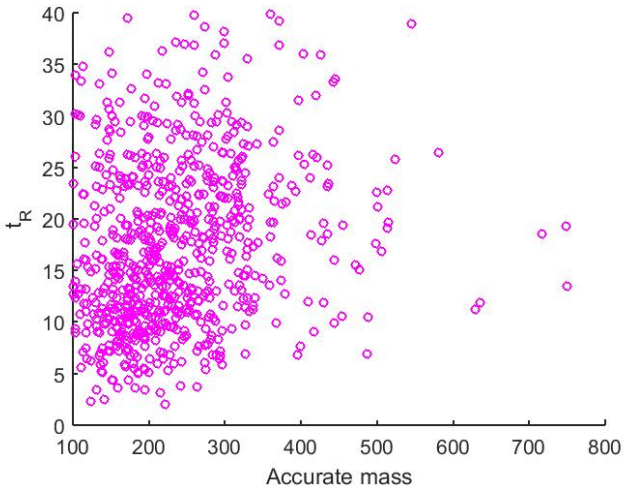


Figure 3-9 The 721 detected peaks plotted for their accurate mass and retention time.

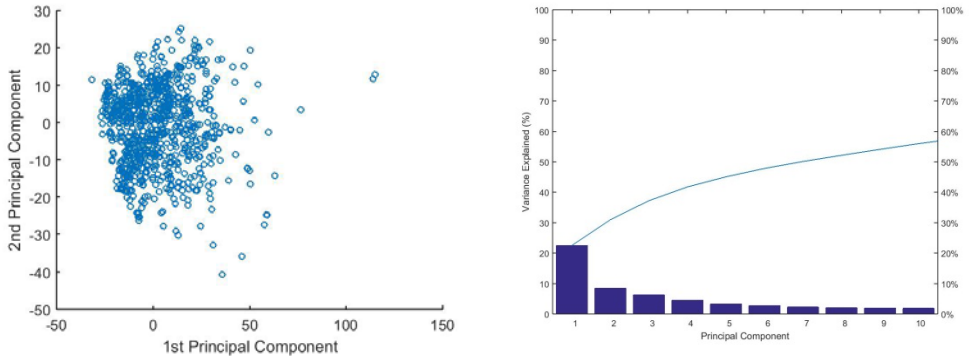


Figure 3-10 Result of the PCA of the data set comprised by the 721 detected peaks and its chemical descriptors.

Similarly to the analysis regarding the occurrence of compounds, the results of the PCA show again a high variability of chemical properties between the compounds. These results indicate that, also for this data set, it is not feasible to catch all these compounds with two newly defined variables (the two first principle components).

Also for this data set, a clustering analysis is performed. The data set was clustered into clusters of suspects having specific properties which could pinpoint to similar behaviour in a specific water matrix. The water matrices were specified as effluent, surface -, ground- and drinking water. The Self-Organising Map (SOM), a nonlinear generalisation of PCA, structures compounds of alike properties. The U-matrix (Figure 3-11 left) is a representation of the SOM which visualises the distances between the neurons. On the nodes of the U-matrix of the SOM the data 'hits' are plotted. The pie-diagrams show the distribution of compounds detected in various water types. From this map no specific patterns can be distinguished with the eye. For example, compounds occurring in drinking water (red) do not seem clustered, but spread over the map. This suggests that suspects that occur in drinking water do not have distinct values for the 1200 descriptors, while the retention time and total concentration clearly deviated from the other water types (Figure 3-2 and Figure 3-4)

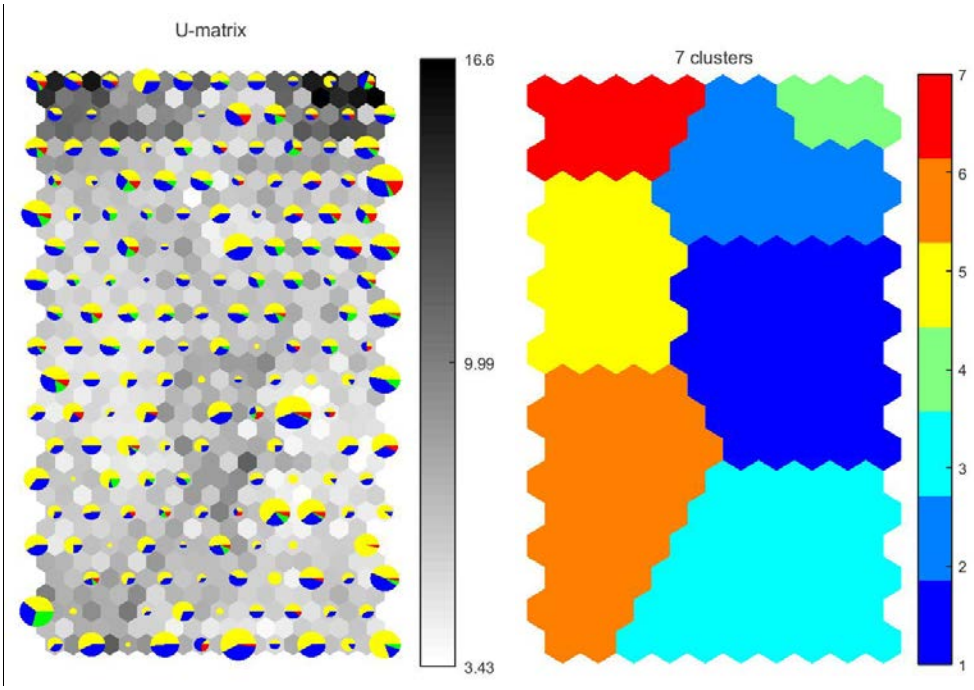


Figure 3-11 Result of the clustering on a Self-Organising Map (SOM). Left: The U-matrix of the SOM with data 'hits' plotted on the nodes of the compound occurrence in drinking water (red), groundwater (green), surface water (blue) and waste water effluent (yellow). Right: Results of the clustering on the SOM by k-means.

Clustering by k-means leads to 7 clusters (Figure 3-11 right). These clusters do not differentiate significantly in compounds that occur in different water types (Figure 3-12). There are however some differences in cluster compositions: clusters 2 and has a large part of compounds present in drinking water; cluster 5 has a large part of compounds present in ground water, two third of clusters 3 and 6 relates to sewage water effluent.

Whether the chemical descriptors are distinct for each cluster was studied by the median z-score Figure 3-13). The Figure looks similar to Figure 3-8 where only several descriptors show distinct median values between the clusters. The chemicals descriptors that show distinct values between the clusters are: the number of atoms and the Broto-Moreau autocorrelation [1-80], the Barysz Matrix Descriptors [370-480], the Burden Modified Eigenvalues Descriptors [480-580] and the Walk Count Descriptors [1185-1210]. All unique descriptors are shown in Attachment III.

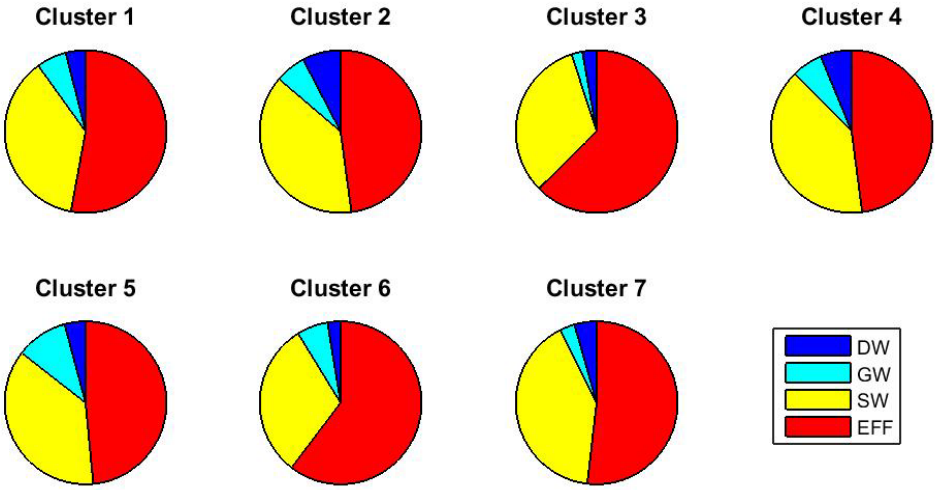


Figure 3-12 Distribution of compounds occurring in different water types (dw: drinking water, gw: groundwater, sw: sewage water and eff: effluent) for each cluster.

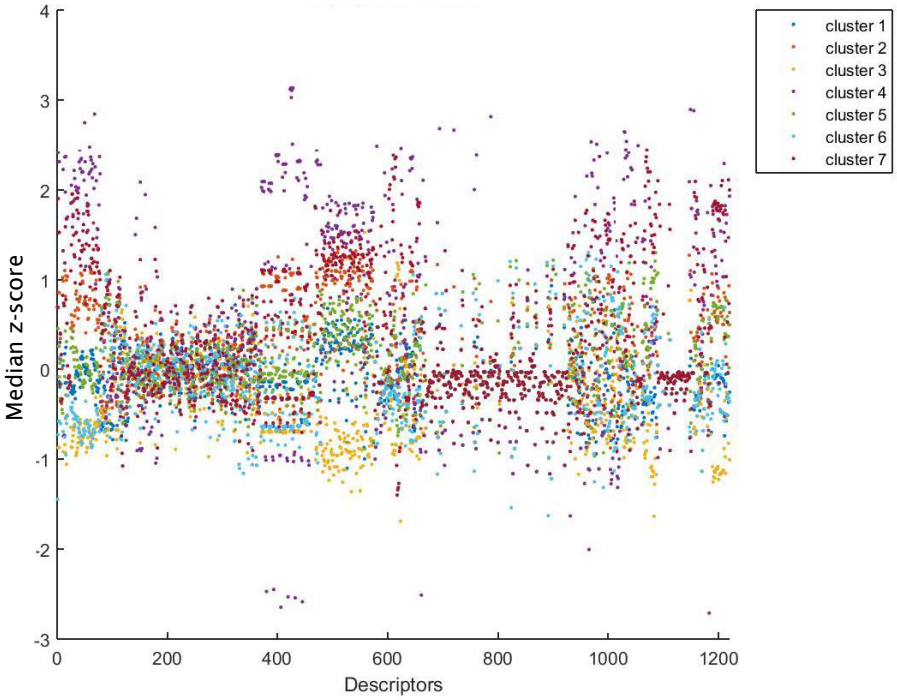


Figure 3-13 Median z-score of the 1220 descriptor values per cluster.

3.3.3 Reproducibility tests

The robustness of the statistical procedure was analysed by testing the reproducibility of the clustering analysis. The SOM is reproducible in all cases. Clustering however depends on the number of iterations and initialisation of the clusters. The clustering can result in a different optimal number of clusters. In this case, the optimal number varies between 6 or 7 clusters.

The descriptors could have mutual correlation (**Error! Reference source not found.**). The removal of five descriptors with the highest mutual correlation coefficient changes both the results obtained with SOM and clustering. The removed descriptors are: ATS1e, VP-0, Sv, McGowan Volume and VABC.

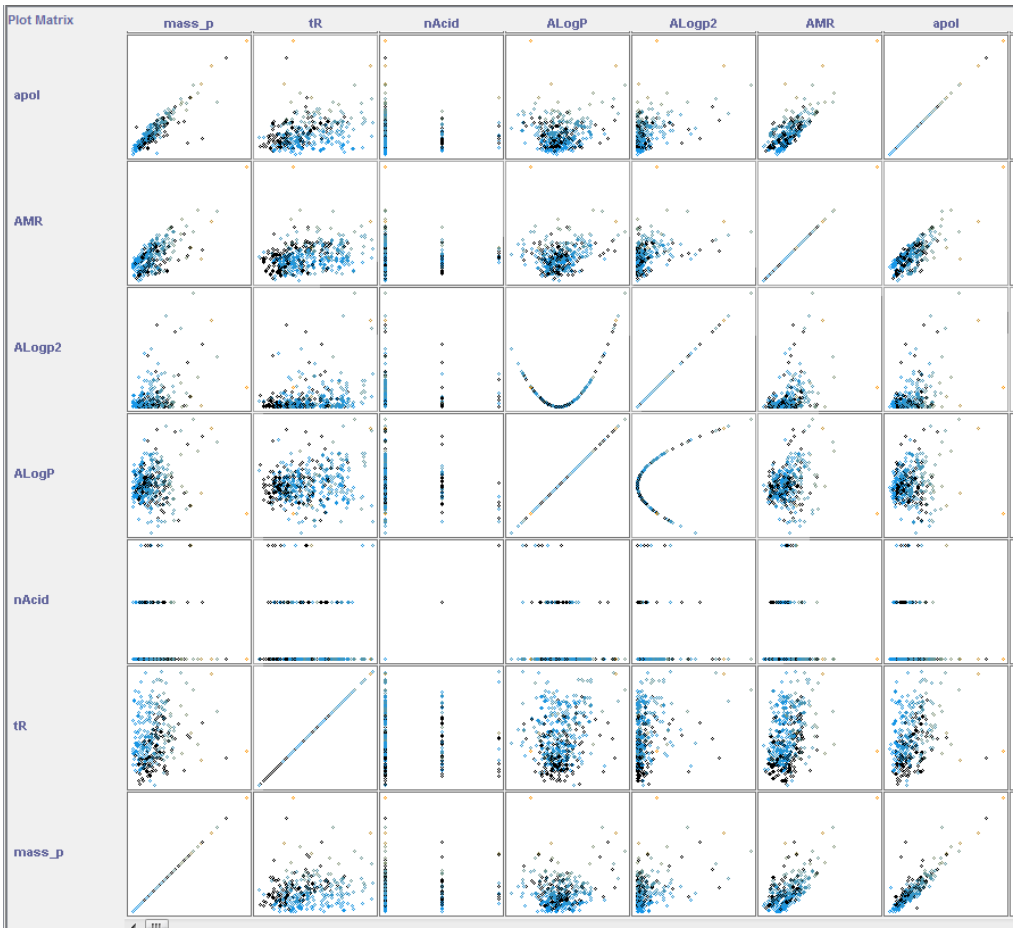


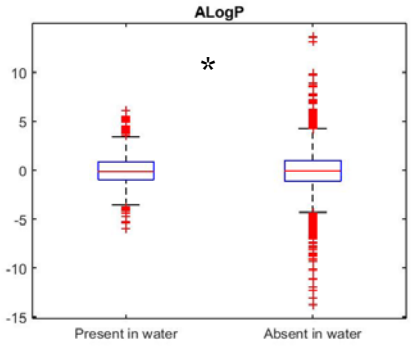
Figure 3-14 Correlation between descriptors (a selection).

3.3.4 Chemical descriptors

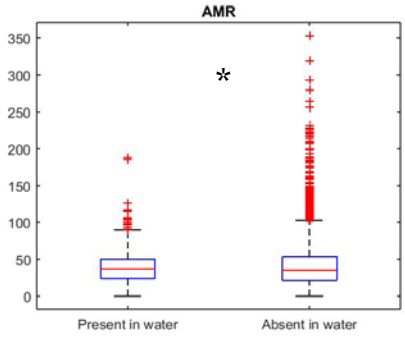
At first sight, clustering did not lead to clusters each having a unique set of chemical descriptors that could be related to their presence in water or to their presence in a specific water type. To study whether there are any significant differences between descriptors occurring in water (first data set) or belonging to a specific water type (second data set), we selected a small set of descriptors and studied their distribution by means of Box-Whisker (B-W) diagrams. In the B-W diagrams, the central mark is the median, edges of the box are the 25th and 75th percentiles, the whiskers extend to the most extreme data points not considered outliers, and outliers (that is, a 99%-confidence region is considered under the assumption that data is normally distributed), are plotted individually (+ sign).

3.3.4.1 B-W diagrams of selected descriptors according to their presence in water

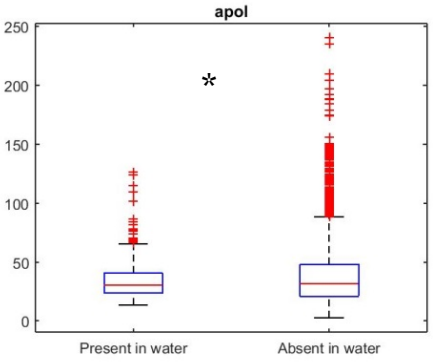
Box-whisker (B-W) diagrams are plotted for a selection of descriptors that are expected to differ between compounds that are present and absent in water: nAcid (number of acidic groups), nAtom (number of atoms), AMR (molar refractivity), apol (sum of the atomic polarizabilities), nN (number of nitrogen atoms), FMF (complexity of a molecule), see Figure 3-15. Generally speaking, (more) extreme values of these descriptors are found for compounds not found in water as well as a higher variability of descriptor values compared to the compounds that are present in water. However, the means for the two classes of all shown chemical descriptors are tested (t-test) statistically different (Figure 3-13).



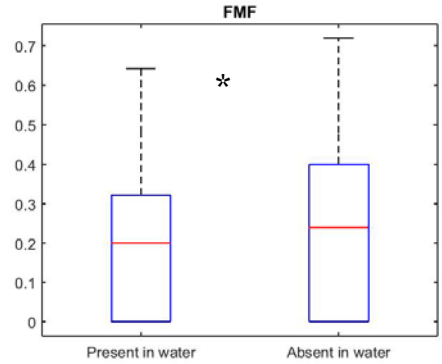
Ghose-Crippen LogKow



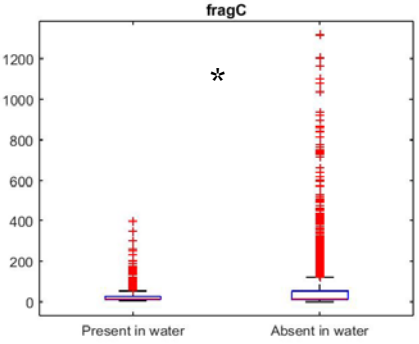
Molar refractivity



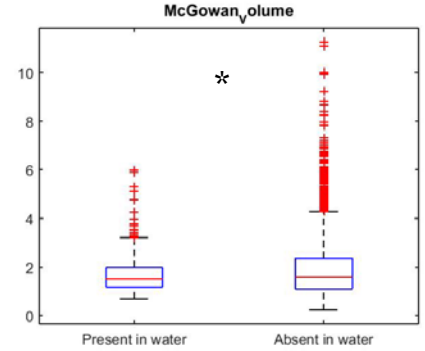
Sum of the atomic polarizabilities (including implicit hydrogens)



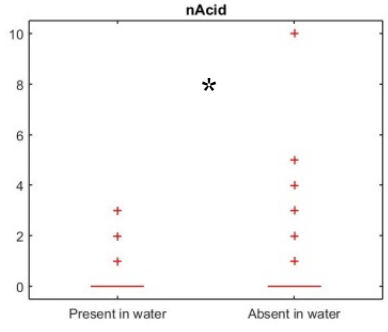
Complexity of a molecule

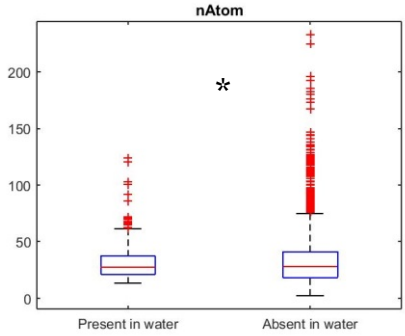


Complexity of a system



McGowan characteristic volume





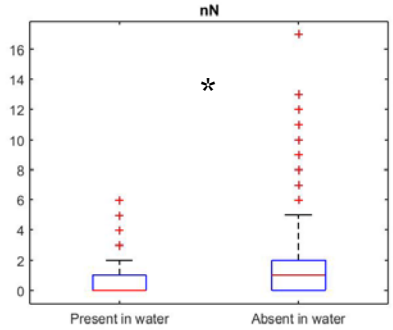
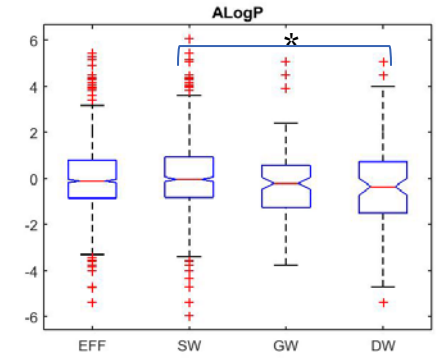
Number of acidic groups. The list of acidic groups is defined by these SMARTS "$([O;H1]-[C,S,P]=O)", "$([;-;!$(*~[*;+])])", "$([NH](S(=O)=O)C(F)(F)F)", and "$(n1nnnc1)" originally presented in JOELib*	*Number of atoms*
 *Number of nitrogen atoms*	

Figure 3-15 Distributions of chemical descriptor values for selected descriptors according to their presence in water. All descriptor values have significant different means for the two groups, indicated with an asterix (*).

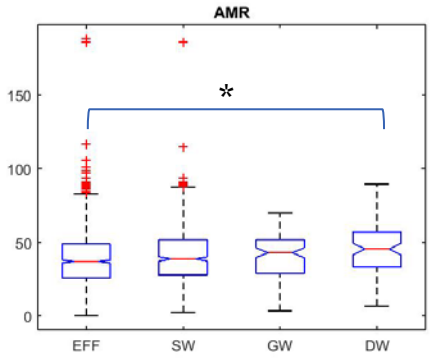
3.3.4.2 B-W diagrams of selected descriptors according to a specific water type

B-W diagrams are plotted for a set of descriptors, slightly different compared to Paragraph 3.3.4.1. Selection is based on the descriptors that are expected to differ between the compounds in the water types. The B-W diagrams are shown in *Figure 3-16*. ANOVA statistics indicate that one of the water types have different means, except for the descriptor complexity of a system (fragC). The water types with significant means are indicated with an asterisk (*). For most descriptors a significant difference is found between effluent and drinking water. This can be expected since these water types are very distinct. The detected outliers are mostly present in effluent and sewage water. This observation corresponds to the expectation that these water types can contain a very specific type of compound not found elsewhere.

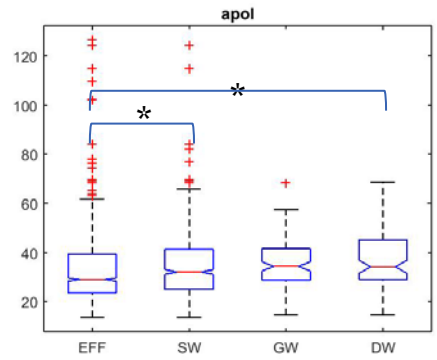
AlogP, the chemical descriptor for the Chose-Crippen log K_{ow}, is a measure for hydrophobicity. However, the log K_{ow} values of the chemicals show only significant differences between surface water compared to drinking water. This deviates from the significant different of the retention time, another measure for hydrophobicity (Figure 3-3). This could be caused a number of suspects that aren't the compound of interest, which causes 'noise' within the dataset that influence potential trends within the dataset. The K_{ow} values do not have a relation with the retention time of each chemical (Figure 3-15). This implies that a large part of the suspects is probably false positives or that the descriptor values for AlogP are of no good quality.



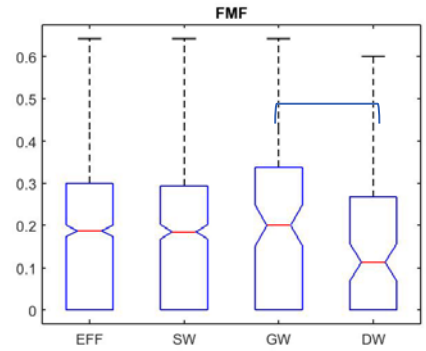
Ghose-Crippen LogKow



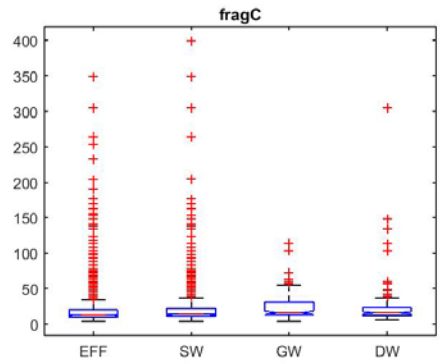
Molar refractivity



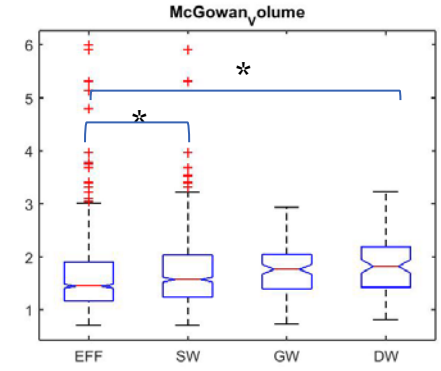
Sum of the atomic polarizabilities (including implicit hydrogens)



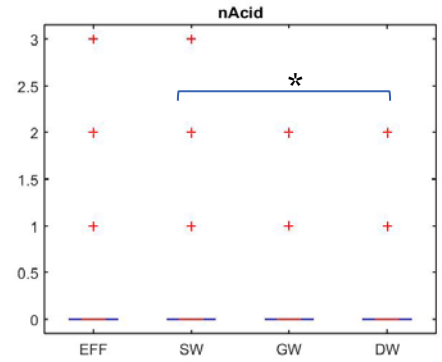
Complexity of a molecule



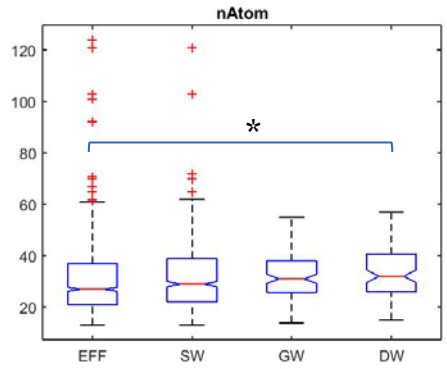
Complexity of a system



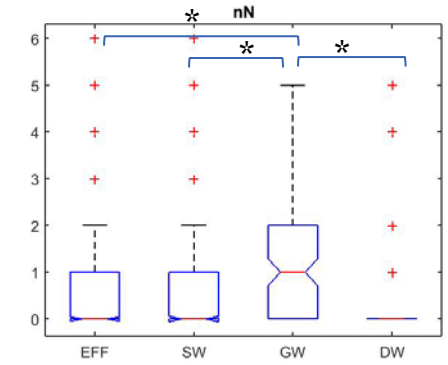
McGowan characteristic volume



Number of acidic groups. The list of acidic groups is defined by these SMARTS "$([O;H1]-[C,S,P]=O)", "$([;-;!$(*~[*;+])])", "$([NH](S(=O)=O)C(F)(F)F)", and "$(n1nnnc1)" originally presented in JOELib*



Number of atoms



Number of nitrogen atoms

Figure 3-16 Distributions of selected chemical descriptor values of compounds in specific water type. Combinations with significant different means are indicated with an asterisk (*).

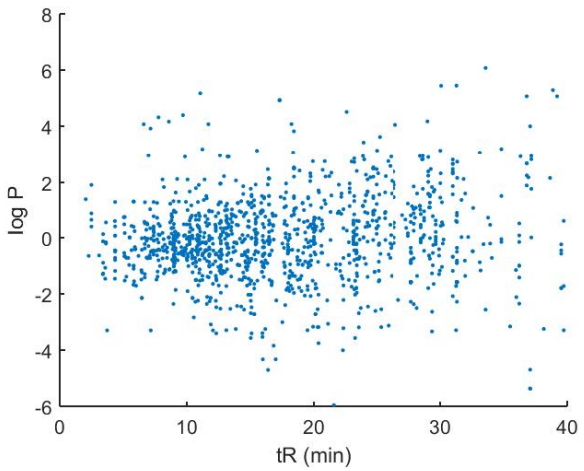


Figure 3-17 Distribution of K_{ow} (Log P) plotted for the retention time (tR).

3.4 Discussion and recommendations

A clear difference between the chromatographical parameters (total concentration and retention time), was shown for the different water types (Figure 3-2 and Figure 3-4). This result could however not be repeated with the distinctive features of the suspect data, the chemical descriptors. It should be noted that the found clusters do relate to these descriptor values. However, it is not clear whether these groups relate their occurrence in water or to a specific water type.

Based on the suspect data used and the broad set of descriptors used, the applied methods (PCA and cluster analysis) did currently not contribute to better knowledge and understanding of the occurrence of chemicals in the various water types. Application of these methods in the daily practice by water utilities is therefore currently not recommended.

Several reasons may explain the inability to successfully link the descriptor values to the occurrence in different water types:

- False positive suspects. As one suspect represents only the potential identity of the peak and peaks can be linked to multiple suspects. Of the 158 prioritized compounds currently 45 compounds (28%) were false postives. Clustering of data points is thus inherently troubled with many uncertainties. Identification processes could 'clean up' the dataset, to make it usable for statistical analyses.

- Not all samples analyzed in the negative mode are included in the study, hence critical information might be absent in the current dataset.

- The heterogenic dataset containing many samples makes it hard to pinpoint differences between water types. Using a homogenic dataset, for example in- and effluent of a STP, source water and the produced drinking water are easier to interpret.

- The quality of the estimated data for the various descriptors (the models were originally made for pharmaceuticals).

- The descriptors, many of which are not clearly related to environmental fate processes and/or are autocorrelated.

- The statistical method might not be appropriate for the high dimensionality of the dataset as suggested by other studies in e.g. Kuncheva et al., 2006, García-Escudero et al., 1999).

Several recommendations for improving the analysis can be made:

- Improve the data quality by increasing the confirmation level of suspect identity and only perform analyses for a selection of identified compounds to reduce uncertainties of identification (currently 21 and 92 of the prioritized compounds have respectively a confirmed structure and a molecular formula).

- Improve the quality of data by pre-processing: select descriptors which have a very small, mutual correlation. This limits or selects descriptors which are known to influence environmental fate.

- Improve the statistical method by a heuristical method (problem solving by learning) to find the most descriptive descriptors for of the identified compounds related to their

presence in water. An approach similar to that of obtaining QSARs can be applied: (i) generate a SOM, (ii) select a training and validation set, (iii) apply genetic or other optimization routines to find a small set of most distinctive descriptors within each cluster as well as the whole data set, (iv) (cross-)validate the results.

Note that the QSAR methodology as explained in the third bullet also lends itself for relating chemical properties to ionization efficiency in the mass spectrometer (BTO project 'Hoe breed is brede screening?') or to retention time in the HPLC column (Barron, 2015).

In short, the used statistical method was not suitable to link chemicals descriptors that relate to different water types from the current dataset (as was shown for the chromatographical parameters). For future data-analyses it is recommended to increase the identity confidence and to select a smaller subset of chemical properties (expert- or data-driven).

4 Conclusion

4.1 Conclusion

In the suspect screening, data was screened for the presence of a large set of anthropogenic chemicals. The relatively fast approach for handling numerous non-target screening data shows to be complementary to currently used target-based approaches. 700 detected masses from LC-HRMS screening data were linked to one or multiple suspects. The interpretation of non-target screening data containing unknown and natural compounds is improved by the selection of the potential relevant compounds of anthropogenic origin. However, uncertainties remain for the identity of the detected suspects, and should be confirmed with detailed MS data and preferably with pure reference standards in future studies. For a selection of compounds, the prioritized compounds (BTO 2015.003), further indentification steps will be carried out. Currently, out of 158 prioritized compounds, 45 compouds were false positives (28%), 21 compounds have a confirmed structure (13%) and 92 of the prioritized compounds have a confirmed molecular formula (58%) and need further identification steps in a future project.

A clear difference between the analytical parameters (total concentration and retention time), was shown for the different water types. This result could however not be repeated with the distinctive features of the suspect data, the chemical descriptors. It should be noted that the found clusters do relate to these descriptor values. However, it is not clear whether these groups relate their occurrence in water or to a specific water type.

Based on the suspect data and the broad set of descriptors used, the applied methods (PCA and cluster analysis) did currently not contribute to better knowledge and understanding of the occurrence of chemicals in the various water types. Several reasons may explain the inability to successfully link the descriptor values to the occurrence in different water types: the false positive suspects, the incomplete dataset (negative mode samples), the heterogenic dataset, the quality of the estimated descriptor values, the descriptors itself (maybe not relevant for environmental fate) and the statistical method (not suitable for a high dimensionality dataset). For future data-analyses it is recommended to increase the identity confidence and to select a smaller subset of chemical properties (expert- or data-driven).

4.2 Future studies

Chemical datamining and prioritization techniques cope with large datasets to filter out the most relevant information on (drinking) water contaminants. Datamining and prioritization can be applied using monitoring or modelling data. Monitoring studies include target, non-target and suspect screening. Modelling studies are often based on emission data and environmental fate of chemicals. Below we list several datamining approaches for future studies.

Target screening monitoring data provides accurate en quantitative data of the occurrence of microcontaminants in water matrices. The development and implementation of target monitoring methods is time and cost consuming. However, approaches for datamining in target-screening data are straightforward.

Non-target screening data provides information about a large amount of (unknown) compounds. Targeted and non-targeted detected compounds can have mutual correlations.

Correlating chemicals give the opportunity to select chemical indicators, compounds that indicate the presence of other (related) compounds. A prioritization method could be set up to select the best chemical indicators. These compounds could be relevant for identification and for implementation in future monitoring.

Non-target screening contains numerous of chemicals, natural compounds, known and unknown compounds. One important group of chemicals is the transformation products. Recent research illustrated that transformation products and their parent compounds can be connected from non-target screening data. For influent and effluent wastewater chemicals and their transformation products were prioritized based on peak intensity, biotransformation reactions and used MS/MS data (Schollee, 2015). This approach can also be adopted tot the drinking water sector to compare infiltrated and abstracted water (dune filtrate or bank filtrate) or raw water and drinking water.

The suspect screening shows to be a useful tool for handling numerous non-target screening data. The approach quickly filters non-target data for the presence of relevant compounds. However, the identity of the detected suspects should be confirmed with detailed MS data and preferably with pure reference standards.

Modelling studies estimate the exposure of contaminants in the environment by their emissions and chemical properties. Recently, a shift is shown for chemical assessment from the Persistent Bioaccumulative and Toxic (PBT) chemicals to the more polar compounds, Persistent Mobile Organic Compounds (PMOC). For example, the German Environmental Protection Agency proposed to include the chemical risk assessment for the protection of raw water sources under the REACH legislation (Neumann, 2015). Compounds are considered persistent as defined by REACH Annex XIII: fresh water half-life > 40 days. Compounds are considered mobile if the water solubility is larger than 150 µg/L and log K_{oc} is smaller than 4.5 (Neumann, 2015). Similar approaches are shown in other studies from KWR (ter Laak, 2015) and within the research program PROMOTE (Arp, pers. comm.).

For both type of studies heuristic optimization methods (cf. QSARs) and clustering or neural network methods can be used to search for a small set of chemical descriptors that can explain occurrence in water matrices. It is recommended that the method is applied on a dataset containing compounds with confirmed identities to reduce the amount of uncertainties related to the found clusters or relationships.

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SOM toolbox software package. Version SOM Toolbox 2.0 (C) 1999

Attachment I

Suspect list

Composition of suspect list covering 5219 individual chemicals, classified per origin list.

Cas-number	Molecular Formula	Suspect
Authorized chemicals		
REACH >1000 ton		
100-00-5	C6H4ClNO2	1-chloro-4-nitrobenzene
100-02-7	C6H5NO3	4-nitrophenol
1001354-72-8	C8H19NO	3-Aminooctan-4-ol
100-20-9	C8H4Cl2O2	terephthaloyl dichloride
100-21-0	C8H6O4	terephthalic acid
1003-14-1	C5H10O	propyloxirane
1003-52-7	C5H4N2O	4-methyloxazole-5-carbonitrile
100-37-8	C6H15NO	2-diethylaminoethanol
100-40-3	C8H12	4-vinylcyclohexene
100-41-4	C8H10	ethylbenzene
100-42-5	C8H8	styrene
10042-59-8	C10H22O	2-propylheptan-1-ol
100442-33-9	C20H27NO	1-[(3,3-diphenylpropyl)(methyl)amino]-2-methyl-2-propanol
100-44-7	C7H7Cl	α-chlorotoluene
100453-11-0	C12H21NO2	Ethyl 2-cyano-2-ethyl-3-methylhexanoate
100-46-9	C7H9N	benzylamine
100-47-0	C7H5N	benzonitrile
100-51-6	C7H8O	benzyl alcohol
100-52-7	C7H6O	benzaldehyde
100-54-9	C6H4N2	nicotinonitrile
10061-01-5	C3H4Cl2	(Z)-1,3-dichloropropene
10061-02-6	C3H4Cl2	trans-1,3-Dichloropropene
100-61-8	C7H9N	N-methylaniline
100-63-0	C6H8N2	phenylhydrazine
100-66-3	C7H8O	anisole
100-68-5	C7H8S	methyl phenyl sulphide
100-69-6	C7H7N	2-vinylpyridine
100-83-4	C7H6O2	3-hydroxybenzaldehyde
1009-22-9	C8H7BrFNO	N-(2-bromo-4-fluorophenyl)acctamide
100-97-0	C6H12N4	methenamine
10097-02-6	C6H12O4	2,2-bis(hydroxymethyl)butanoic acid

101-02-0	C18H15O3P	triphenyl phosphite
10109-95-2	C20H16N2O4	2,5-dianilinoterephthalic acid
101-14-4	C13H12Cl2N2	4,4'-methylenebis[2-chloroaniline]
101-37-1	C12H15N3O3	2,4,6-triallyloxy-1,3,5-triazine
101377-47-3	C16H15F2N3Si	bis(4-fluorophenyl)methyl(4H-1,2,4-triazol-4yl-methyl)silane
1013-88-3	C13H11N	no name
101-39-3	C10H10O	α-methylcinnamaldehyde
101-43-9	C10H16O2	cyclohexyl methacrylate
101513-70-6	C7HCl2F3O	3,5-dichloro-2,4-difluorobenzoyl fluoride
101-54-2	C12H12N2	N-(4-aminophenyl)aniline
101-68-8	C15H10N2O2	4,4'-methylenediphenyl diisocyanate
101-72-4	C15H18N2	N-isopropyl-N'-phenyl-p-phenylenediamine
101-77-9	C13H14N2	4,4'-methylenedianiline
101-80-4	C12H12N2O	4,4'-oxydianiline
101-83-7	C12H23N	dicyclohexylamine
101-84-8	C12H10O	diphenyl ether
101-86-0	C15H20O	Hexylcinnamaldehyde
101990-44-7	C8H12ClN3	N-[(6-chloro-3-pyridinyl)methyl]-1,2-ethane-diamine
102-01-2	C10H11NO2	acetoacetanilide
102-06-7	C13H13N3	1,3-diphenylguanidine
102-09-0	C13H10O3	diphenyl carbonate
10221-57-5	C7H16O2	1,2-diethoxypropane
10233-13-3	C15H30O2	isopropyl laurate
102-36-3	C7H3Cl2NO	3,4-dichlorophenyl isocyanate
102387-48-4	C20H24ClN3O2	2-acetylamino-6-chloro-4-[(4-diethylamino)-2-methylphenyl-imino]-5-methyl-1-oxo-2,5-cyclohexadiene
102561-46-6	C29H41NO4S	benzyltributylammonium 4-hydroxynaphthalene-1-sulfonate
102-56-7	C8H11NO2	2,5-dimethoxyaniline
102-60-3	C14H32N2O4	1,1',1'',1'''-ethylenedinitrilotetrapropan-2-ol
102625-64-9	C16H15F2N3O3S	5-difluoromethoxy-2-[[(3,4-dimethoxy-2-pyridyl)methyl]thio]-1H-benzimidazole
102-71-6	C6H15NO3	2,2',2''-nitrilotriethanol
102-76-1	C9H14O6	triacetin
102-77-2	C11H12N2OS2	2-(morpholinothio)benzothiazole
102-82-9	C12H27N	tributylamine
10291-28-8	C22H20N2O4	2,5-bis(p-toluidino)terephthalic acid
103041-38-9	C10H14N2O2	3-(Pyridin-2-ylamino)-propionic acid ethyl ester
103-09-3	C10H20O2	2-ethylhexyl acetate
103-11-7	C11H20O2	2-ethylhexyl acrylate
103122-66-3	C8H15NO3S	O-isobutyl-N-ethoxy carbonylthiocarbamate
103201-78-1	C11H19NO2	(4S)-4-cyclohexyl-L-proline
103-23-1	C22H42O4	bis(2-ethylhexyl) adipate
10326-41-7	C3H6O3	(R)-lactic acid

103312-62-5	C14H12ClN3S	2-{[(4-chloro-3-methylpyridin-2-yl)methyl]thio}-1H-Benzimidazole.
103-34-4	C8H16N2O2S2	di(morpholin-4-yl) disulphide
103429-90-9	C8H16O3	3-Methoxy-3-methylbutyl acetate
103-50-4	C14H14O	dibenzyl ether
103577-40-8	C16H14F3N3OS	2-[[[3-Methyl-4-(2,2,2-trifluoroethoxy)-2-pyridinyl]methyl]thio]-1H-benzimidazole
103-74-2	C7H9NO	2-(2-pyridyl)ethanol
103-83-3	C9H13N	benzyldimethylamine
103953-71-5	C14H21NO2	1-[(2E)-3,7-dimethylocta-2,6-dien-1-yl]pyrrolidine-2,5-dione
104-12-1	C7H4ClNO	4-chlorophenyl isocyanate
104146-10-3	C24H23ClN2O5S	4-methoxybenzyl 3-chloromethyl-5-oxo-6-phenylacetamido-(2H)5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate
104147-32-2	C8H5Cl2F4NO	2,6-dichloro-4-amino-(1,1,2,2-tetrafluoroethoxy)benzene
104-15-4	C7H8O3S	toluene-4-sulphonic acid
10420-33-4	C8H12O5	dimethyl acetylsuccinate
10425-11-3	C13H10O3	3,4-dihydroxybenzophenone
104366-82-7	C11H18N2O2	HMDAPP
104468-21-5	C10H18O2	2,2-dimethyl 3-methyl-3-butenyl propanoate
10461-98-0	C14H15N	Peonile
104632-26-0	C10H17N3S	(S)-2-Amino-6-propylamino-4,5,6,7-tetrahydrobenzothiazole
1047-16-1	C20H12N2O2	5,12-dihydroquino[2,3-b]acridine-7,14-dione
104-75-6	C8H19N	2-ethylhexylamine
104-76-7	C8H18O	2-ethylhexan-1-ol
1048007-94-8	C15H12N4O2S	N-(2-Methyl-5-nitrophenyl)-4-(pyridin-3-yl)-1,3-thiazol-2-amine
104-83-6	C7H6Cl2	α,4-dichlorotoluene
104-88-1	C7H5ClO	4-chlorobenzaldehyde
104-93-8	C8H10O	4-methylanisole
104958-67-0	C16H22N2O3	N-butyl-2-(4-morpholinylcarbonyl)benzamide
104966-97-4	C19H30O5	10-hydroxy-1-(2-hydroxy-3,4-dimethoxy-6-methylphenyl) decan-1-one
104987-12-4	C43H69NO12	no name
105024-66-6	C25H29FO2Si	(4-ethoxyphenyl)(3-(4-fluoro-3-phenoxyphenyl)propyl)dimethylsilane
105-08-8	C8H16O2	cyclohex-1,4-ylenedimethanol
105247-17-4	C22H27NOS2	3-(3,5-di-tert-butyl-4-hydroxybenzyl)benzothiazole-2-thione
105-34-0	C4H5NO2	methyl cyanoacetate
105-39-5	C4H7ClO2	ethyl chloroacetate
10540-29-1	C26H29NO	tamoxifen
10543-57-4	C10H16N2O4	N,N'-ethylenebis[N-acetylacetamide]
105-45-3	C5H8O3	methyl acetoacetate
105-53-3	C7H12O4	diethyl malonate
105-56-6	C5H7NO2	ethyl cyanoacetate
105-59-9	C5H13NO2	2,2'-methyliminodiethanol

105-60-2	C6H11NO	ε-caprolactam
105-74-8	C24H46O4	dilauroyl peroxide
105-75-9	C12H20O4	dibutyl fumarate
105-76-0	C12H20O4	dibutyl maleate
105812-81-5	C13H18FNO	(-)-trans-4-(4'-fluorophenyl)-3-hydroxymethyl-N-methylpiperidine
105827-91-6	C4H3Cl2NS	2-chloro-5-chloromethylthiazole
10584-98-2	C28H56O4S2Sn	2-ethylhexyl 4,4-dibutyl-10-ethyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
10591-85-2	C30H28N2S4	tetrakis(phenylmethyl)thioperoxydi(carbothioamide)
10605-40-0	C5H12Cl2Si	chloro(3-chloropropyl)dimethylsilane
106-14-9	C18H36O3	12-hydroxystearic acid
106185-75-5	C14H24O	2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol
106-22-9	C10H20O	citronellol
106-23-0	C10H18O	citronellal
106-24-1	C10H18O	geraniol
106246-33-7	C21H28Cl2N2	4,4'-METHYLEN-BIS-(3-CHLOR-2,6-DIETHYLANILIN)
1062580-52-2	C14H24Cl2N2	(3R,4R)-N,4-Dimethyl-1-(phenylmethyl)-3-piperidinamine dihydrochloride
106-31-0	C8H14O3	butyric anhydride
1064076-86-3	C33H46F4N2O4S	N-Cyclohexylcyclohexanamine (2S)-4-fluoro-4-methyl-2-{[(1S)-2,2,2-trifluoro-1-{4'-(methylsulfonyl)[1,1'-biphenyl]-4-yl}ethyl]amino}pentanoate
106-42-3	C8H10	p-xylene
106-43-4	C7H7Cl	4-chlorotoluene
106-44-5	C7H8O	p-cresol
106447-44-3	C10H12N2O3S	3-(cis-1-propenyl)-7-amino-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
106461-41-0	C22H27N5O2	2,4-dihydro-4-(4-(4-(4-hydroxyphenyl)-1-piperazinyl)phenyl)-2-(1-methylpropyl-3H-1,2,4-triazol-3-one
106-46-7	C6H4Cl2	1,4-dichlorobenzene
106-47-8	C6H6ClN	4-chloroaniline
106-49-0	C7H9N	p-toluidine
106-50-3	C6H8N2	p-phenylenediamine
106-63-8	C7H12O2	isobutyl acrylate
106-65-0	C6H10O4	dimethyl succinate
1067-33-0	C12H24O4Sn	dibutyltin di(acetate)
1067-53-4	C11H24O6Si	tris(2-methoxyethoxy)vinylsilane
1067-55-6	C10H24O2Sn	dibutyldimethoxystannane
106-79-6	C12H22O4	dimethyl sebacate
106797-53-9	C12H16O4	2-hydroxy-4'-hydroxyethoxy-2-methylpropiophenone
106-88-7	C4H8O	1,2-epoxybutane
106-89-8	C3H5ClO	1-chloro-2,3-epoxypropane
106-91-2	C7H10O3	2,3-epoxypropyl methacrylate
106-92-3	C6H10O2	allyl 2,3-epoxypropyl ether

106-94-5	C3H7Br	1-bromopropane
106-97-8	C4H10	butane
106-98-9	C4H8	but-1-ene
106-99-0	C4H6	buta-1,3-diene
106990-43-6	C132H250N32	N,N',N'',N'''-tetrakis(4,6-bis(butyl-(N-methyl-2,2,6,6-tetramethylpiperidin-4-yl)amino)triazin-2-yl)-4,7-diazadecane-1,10-diamine
107-01-7	C4H8	2-butene
107-02-8	C3H4O	acrylaldehyde
107-05-1	C3H5Cl	3-chloropropene
1070-64-0	C10H18Cl2O2	ethyl 6,8-dichlorooctanoate
107-10-8	C3H9N	propylamine
1071-22-3	C3H4Cl3NSi	3-(trichlorosilyl)propiononitrile
107-13-1	C3H3N	acrylonitrile
107-18-6	C3H6O	allyl alcohol
107-19-7	C3H4O	prop-2-yn-1-ol
107-25-5	C3H6O	methyl vinyl ether
1073-69-4	C6H7ClN2	(4-chlorophenyl)hydrazine
107-41-5	C6H14O2	2-methylpentane-2,4-diol
107-43-7	C5H11NO2	betaine
107-45-9	C8H19N	1,1,3,3-tetramethylbutylamine
107-46-0	C6H18OSi2	hexamethyldisiloxane
1075-89-4	C9H13NO2	8-azaspiro[4.5]decane-7,9-dione
107-86-8	C5H8O	3-methyl-2-butenal
107-88-0	C4H10O2	butane-1,3-diol
107898-54-4	C15H26O	(+/-) trans-3,3-dimethyl-5-(2,2,3-trimethyl-cyclopent-3-en-1-yl)pent-4-en-2-ol
107-92-6	C4H8O2	butyric acid
107-94-8	C3H5ClO2	3-chloropropionic acid
107-95-9	C3H7NO2	β-alanine
107-96-0	C3H6O2S	3-mercaptopropionic acid
107-98-2	C4H10O2	1-methoxypropan-2-ol
108-01-0	C4H11NO	2-dimethylaminoethanol
108-03-2	C3H7NO2	1-nitropropane
108-05-4	C4H6O2	vinyl acetate
108-10-1	C6H12O	4-methylpentan-2-one
108-11-2	C6H14O	4-methylpentan-2-ol
108-18-9	C6H15N	diisopropylamine
108-20-3	C6H14O	diisopropyl ether
108-21-4	C5H10O2	isopropyl acetate
108-22-5	C5H8O2	isopropenyl acetate
108-24-7	C4H6O3	acetic anhydride
108-30-5	C4H4O3	succinic anhydride
108-31-6	C4H2O3	maleic anhydride
108-32-7	C4H6O3	propylene carbonate
108-38-3	C8H10	m-xylene

108-39-4	C7H8O	m-cresol
108-44-1	C7H9N	m-toluidine
108-45-2	C6H8N2	m-phenylenediamine
108-46-3	C6H6O2	resorcinol
108-55-4	C5H6O3	glutaric anhydride
108-59-8	C5H8O4	dimethyl malonate
108-65-6	C6H12O3	2-methoxy-1-methylethyl acetate
108-67-8	C9H12	mesitylene
108-68-9	C8H10O	3,5-xylenol
108-74-7	C6H15N3	hexahydro-1,3,5-trimethyl-1,3,5-triazine
108-77-0	C3Cl3N3	2,4,6-trichloro-1,3,5-triazine
108-78-1	C3H6N6	melamine
108-80-5	C3H3N3O3	cyanuric acid
108-83-8	C9H18O	2,6-dimethylheptan-4-one
108-87-2	C7H14	methylcyclohexane
108-88-3	C7H8	toluene
108-90-7	C6H5Cl	chlorobenzene
108-91-8	C6H13N	cyclohexylamine
108-93-0	C6H12O	cyclohexanol
108-94-1	C6H10O	cyclohexanone
108-95-2	C6H6O	phenol
108-98-5	C6H6S	benzenethiol
108-99-6	C6H7N	3-methylpyridine
109-09-1	C5H4ClN	2-chloropyridine
1093205-93-6	C15H21N3O2	Propanamide,3-(3-amino-2-cyanophenoxy)-2,2-dimethyl-Npropyl-
109-52-4	C5H10O2	valeric acid
109-53-5	C6H12O	isobutyl vinyl ether
109-55-7	C5H14N2	3-aminopropyldimethylamine
109-59-1	C5H12O2	2-isopropoxyethanol
109-60-4	C5H10O2	propyl acetate
109-61-5	C4H7ClO2	propyl chloroformate
109-66-0	C5H12	pentane
109-67-1	C5H10	pent-1-ene
109-69-3	C4H9Cl	1-chlorobutane
109-70-6	C3H6BrCl	1-bromo-3-chloropropane
109-72-8	C4H9Li	butyllithium
109-73-9	C4H11N	butylamine
109-75-1	C4H5N	but-3-enenitrile
109-77-3	C3H2N2	malononitrile
109-78-4	C3H5NO	3-hydroxypropiononitrile
109-83-1	C3H9NO	2-methylaminoethanol
109-86-4	C3H8O2	2-methoxyethanol
109-87-5	C3H8O2	dimethoxymethane
109-89-7	C4H11N	diethylamine

109-92-2	C4H8O	ethyl vinyl ether
109-99-9	C4H8O	tetrahydrofuran
110-00-9	C4H4O	furan
110-01-0	C4H8S	tetrahydrothiophene
110-05-4	C8H18O2	di-tert-butyl peroxide
110-12-3	C7H14O	5-methylhexan-2-one
110-15-6	C4H6O4	succinic acid
110-16-7	C4H4O4	maleic acid
110-17-8	C4H4O4	fumaric acid
110-19-0	C6H12O2	isobutyl acetate
110-25-8	C21H39NO3	(Z)-N-methyl-N-(1-oxo-9-octadecenyl)glycine
110-27-0	C17H34O2	isopropyl myristate
110-42-9	C11H22O2	methyl decanoate
110-43-0	C7H14O	heptan-2-one
110-54-3	C6H14	n-hexane
110553-27-0	C25H44OS2	4,6-bis(octylthiomethyl)-o-cresol
110-60-1	C4H12N2	tetramethylenediamine
110-62-3	C5H10O	valeraldehyde
110-63-4	C4H10O2	butane-1,4-diol
110-64-5	C4H8O2	but-2-ene-1,4-diol
110-65-6	C4H6O2	but-2-yne-1,4-diol
11070-44-3	C9H10O3	tetrahydromethylphthalic anhydride
110-71-4	C4H10O2	1,2-dimethoxyethane
11071-47-9	C8H16	isooctene
110-77-0	C4H10OS	2-(ethylthio)ethanol
110-80-5	C4H10O2	2-ethoxyethanol
110-82-7	C6H12	cyclohexane
110-83-8	C6H10	cyclohexene
110-85-0	C4H10N2	piperazine
110-86-1	C5H5N	pyridine
110-88-3	C3H6O3	1,3,5-trioxane
110-91-8	C4H9NO	morpholine
110964-79-9	C8H7NO6S	2-Nitro-4-(methylsulfonyl)benzoic acid
110-97-4	C6H15NO2	1,1'-iminodipropan-2-ol
111-11-5	C9H18O2	methyl octanoate
111-14-8	C7H14O2	heptanoic acid
111-17-1	C6H10O4S	3,3'-thiodi(propionic acid)
111-20-6	C10H18O4	sebacic acid
111-27-3	C6H14O	hexan-1-ol
111-29-5	C5H12O2	pentane-1,5-diol
111-30-8	C5H8O2	glutaral
111360-16-8	C17H36O3S	2-hexyldecyl mesylate
111-36-4	C5H9NO	butyl isocyanate
11138-60-6	C32H60O6	Decanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol octanoate

111-40-0	C4H13N3	2,2'-iminodi(ethylamine)
111-41-1	C4H12N2O	2-(2-aminoethylamino)ethanol
111-42-2	C4H11NO2	2,2'-iminodiethanol
111439-76-0	C9H22O2Si	isobutylisopropyldimethoxysilane
111453-32-8	C11H11I3N2O5	rac-5-Amino-N-(2,3-dihydroxypropyl)-2,4,6-triiodoisophthalamic acid
111-46-6	C4H10O3	2,2'-oxydiethanol
111-48-8	C4H10O2S	thiodiglycol
1115-20-4	C10H20O4	3-hydroxy-2,2-dimethylpropyl 3-hydroxy-2,2-dimethylpropionate
111-64-8	C8H15ClO	octanoyl chloride
111-65-9	C8H18	octane
111-66-0	C8H16	oct-1-ene
1116-70-7	C12H27Al	tributylaluminium
111-69-3	C6H8N2	adiponitrile
111-70-6	C7H16O	heptan-1-ol
111-71-7	C7H14O	heptanal
1117-37-9	C7H13NO2	ethyl trans-3-dimethylaminoacrylate
111-76-2	C6H14O2	2-butoxyethanol
111-77-3	C5H12O3	2-(2-methoxyethoxy)ethanol
111-78-4	C8H12	cycloocta-1,5-diene
111-81-9	C12H22O2	methyl undec-10-enoate
111-82-0	C13H26O2	methyl laurate
111-84-2	C9H20	nonane
1118-46-3	C4H9Cl3Sn	n-butyltin trichloride
111-85-3	C8H17Cl	1-chlorooctane
111-86-4	C8H19N	octylamine
111-87-5	C8H18O	octan-1-ol
111-88-6	C8H18S	octane-1-thiol
111-90-0	C6H14O3	2-(2-ethoxyethoxy)ethanol
111-91-1	C5H10Cl2O2	bis(2-chloroethoxy)methane
111-92-2	C8H19N	dibutylamine
1119-40-0	C7H12O4	dimethyl glutarate
111-96-6	C6H14O3	bis(2-methoxyethyl) ether
111974-74-4	C17H19Cl2N3S	10-(piperazin-1-yl)-2-thia-9- azatricyclo[9.4.0.0^{3,8}]pentadeca-1(15),3,5,7,9,11,13-heptaene dihydrochloride
1120-21-4	C11H24	undecane
1120-24-7	C12H27N	decyldimethylamine
1120-36-1	C14H28	tetradec-1-ene
1120-49-6	C20H43N	didecylamine
112-05-0	C9H18O2	nonanoic acid
1120-71-4	C3H6O3S	1,3-propanesultone
112-07-2	C8H16O3	2-butoxyethyl acetate
112-16-3	C12H23ClO	lauroyl chloride
112-18-5	C14H31N	dodecyldimethylamine

112-25-4	C8H18O2	2-hexyloxyethanol
112-27-6	C6H14O4	2,2'-(ethylenedioxy)diethanol
112-30-1	C10H22O	decan-1-ol
112-34-5	C8H18O3	2-(2-butoxyethoxy)ethanol
112-35-6	C7H16O4	2-(2-(2-methoxyethoxy)ethoxy)ethanol
112-38-9	C11H20O2	undec-10-enoic acid
112-39-0	C17H34O2	methyl palmitate
112-40-3	C12H26	dodecane
112-41-4	C12H24	dodec-1-ene
112-42-5	C11H24O	undecan-1-ol
112-44-7	C11H22O	undecanal
112-49-2	C8H18O4	1,2-bis(2-methoxyethoxy)ethane
112-50-5	C8H18O4	2-(2-(2-ethoxyethoxy)ethoxy)ethanol
112-53-8	C12H26O	dodecan-1-ol
112-55-0	C12H26S	dodecane-1-thiol
112-61-8	C19H38O2	methyl stearate
112-67-4	C16H31ClO	palmitoyl chloride
112-69-6	C18H39N	hexadecyldimethylamine
1127-01-1	C9H16O3	no name
112-72-1	C14H30O	tetradecanol
112-75-4	C16H35N	dimethyl(tetradecyl)amine
112-76-5	C18H35ClO	stearoyl chloride
1128026-41-4	C12H30O3SSi2	3,3-dimethoxy-8,8,9,9-tetramethyl-2-oxa-7-thia-3,8-disiladecane
112-84-5	C22H43NO	Amides, C22 (unsaturated)
112-85-6	C22H44O2	docosanoic acid
112-88-9	C18H36	octadec-1-ene
112-91-4	C18H33N	oleonitrile
112-92-5	C18H38O	octadecan-1-ol
1132-95-2	C12H24O2	1,1-diisopropoxycyclohexane
1134-94-7	C12H11NS	2-phenylthioaniline
1135-22-4	C10H18O3S	3-Thiophenebutanol, 2,5-dihydro-a,a-dimethyl-, 1,1-dioxide
114772-54-2	C14H10BrN	4'-Bromomethylbiphenyl-2-carbonitrile
114798-26-4	C22H20ClN6O	Losartan
115-07-1	C3H6	propene
115-11-7	C4H8	2-methylpropene
115-19-5	C5H8O	2-methylbut-3-yn-2-ol
115-27-5	C9H2Cl6O3	1,4,5,6,7,7-hexachloro-8,9,10-trinorborn-5-ene-2,3-dicarboxylic anhydride
115-77-5	C5H12O4	pentaerythritol
115-84-4	C9H20O2	2-butyl-2-ethylpropanediol
115-86-6	C18H15O4P	triphenyl phosphate
115895-09-5	C26H40Cl2O5	ethyl 3,5-dichloro-4-hexadecyloxycarbonyloxybenzoate
115-95-7	C12H20O2	linalyl acetate

115-96-8	C6H12Cl3O4P	tris(2-chloroethyl) phosphate
116-02-9	C9H18O	3,3,5-trimethylcyclohexanol
116091-63-5	C10H13NO4S	2-methoxy-5-(2-oxopropyl)benzenesulfonamide
116-15-4	C3F6	hexafluoropropene
1163-19-5	C12Br10O	bis(pentabromophenyl) ether
116-37-0	C21H28O4	1,1'-isopropylidenebis(p-phenyleneoxy)dipropan-2-ol
1164-92-7	C21H32O3	17 beta-Acetoxy-5 alpha-androstan-3-one
116817-12-0	C21H23NO5S	N,N-dimethyl-3-(1-naphthyloxy)-3-(2-thienyl)propan-1-amine oxalate
117-08-8	C8Cl4O3	tetrachlorophthalic anhydride
1172131-64-4	C21H27FN4O4	2-(2-aminopropan-2-yl)-4-[(4-fluorobenzyl)carbamoyl]-1-methyl-6-oxo-1,6-dihydropyrimidin-5-yl 2,2-dimethylpropanoate
117-21-5	C8H3ClO3	3-chlorophthalic anhydride
1174050-26-0	C42H34O16	(3R,3aR,6R,6aR)-6-[(4-{[4-(acryloyloxy)benzoyl]oxy}-3-methoxybenzoyl)oxy]hexahydrofuro[3,2-b]furan-3-yl 4-{[4-(acryloyloxy)benzoyl]oxy}-3-methoxybenzoate
117570-53-3	C17H14O4	(5,6-Dimethyl-9-oxo-9H-xanthen-4-yl)acetic acid
117570-93-1	C17H16O5	2-[2-(carboxymethyl)phenoxy]-3,4-dimethylbenzoic acid
117-81-7	C24H38O4	bis(2-ethylhexyl) phthalate
117827-06-2	C24H39Cl2NO2	3',5'-dichloro-4'-ethyl-2'-hydroxypalmitanilide
117829-74-0	C5H14ClNO	3-(dimethylamino)-1-propanol hydrochloride
1180558-15-9	C15H11F3KNO4	potassium (2R)-2-[4-[[5-trifluoromethyl-2-pyridinyl]oxy]phenoxy]propanoate
118135-28-7	C13H23ClO2	2-Chlormethyl-8-(1,1-dimethylethyl)-1,4-dioxaspiro[4.5]decan
118-45-6	C8H3ClO3	4-chlorophthalic anhydride
1184648-08-5	C9H9KO4	potassium (R)-2-(4-hydroxy-phenoxy)-propionate
1184-85-6	C2H7NO2S	sulfonamide derivative
118-48-9	C8H5NO3	4H-3,1-benzoxazine-2,4(1H)-dione
1185-55-3	C4H12O3Si	trimethoxy(methyl)silane
1185-81-5	C32H68S2Sn	dibutylbis(dodecylthio)stannane
118-75-2	C6Cl4O2	tetrachloro-p-benzoquinone
1187-74-2	C11H18O5	diethyl 4-oxopentane-1,2-dicarboxylate
118-79-6	C6H3Br3O	2,4,6-tribromophenol
118-96-7	C7H5N3O6	2,4,6-trinitrotoluene
119018-29-0	C16H21N3O4S	4-(2-((3-ethyl-4-methyl-2-oxo-pyrrolin-1-yl)carboxamido)ethyl)benzenesulfonamide)
119313-12-1	C23H30N2O2	2-benzyl-2-dimethylamino-4'-morpholinobutyrophenone
1193-21-1	C4H2Cl2N2	4,6-dichloropyrimidine
1193-24-4	C4H4N2O2	6-hydroxy-1H-pyrimidin-4-one
119-36-8	C8H8O3	methyl salicylate
119-47-1	C23H32O2	6,6'-di-tert-butyl-2,2'-methylenedi-p-cresol
119-53-9	C14H12O2	benzoin
119-56-2	C13H11ClO	4-chlorobenzhydryl alcohol
119-61-9	C13H10O	benzophenone

119-64-2	C10H12	1,2,3,4-tetrahydronaphthalene
119-65-3	C9H7N	isoquinoline
119738-06-6	C21H19ClN2O5	(±) tetrahydrofurfuryl (R)-2-[4-(6-chloroquinoxalin-2-yloxy)phenyloxy]propionate
119851-28-4	C14H10Cl2O2	1-[2-chloro-4-(4-chlorophenoxy)phenyl]ethanone
119895-68-0	C8H4F2O3	2,2-difluoro-benzo[1,3]dioxole-4-carbaldehyde
120118-14-1	C11H8ClN3	5-chloro-4-(4-methylphenyl)-1H-imidazole-2-carbonitrile
120-12-7	C14H10	anthracene
1201-31-6	C7H2F4O2	Tetrafluorbenzoesäure
120279-88-1	C8H9NO3S3	6-methyl-4-oxo-5,6-dihydro-4H-thieno[2,3-b]thiopyran-2-sulfonamide
1203-17-4	C14H20	1,1,2,3,3-pentamethylindan
120-55-8	C18H18O5	oxydiethylene dibenzoate
120-61-6	C10H10O4	dimethyl terephthalate
120-71-8	C8H11NO	6-methoxy-m-toluidine
12075-68-2	C6H15Al2Cl3	triethyldialuminium trichloride
1207628-34-9	C10H15NO3	Methyl (3aR,7aR)-4-oxooctahydro-1Hindole-1-carboxylate
120-78-5	C14H8N2S4	di(benzothiazol-2-yl) disulphide
120-80-9	C6H6O2	pyrocatechol
120-82-1	C6H3Cl3	1,2,4-trichlorobenzene
120-83-2	C6H4Cl2O	2,4-dichlorophenol
120-92-3	C5H8O	cyclopentanone
120983-72-4	C5H6Cl2O	JAU 6476-Chlormethylketon
121-03-9	C7H7NO5S	4-nitrotoluene-2-sulphonic acid
12108-13-3	C9H7MnO3	tricarbonyl(methylcyclopentadienyl)manganese
121158-58-5	C16H26O	Phenol, dodecyl-, branched
121-17-5	C7H3ClF3NO2	4-chloro-α,α,α-trifluoro-3-nitrotoluene
121219-07-6	C8H8F2O	1-ethoxy-2,3-difluorobenzene
121240-56-0	C16H37F2P	Tetrabutylphosphonium hydrogen difluoride
121-33-5	C8H8O3	vanillin
121-44-8	C6H15N	triethylamine
121451-05-6	C9H4Cl2F7NO	3,5-dichloro-2-fluoro-4-(1,1,2,3,3,3-hexafluoropropoxy)aniline
121-86-8	C7H6ClNO2	2-chloro-4-nitrotoluene
121-91-5	C8H6O4	isophthalic acid
1220100-43-5	C18H34Cl2F8N2O4	N,N'-bis[2-hydroxy-3-(2,2,3,3-tetrafluoropropoxy)propyl]-N,N,N',N'-tetramethylethane-1,2-diaminium dichloride
122-09-8	C10H15N	phentermine
122-20-3	C9H21NO3	1,1',1''-nitrilotripropan-2-ol
1222-05-5	C18H26O	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyran
122-39-4	C12H11N	diphenylamine
12239-87-1	C32H15ClCuN8	copper chlorophthalocyanine
122-51-0	C7H16O3	triethyl orthoformate
122-52-1	C6H15O3P	triethyl phosphite

122586-52-1	C44H84N2O6	bis(2,2,6,6-tetramethyl-1-octyloxypiperidin-4-yl)-1,10-decanedioate
122-60-1	C9H10O2	2,3-epoxypropyl phenyl ether
122731-58-2	C11H12N2O7	rac-N-(2,3-Dihydroxypropyl)-5-nitroisophthalamic acid
122731-59-3	C15H15I3N2O7	rac-5-Amino-N-(2,3-diacetoxypropyl)-2,4,6-triiodoisophthalamic acid
122-79-2	C8H8O2	phenyl acetate
1229457-94-6	C8H12IN3	4-(4-Iodo-1H-pyrazol-1-yl)piperidine
122-99-6	C8H10O2	2-phenoxyethanol
123-05-7	C8H16O	2-ethylhexanal
123-30-8	C6H7NO	4-aminophenol
123-31-9	C6H6O2	hydroquinone
123-35-3	C10H16	7-methyl-3-methyleneocta-1,6-diene
123-38-6	C3H6O	propionaldehyde
123-42-2	C6H12O2	4-hydroxy-4-methylpentan-2-one
123-51-3	C5H12O	3-methylbutan-1-ol
1235-23-0	C21H19ClO	2-chloroethyl trityl ether
123-54-6	C5H8O2	pentane-2,4-dione
123-62-6	C6H10O3	propionic anhydride
123-72-8	C4H8O	butyraldehyde
123-86-4	C6H12O2	n-butyl acetate
123-91-1	C4H8O2	1,4-dioxane
123-92-2	C7H14O2	isopentyl acetate
123-96-6	C8H18O	octan-2-ol
123968-25-2	C37H56O3	2-(1-(2-hydroxy-3,5-di-tert-pentyl-phenyl)ethyl)-4,6-di-tert-pentylphenyl acrylate
123989-29-7	C12H13ClO	1-(4-chlorophenyl)-2-cyclopropylpropan-1-one
123989-31-1	C11H13ClO	1-(4-chloro-phenyl)-2-methyl-but-3-en-1-ol
123-99-9	C9H16O4	azelaic acid
124-04-9	C6H10O4	adipic acid
124-07-2	C8H16O2	octanoic acid
124-09-4	C6H16N2	hexamethylenediamine
124-10-7	C15H30O2	methyl myristate
124-13-0	C8H16O	octanal
124172-53-8	C26H50N4O2	N,N'-1,6-hexanediylbis(N-(2,2,6,6-tetramethyl-piperidin-4-yl)formamide
124-17-4	C10H20O4	2-(2-butoxyethoxy)ethyl acetate
124-18-5	C10H22	decane
1241-94-7	C20H27O4P	2-ethylhexyl diphenyl phosphate
124-22-1	C12H27N	dodecylamine
124-28-7	C20H43N	dimantine
124-30-1	C18H39N	octadecylamine
1246610-75-2	C18H22ClN5O2	2-({6-[(3R)-3-Aminopiperidin-1-yl]-3-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl}methyl)benzonitrile hydrochloride
124-68-5	C4H11NO	2-amino-2-methylpropanol
124-70-9	C3H6Cl2Si	dichloro(methyl)(vinyl)silane

124750-51-2	C33H25BrN4	5-[4'-(bromomethyl)biphenyl-2-yl]-1-trityl-1H-tetrazole
124832-31-1	C21H26N6O6	2-[(2-amino-6-oxo-3,6-dihydro-9H-purin-9-yl)methoxy]ethyl N-[(benzyloxy)carbonyl]-L-valinate
125109-85-5	C13H18O	β-methyl-3-(1-methylethyl)benzenepropanal
125-12-2	C12H20O2	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate
12567-73-6	C16H28O8Zr	Tetrakis(isobutyrato)zirconium
125700-67-6	C11H16BF4N5O	2-(1-H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate
12578-12-0	C36H70O6Pb3	dioxobis(stearato)trilead
125971-57-5	C19H19NO2	2-Isobutyryl-3,N-diphenylacrylamide
125971-95-1	C40H47FN2O5	(4R,6R)-6-[2-[2-(4-fluorophenyl)-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-1H-pyrrol-1-yl]ethyl]-2,2-dimethyl-1,3-Dioxane-4-acetic acid 1,1-dimethylethyl ester
126-30-7	C5H12O2	2,2-dimethylpropane-1,3-diol
126-33-0	C4H8O2S	tetrahydrothiophene 1,1-dioxide
12645-31-7	C8H19O4P	Phosphoric acid, 2-ethylhexyl ester
126-58-9	C10H22O7	2,2,2',2'-tetrakis(hydroxymethyl)-3,3'-oxydipropan-1-ol
1266664-66-7	C13H17Cl2N3O	(7R)-4-(5-Chloro-1,3-benzoxazol-2-yl)-7-methyl-1,4-diazepan-1-ium chloride
126-73-8	C12H27O4P	tributyl phosphate
126-81-8	C8H12O2	5,5-dimethylcyclohexane-1,3-dione
126-98-7	C4H5N	methacrylonitrile
126990-35-0	C12H24O2Si	dicyclopentyldimethoxysilane
126-99-8	C4H5Cl	2-chlorobuta-1,3-diene
127-06-0	C3H7NO	acetone oxime
1271488-66-4	C12H20O3	methyl trans-3-oxo-2-pentylcyclopentanecarboxylate
127-19-5	C4H9NO	N,N-dimethylacetamide
127474-91-3	C28H40O4	CORAPAN TQ
127-47-9	C22H32O2	retinyl acetate
128275-31-0	C14H15NO5	6-(phthalimido)peroxyhexanoic acid
128-37-0	C15H24O	2,6-di-tert-butyl-p-cresol, BHT
128-39-2	C14H22O	2,6-di-tert-butylphenol
128-44-9	C7H5NO3S	1,2-benzisothiazol-3(2H)-one 1,1-dioxide
128-69-8	C24H8O6	perylene-3,4:9,10-tetracarboxylic dianhydride
128740-14-7	C14H20N2	6-benzyloctahydro-1H-pyrrolo[3,4-b]pyridine
129-00-0	C16H10	pyrene
129423-54-7	C17H13CaClN4O7S2	calcium 4-chloro-2-(5-hydroxy-3-methyl-1-(3-sulfonatophenyl)pyrazol-4-ylazo)-5-methylbenzenesulfonate
129738-34-7	C19H34	trans-4-pentyl-trans-4'-vinylbicyclohexyl
129909-90-6	C10H19N5O2	4-amino-N-(1,1-dimethylethyl)-4,5-dihydro-3-(1-methylethyl)-5-oxo-1H-1,2,4-triazole-1-carboxamide
13014-24-9	C7H3Cl5	1,2-dichloro-4-(trichloromethyl)benzene
130198-05-9	C15H24ClNO2	1-[2-amino-1-(4-methoxyphenyl)ethyl]cyclohexan-1-ol hydrochloride

13031-41-9	C9H7NO2	4-cyanophenyl acetate
13048-33-4	C12H18O4	hexamethylene diacrylate
13051-49-5	C7H11ClO3	2-chloro-3-oxopentyl acetate
130603-71-3	C33H40O21	2-(3,4-Dihydroxyphenyl)-5,7-dihydroxy-4-oxo-4H-chromen-3-yl 6-deoxy-α-L-mannopyranosyl-(1->6)-[α-D-glucopyranosyl-(1->4)]-β-D-glucopyranoside
13076-17-0	C6H8O4	(3R,6R)-3,6-Dimethyl-1,4-dioxane-2,5-dione
130841-23-5	C9H3Cl2F6NO3	1,4-dichloro-2-(1,1,2,3,3,3-hexafluoropropoxy)-5-nitrobenzene
131-11-3	C10H10O4	dimethyl phthalate
13115-71-4	C7H13N3O4	(2S)-5-amino-2-[(aminoacetyl)amino]-5-oxopentanoic acid
131-17-9	C14H14O4	diallyl phthalate
13122-18-4	C13H26O3	tert-butyl 3,5,5-trimethylperoxyhexanoate
13127-18-9	C37H68N2O13	(3R,4S,5S,6R,7R,9R,10E,11S,12R,13S,14R)-6-{[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyltetrahydro-2Hpyran-2-yl]oxy}-14-ethyl-7,12,13-trihydroxy-10-(hydroxyimino)-4-{[(2R,4R,5S,6S)-5-hydroxy-4-methoxy-4,6-dimethyltetrahydro-2H-pyran-2-yl]oxy}-3,5,7,9,11,13-hexamethyloxacyclotetradecan-2-one
13162-05-5	C3H5NO	N-vinylformamide
131860-97-4	C15H13ClN2O4	methyl (2E)-2-{2-[(6-chloropyrimidin-4-yl)oxy]phenyl}-3-methoxyprop-2-enoate
1319-77-3	C7H8O	cresol
1321-12-6	C7H7NO2	nitrotoluene
13222-26-9	C4H6Cl2O	2-chloro-2-methylpropanoyl chloride
13223-43-3	C7H9N5O2	5,7-Dimethoxy[1,2,4]triazolo[1,5-a]pyrimidin-2-amine
132335-44-5	C9H15NOS	(1S)-3-(dimethylamino)-1-(thiophen-2-yl)propan-1-ol
132335-47-8	C21H23NO5S	(3S)-N,N-dimethyl-3-(naphthalen-1-yloxy)-3-(thiophen-2-yl)propan-1-amine ethanedioate
132900-75-5	C35H36O10	2-methylbenzene-1,4-diyl bis{4-[4-(acryloyloxy)butoxy]benzoate}
1330-20-7	C8H10	xylene
133047-57-1	C24H24Cl2N6O8S2	3,10-bis[(2-aminopropyl)amino]-6,13-dichloro[1,4]benzoxazino[2,3-b]phenoxazine-4,11-disulfonic acid
1330-78-5	C21H21O4P	tris(methylphenyl) phosphate
1333488-95-1	C12H7F2NO4	methyl (2E)-2-cyano-3-(2,2-difluoro-1,3-benzodioxol-4-yl)prop-2-enoate
13349-82-1	C8H18N2O2	1-[2-(2-Hydroxyethoxy)-ethyl]-piperazine
1335-46-2	C14H22O	Ionone, methyl-
13361-34-7	C11H19NO2	2-ethylhexyl cyanoacetate
1338-23-4	C8H14O4	2-Butanone, peroxide
1338-24-5	C10H18O2	Naphthenic acids
133865-89-1	C17H19FN2O2	(S)-2-(4-(3-Fluorbenzyl)oxobenzyl)aminopropanamid
133909-99-6	C41H37ClN6O	2-butyl-4-chloro-4,5-dihydro-5-hydroxymethyl-1-[2'-(2-triphenylmethyl-1,2,3,4-2H-tetrazol-5-yl)-1,1'-biphenyl-4-methyl]-1H-imidazole

134-32-7	C10H9N	1-naphthylamine
134568-16-4	C8H8O3S	methyl 3-oxo-3-(thiophen-2-yl)propanoate
134620-00-1	C2H14N4O6Pd	Tetraamminepalladiumdihydrogencarbonate
13463-40-6	C5FeO5	pentacarbonyliron
13463-41-7	C10H8N2O2S2Zn	pyrithione zinc
134652-60-1	C13H26O2Si	tripropan-2-ylsilyl 2-methylprop-2-enoate
13466-78-9	C10H16	3,7,7-trimethylbicyclo[4.1.0]hept-3-ene
13475-82-6	C12H26	Hydrocarbons, C4, 1,3-butadiene-free, polymd., triisobutylene fraction, hydrogenated
13482-23-0	C7H12O2	4-Methoxycyclohexanon
135-19-3	C10H8O	2-naphthol
135-57-9	C26H20N2O2S2	N,N'-dithiodi-o-phenylenedibenzamide
135590-91-9	C16H18Cl2N2O4	MEFENPYRDIETHYL, diethyl 1-(2,4-dichlorophenyl)-5-methyl-4,5-dihydro-1H-pyrazole-3,5-dicarboxylate
135-61-5	C18H15NO2	3-hydroxy-2'-methyl-2-naphthanilide
135861-56-2	C24H30O6	1,3:2,4-bis-O-(3,4-dimethylbenzylidene)-D-glucitol
136210-30-5	C29H50N2O8	tetraethyl N,N'-(methylenedicyclohexane-4,1-diyl)bis-DL-aspartate
136210-32-7	C31H54N2O8	bis(4-(1,2-bis(ethoxycarbonyl)ethylamino)-3-methylcyclohexyl)methane
136-23-2	C18H36N2S4Zn	zinc bis(dibutyldithiocarbamate)
13636-02-7	C9H15NOS	3-(Dimethylamino)-1-(2-thienyl)-1-propanol
136465-81-1	C14H26N2O	(3S,4aS,8aS)-Ntertbutyldecahydroisoquinoline-3-carboxamide
136522-17-3	C24H39N3O2	(3S,4aS,8aS)-2-[(2R,3S)-3-amino-2-hydroxy-4-phenylbutyl]-N-tert-butyldecahydroisoquinoline-3-carboxamide
13674-84-5	C9H18Cl3O4P	tris(2-chloro-1-methylethyl) phosphate
13674-87-8	C9H15Cl6O4P	tris[2-chloro-1-(chloromethyl)ethyl] phosphate
136890-21-6	C22H40O3	(±)-3-hexyl-5,6-dihydro-4-hydroxy-6-undecyl-2H-Pyran-2-one
137-26-8	C6H12N2S4	thiram
137281-39-1	C15H14N4O3	4-[2-(2-amino-4,7-dihydro-4-oxo-3H-pyrrolo[2,3-d]pyrimidin-5-yl)ethyl]benzoic acid
137-30-4	C6H12N2S4Zn	ziram
137309-88-7	C16H18O5S	2-(2-methoxyphenoxy)ethyl 4-toluenesulfonate
137-32-6	C5H12O	2-methylbutan-1-ol
13752-51-7	C9H16N2O2S2	4-[(morpholinothio)thioxomethyl]morpholine
137796-06-6	C11H23NO	4-ethyl-2-methyl-2-isopentyl-1,3-oxazolidine
137863-20-8	C31H35N5O3	PBS859DS
138113-08-3	C13H11NO	(7-methoxynaphthalen-1-yl)acetonitrile
13822-56-5	C6H17NO3Si	3-(trimethoxysilyl)propylamine
138401-24-8	C25H27N3O	4'-((2-butyl-4-oxo-1,3-diazaspiro[4.4]non-1-ene-3-yl)methyl)(1,1'-biphenyl)-2-carbonitrile
138526-69-9	C6H2BrF3	1-bromo-3,4,5-trifluorobenzene
138679-81-9	C15H21F	1-fluoro-3-(trans-4-propylcyclohexyl)benzene
138776-88-2	C52H56O6P2	Biphosphite
13893-53-3	C6H12N2	2-amino-2,3-dimethylbutanenitrile
139122-17-1	C17H14ClNO3	2-(3-chloro-2-oxo-2,3-dihydro-1H-indol-4-yl) ethyl benzoate

139-13-9	C6H9NO6	nitrilotriacetic acid
139147-73-2	C10H18Cl2Si	Dichlorodicyclopentylsilane
139189-30-3	C38H40O8P2	Tetrakis(2,6-dimethylphenyl) 1,3-phenylene phosphate
139306-10-8	C10H15NO	Dimetol
139-40-2	C9H16ClN5	propazine
13940-94-8	C7H5Cl3	4-chloro-1-(dichloromethyl)benzene
139504-68-0	C14H28O2	1-[(2-tert-butylcyclohexyl)oxy]butan-2-ol
13963-57-0	C15H21AlO6	aluminium tris(2,4-pentanedionato-O,O')
140-11-4	C9H10O2	benzyl acetate
14024-48-7	C10H14CoO4	cobalt(II) 4-oxopent-2-en-2-olate
140-29-4	C8H7N	phenylacetonitrile
140-31-8	C6H15N3	2-piperazin-1-ylethylamine
140391-39-5	C17H16N4O6	PRNIBA
140623-89-8	C5H3BCl2F5N	2,6-dichloro-1-fluoropyridiniumtetrafluoroborate
140-66-9	C14H22O	4-(1,1,3,3-tetramethylbutyl)phenol
140-88-5	C5H8O2	ethyl acrylate
140921-24-0	C56H108N6O8	1,6-hexanediyl-bis(2-(2-(1-ethylpentyl)-3-oxazolidinyl)ethyl)carbamate
141-02-6	C20H36O4	bis(2-ethylhexyl) fumarate
141-05-9	C8H12O4	diethyl maleate
141-10-6	C13H20O	6,10-dimethylundeca-3,5,9-trien-2-one
141-27-5	C10H16O	(E)-3,7-dimethylocta-2,6-dienal
141-32-2	C7H12O2	butyl acrylate
141-57-1	C3H7Cl3Si	trichloro(propyl)silane
141573-95-7	C8H10F2N2O2	Ethyl 3-difluoromethyl-1-methyl-4-pyrazole carboxylate
141645-16-1	C19H17NO5	(2-Butyl-5-nitro-1-benzofuran-3-yl)(4-hydroxyphenyl)methanone
141645-23-0	C30H40N2O5	(2-butyl-5-nitrobenzofuran-3-yl)[4-(3-dibutylaminopropoxy)phenyl]methanone
141773-73-1	C17H32O3	2-(1-(3',3'-dimethyl-1'-cyclohexyl)ethoxy)-2-methyl propyl propanoate
141-78-6	C4H8O2	ethyl acetate
141-79-7	C6H10O	4-methylpent-3-en-2-one
141818-73-7	C18H22N2O4S	allyl (2S,4S)-4-benzoylsulfanyl-2-(dimethylcarbamoyl)pyrrolidine-1-carboxylate
141-97-9	C6H10O3	ethyl acetoacetate
14214-31-4	C4H4ClNS	2-Chlor-3-isothiocyanato-1-propene
142-16-5	C20H36O4	bis(2-ethylhexyl) maleate
142-19-8	C10H18O2	allyl heptanoate
142-22-3	C12H18O7	diallyl 2,2'-oxydiethyl dicarbonate
142-29-0	C5H8	cyclopentene
1424-00-6	C20H32O2	mesterolone
14246-53-8	C10H19NO3	N-(1-oxooctyl)glycine
14264-16-5	C36H30Cl2NiP2	bis(triphenylphosphine)nickel(II) chloride
142653-61-0	C9H15NO	3-(cis-3-hexenyloxy)propanenitril
142770-42-1	C16H13ClO2S	1-chloro-4-(n-propoxy)-5-thioxanthen-10-one

142-82-5	C7H16	heptane
142-84-7	C6H15N	dipropylamine
142-90-5	C16H30O2	dodecyl methacrylate
142-91-6	C19H38O2	isopropyl palmitate
14302-13-7	C32Br6Cl10CuN8	[1,3,8,16,18,24-hexabromo-2,4,9,10,11,15,17,22,23,25-decachloro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]copper
143-07-7	C12H24O2	lauric acid
143-08-8	C9H20O	nonan-1-ol
143183-03-3	C31H22N4O2S3	S-1,3-benzothiazol-2-yl (2Z)-(2-amino-1,3-thiazol-4-yl)[(trityloxy)imino]ethanethioate
143-22-6	C10H22O4	2-(2-(2-butoxyethoxy)ethoxy)ethanol
14324-55-1	C10H20N2S4Zn	zinc bis(diethyldithiocarbamate)
143-28-2	C18H36O	(Z)-octadec-9-enol
143-29-3	C17H36O6	bis(2-(2-butoxyethoxy)ethoxy)methane
143418-49-9	C6H4BF3O2	3,4,5-Trifluorophenylboronic acid
1435-71-8	C13H11N3O3	2-[(o-nitrophenyl)azo]-p-cresol
143860-04-2	C11H23NO	3-ethyl-2-methyl-2-(3-methylbutyl)-1,3-oxazolidine
143878-20-0	C23H18N2O2	6-N-Phthalimidomethyl-6,11-dihydro-5H-dibenz[b,e]azepine
144020-22-4	C17H26O	Reaction products of acetic anhydride and 1,5,10-trimethyl-1,5,9-cyclodecatriene
144333-84-6	C9H12N6O2	1,1'-(1,3-dioxolane-2,2-diyldimethanediyl)bis(1H-1,2,4-triazole)
14433-76-2	C12H25NO	N,N-dimethyldecan-1-amide
144377-42-4	C4H5F5	1,1,1,3,3-pentafluorobutane
144447-11-0	C20H22O5	4-methoxyphenyl-4(5,6-epoxyhexyloxy)benzoate
144-83-2	C11H11N3O2S	Sulfapyridine
144900-34-5	C11H10Cl2O2	4-(2,2-dichlorocyclopropyl)phenyl acetate
145641-35-6	C16H22ClNO2	Benzyl (2S,3aR,7aS)-octahydro-1H-indole-2-carboxylate hydrochloride
145783-14-8	C7H7Cl2N3O2S	4,6-dichloro-5-nitro-2-(propylthio)pyrimidine
1461-22-9	C12H27ClSn	tributyltin chloride
1461-25-2	C16H36Sn	tetrabutyltin
146805-74-5	C4H7FO2	Methyl (R)-2-fluoropropanoate
14691-89-5	C11H21N2O2	AA-TEMPO
147086-81-5	C7H6OS2	trans-(4S,6S)-5,6-dihydro-6-methyl-4H-thieno[2,3-b]thiopyran-4-ol, 7,7-dioxide
147-14-8	C32H16CuN8	29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32 copper
147200-03-1	C10H14N2O5S3	(S,S)-trans-4-(acetylamino)-5,6-dihydro-6-methyl-7,7-dioxo-4H-thieno[2,3-b]thiopyran-2-sulfonamide
14726-36-4	C30H28N2S4Zn	zinc bis(dibenzyldithiocarbamate)
147315-50-2	C27H27N3O2	2-(4,6-diphenyl-1,3,5-triazin-2-yl)-5-((hexyl)oxy)phenol
1477-55-0	C8H12N2	m-phenylenebis(methylamine)
147770-06-7	C29H40N2O4	2-Ethoxy-4-{3-[(S)-3-methy-1-(2-piperidin-1-yl-phenyl)-butylamino]-2-oxo-propyl}-benzoic acid ethyl ester

147783-69-5	C31H48N2O5	bis(1,2,2,6,6-pentamethyl-4-piperidinyl) 2-(4-methoxybenzylidene)malonate
14818-35-0	C12H16O2	6-cyclohexyl-4-methyl-2H-pyran-2-one
148348-13-4	C16H32N2O	isobutylidene-(2-(2-isopropyl-4,4-dimethyloxazolidine-3-yl)-1,1-dimethylethyl)amine
148528-05-6	C9H22N2	2-Methyloctane-1,8-diamine
1490-04-6	C10H20O	DL-menthol
14907-27-8	C12H15ClN2O2	methyl (2R)-2-amino-3-(1H-indol-3-yl)propanoate hydrochloride
149-30-4	C7H5NS2	benzothiazole-2-thiol
149-57-5	C8H16O2	2-ethylhexanoic acid
149-73-5	C4H10O3	trimethyl orthoformate
15022-08-9	C7H10O3	diallyl carbonate
1506-02-1	C18H26O	tonalide (AHTN)
150-76-5	C7H8O2	mequinol
150-78-7	C8H10O2	1,4-dimethoxybenzene
150928-21-5	C18H18ClI3N2O8	rac-3-(2,3-Diacetoxypropylcarbamoyl)-2,4,6-triiodo-5-methoxyacetylaminobenzoyl chloride
151012-31-6	C15H18BrClN2O	[1-(4-bromobenzyl)-2-butyl-4-chloro-1H-imidazol-5-yl]methanol
151213-15-9	C20H21F2N3O3	7-[(4aS,7aS)-1,2,4a,5,7,7a-hexahydropyrrolo[3,4-b]pyridin-6-yl]-1-cyclopropyl-6,8-difluoro-4-oxo-3H-quinoline-3-carboxylic acid
15121-89-8	C12H12O3	E-ethyl-4-oxo-4-phenylcrotonate
15214-89-8	C7H13NO4S	2-acrylamido-2-methylpropanesulphonic acid
152402-98-7	C14H12N4O2S	2-[(3-methyl-4-nitropyridin-2-yl)methylsulfanyl]-1H-benzimidazole
152628-03-0	C12H14N2O2	4-Methyl-2-propylbenzimidazole-6-carboxylic acid
152827-98-0	C32H48ClN5O3	218 DO
15290-77-4	C5H3F7	1,1,2,2,3,3,4-Heptafluorocyclopentane
152-97-6	C22H29FO4	fluocortolone
153-00-4	C20H30O2	metenolone
15307-93-4	C12H9Cl2N	2,6-dichloro-N-phenylaniline
15308-01-7	C14H10Cl3NO	2-chloro-N-(2,6-dichlorophenyl)-N-phenylacetamide
15356-60-2	C10H20O	(+)-menthol
153719-38-1	C4H8N4O3	N-Nitro-N-(3-methyl-3,6-dihydro-2H-1,3,5-oxadiazin-4-yl)amine
154279-60-4	C21H42N2	4,4'-methylenebis(N-sec-butylcyclohexamine)
15448-47-2	C3H6O	(2R)-2-Methyloxirane
154702-15-5	C44H59N7O5	Bis(2-ethylhexyl) 4,4’-{6-[4-tert-butylcarbamoyl)anilino]-1,3,5-triazine-2,4-diyldiimino}dibenzoate
154825-97-5	C11H13BrO2	2-(4-bromophenyl)-2-methylpropionic acid methyl ester
155041-85-3	C21H30	(trans(trans))-4'-vinyl-4-(4-methylphenyl)bicyclohexyl
15546-11-9	C18H28O8Sn	methyl (Z,Z)-8,8-dibutyl-3,6,10-trioxo-2,7,9-trioxa-8-stannatrideca-4,11-dien-13-oate
1555-62-0	C18H33N3	3,3'-(dodecylimino)dipropanenitrile
155601-30-2	C5H12N4O5S	1-(2-hydroxyethyl)-1H-pyrazol-4,5-diyldiammoniumsulfate

15571-58-1	C36H72O4S2Sn	2-ethylhexyl 10-ethyl-4,4-dioctyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
15625-89-5	C15H20O6	2-ethyl-2-[[(1-oxoallyl)oxy]methyl]-1,3-propanediyl diacrylate
156366-26-6	C27H29NO4	ethyl 3-oxo-4-(2-(tritylamino)ethoxy)butanoate
156-43-4	C8H11NO	p-phenetidine
156572-81-5	C15H29NaO5S	Sodium 2-(dodecanoyloxy)propane-1-sulfonate
15667-63-7	C6H7NO2	1-cyanoallyl acetate
156755-23-6	C15H11BrO2	6-Bromo-3,4-dihydro-4-phenyl-2H-1-benzopyran-2-one
15687-27-1	C13H18O2	ibuprofen
156-87-6	C3H9NO	3-aminopropan-1-ol
1569-01-3	C6H14O2	1-propoxypropan-2-ol
1569-02-4	C5H12O2	1-ethoxypropan-2-ol
1570-64-5	C7H7ClO	4-chloro-o-cresol
158001-04-8	C13H9F2NO3	1-cyclopropyl-6,7-difluoro-1,4-dihydro-4-oxoquinoline-3-carboxylic acid
15827-60-8	C9H28N3O15P5	[[(phosphonomethyl)imino]bis[ethane-2,1-diylnitrilobis(methylene)]]tetrakisphosphonic acid
15834-04-5	C25H44O8	2,2-bis[[(1-oxopentyl)oxy]methyl]propane-1,3-diyl divalerate
1589-49-7	C4H10O2	3-methoxypropan-1-ol
16004-15-2	C7H6BrI	1-Bromomethyl-4-iodo-benzene
160232-08-6	C19H32N2O3	tert-butyl {(2S,3R)-3-hydroxy-4-[(2-methylpropyl)amino]-1-phenylbutan-2-yl}carbamate
16040-69-0	C32H12Cl4CuN8	[2,9,16,23-tetrachloro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]copper
16066-35-6	C9H12O3S	p-cumenesulphonic acid
160844-75-7	C18H20N2O3S	5-Thiazolecarboxylic acid, 2-[3-cyano-4-(2-methylpropoxy)phenyl]-4-methyl-, ethyl ester
16088-62-3	C3H6O	(S)-1,2-epoxypropane
161596-47-0	C11H9NO3	Epoxyphthalimid
161798-01-2	C14H13NO4S	Ethyl 2-(3-formyl-4-hydroxyphenyl)-4-methyl thiazole-5-carboxylate
161798-03-4	C18H21NO4S	5-Thiazolecarboxylic acid, 2-[3-formyl-4-(2-methylpropoxy)phenyl]-4-methyl-, ethyl ester
16219-75-3	C9H12	5-ethylidene-8,9,10-trinorborn-2-ene
162204-20-8	C19H26FN3O8	2',3'-Di-O-acetyl-5'-deoxy-5-fluoro-N-[(pentyloxy)carbonyl]cytidine
162208-27-7	C10H16N3O5PS2	diethyl thiophosphoryl (Z)-(2-aminothiazol-4-yl)methoxyimino acetate
1624-02-8	C36H30CrO4Si2	bis(triphenylsilyl) chromate
1624-62-0	C19H24O2	3-methoxyoestra-1,3,5(10)-trien-17-one
162881-26-7	C26H27O3P	phenyl bis(2,4,6-trimethylbenzoyl)-phosphine oxide
16298-38-7	C21H30N2	4,4'-methylenebis(2-isopropyl-6-methylaniline)
1634-04-4	C5H12O	tert-butyl methyl ether
1636-27-7	C9H16O4	dipropylmalonic acid
1647-12-7	C7H12O2	Ethyl 2-methylbut-3-enoate
16484-77-8	C10H11ClO3	(R)-2-(4-chloro-2-methylphenoxy)propionic acid
16529-56-9	C5H7N	2-methyl-3-butenenitrile

1653-19-6	C4H4Cl2	2,3-dichlorobuta-1,3-diene
165670-57-5	C16H16N4	5-phenyl-2-(2-phenylpropan-2-yl)-2H-tetrazole
16613-04-0	C19H18O5	2-(4-benzoyl-3-hydroxyphenoxy)ethyl (2-methyl)-2-propenoat
1663-39-4	C7H12O2	tert-butyl acrylate
16673-34-0	C16H17ClN2O4S	N-[2-[4-(aminosulphonyl)phenyl]ethyl]-5-chloro-2-methoxybenzamide
167004-78-6	C11H20NO4P	3-[butoxy(methyl)phosphoryl]-1-cyanopropyl acetate
1671-18-7	C8H9ClO2S	2-Chloro-1-methyl-4-(methylsulfonyl)benzene
1671-49-4	C8H9NO4S	NMST, 4-mesyl-2-nitrotolueen
168253-59-6	C22H40N2O8	1,5-bis[1,2-bis(ethoxycarbonyl)ethylamino]-2-methylpentane
168689-49-4	C35H53ClN2O7	hexadecyl 4-chloro-3-[2-(5,5-dimethyl-2,4-dioxo-1,3-oxazolidin-3-yl)-4,4-dimethyl-3-oxopentamido]benzoate
16874-33-2	C5H8O3	Tetrahydrofuran-2-carboxylic acid
16883-83-3	C27H34O6	benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate
169280-56-2	C20H29N3O3S	4-Amino-N-[(2R,3S)-3-amino-2-hydroxy-4-phenylbutyl]-N-isobutylbenzenesulfonamide
1696-20-4	C6H11NO2	4-acetylmorpholine
1712-70-5	C6H7F3O2	trans-4-Ethoxy-1,1,1-trifluoro-3-buten-2-one
17159-79-4	C9H14O3	ethyl 4-oxocyclohexane-1-carboxylate
1717-00-6	C2H3Cl2F	1,1-dichloro-1-fluoroethane
1724-39-6	C12H24O	cyclododecanol
17247-58-4	C5H9Br	(bromomethyl)cyclobutane
17273-79-9	C11H7NaO2	Sodium naphthalene-2-carboxylate
17351-75-6	C12H20O2	1,4-bis[(vinyloxy)methyl]cyclohexane
1738-25-6	C5H10N2	3-dimethylaminopropiononitrile
173904-11-5	C16H30N2	N,N’-[cyclohexane-1,3-diylbis(methylene)]bis(2-methylpropan-1-imine)
175463-32-8	C10H14N2O3	tert-butyl 3-Cyano-4-oxo-pyrrolidine-1-carboxylate
175481-26-2	C13H18N2O3	2-(acetylamino)-N-benzyl-3-methoxypropanamide
1761-71-3	C13H26N2	4,4'-methylenebis(cyclohexylamine)
17639-93-9	C4H7ClO2	methyl 2-chloropropionate
17689-77-9	C8H14O6Si	triacetoxyethylsilane
176969-33-8	C9H12F2O4	Ethyl-2-(ethoxymethylene-4,4-difluoro (acetoacetate)
176969-34-9	C6H6F2N2O2	3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxylic acid
176972-62-6	C12H16ClNO3	Methyl [(2S,3S)-4-chloro-3-hydroxy-1-phenylbutan-2-yl]carbamate
17742-69-7	C7H5Cl2NO3	1,3-dichloro-2-methoxy-5-nitrobenzene
17773-41-0	C5H9NOS	2-hydroxy-4-(methylthio)butyronitrile
17796-82-6	C14H15NO2S	N-(cyclohexylthio)phthalimide
17832-28-9	C6H12O2	4-(vinyloxy)butan-1-ol
17865-32-6	C9H20O2Si	cyclohexyldimethoxymethylsilane
17890-10-7	C10H17NO2Si	N-((Dimethoxy(methyl)silyl)methyl)-N-phenylamine
179688-27-8	C15H23NO6	Ethyl 2-amino-4,5-bis(2-methoxyethoxy)benzoate

17980-47-1	C10H24O3Si	triethoxyisobutylsilane
18087-70-2	C6H6ClN3	imidazo[1,2-b]pyridazine;hydrochloride
18143-33-4	C4H11ClOSi	(Chloromethyl)methoxydimethylsilane
181587-01-9	C13H9Cl2F3N4OS	Ethiprole
18169-57-8	C4H9Cl3Si	trichloroisobutylsilane
18172-67-3	C10H16	pin-2(10)-ene
18241-31-1	C18H18O4	bis(4-methylbenzyl) oxalate
183065-68-1	C7H3BrF2O2	4-bromo-2,6-difluorobenzoic acid
1836-62-0	C9H13NO2	2-(2-methoxyphenoxy)ethanamine
18379-25-4	C8H17Cl3Si	trichloro(2,4,4-trimethylpentyl)silane
18402-22-7	C14H29Cl3Si	trichloro(tetradecyl)silane
1843-05-6	C21H26O3	octabenzone
18479-58-8	C10H20O	2,6-dimethyloct-7-en-2-ol
18480-53-0	C4HCl2NO2S	3,4-dichloroisothiazole-5-carboxylic acid
18516-18-2	C5H10O3	3-hydroxy-2-(hydroxymethyl)-2-methylpropionaldehyde
1852-17-1	C4H8N2O	perhydropyrimidin-2-one
18531-99-2	C20H14O2	(S)-1,1'-Binaphthalene-2,2'-diol
18595-18-1	C9H11NO2	Methyl 3-amino-4-methylbenzoate
18600-59-4	C22H12N2O4	2,2-(1,4-phenylene)bis((4H-3,1-benzoxazine-4-one)
1860-26-0	C24H51N	2-ethyl-N,N-bis(2-ethylhexyl)hexylamine
18667-19-1	C15H25ClN2O2	1-Chloroacetyl-1,3-dicyclohexyl-urea
186817-80-1	C11H22O3	Propanoic acid, 2-hydroxy-, 2-ethylhexyl ester, (2S)-
18683-91-5	C13H18Br2N2O	ambroxol
1869-24-5	C7H6F3NO2S	2-(trifluoromethyl)benzenesulfonamide
1873-88-7	C7H22O2Si3	1,1,1,3,5,5,5-heptamethyltrisiloxane
187393-00-6	C38H49N3O5	2,2'-[6-(4-methoxyphenyl)-1,3,5-triazine-2,4-diyl]bis{5-[(2-ethylhexyl)oxy]phenol}
18835-33-1	C26H52	hexacos-1-ene
18835-34-2	C28H56	octacos-1-ene
18916-17-1	C27H34O14	3,5-dihydroxy-4-[3-(4-hydroxyphenyl)propanoyl]phenyl 2-O-(6-deoxy-α-Dmannopyranosyl)-β-D-gulopyranoside
18979-61-8	C10H14O2	4-butylbenzene-1,3-diol
739	C6H11NaO4	sodium 2,4-dihyroxy-3,3-dimethylbutanoate
1912-24-9	C8H14ClN5	atrazine
191226-98-9	C6H11NaO4	Carbamic acid, [(1S,2R)-2-hydroxy-3-[(2-methylpropyl)[(4-nitrophenyl)sulfonyl]amino]-1-(phenylmethyl)propyl]-, 1,1-dimethylethyl ester
19130-96-2	C6H13NO4	(2R,3R,4R,5S)-2-(hydroxymethyl)piperidine-3,4,5-triol
1917-44-8	C15H11N3O	1,3,5-Triazin-2(1H)-one, 4,6-diphenyl-
1927-95-3	C8H7BrO2	4-bromophenyl acetate
1939-36-2	C11H18N2O8	N,N'-propylene-1,3-diylbis[N-(hydroxycarbonylmethyl)glycine]
1943-82-4	C9H9NO	2-phenylethylisocyanate
19438-60-9	C9H12O3	hexahydro-4-methylphthalic anhydride
194608-78-1	C10H23N	1-Heptanamine, 2-propyl-

194805-07-7	C16H14BrF2NO4	Ethyl 7-bromo-1-cyclopropyl-8-(difluoromethoxy)-4-oxo-1,4-dihydro-3-quinolinecarboxylate
1962-75-0	C16H22O4	dibutyl terephthalate
19829-42-6	C16H12Cl2O4	bis(4-chlorobenzyl) oxalate
199327-61-2	C16H21N3O4	Morfon, 7-methoxy-6-(3-morfolin-4-yl-propoxy)-3H-quinazolin-4-on
20030-30-2	C9H14O	2,5,6-trimethylcyclohex-2-en-1-one
2004-62-8	C12H22N4	N,N'-Bis(2-cyanoethyl)hexamethylenediamine
20208-39-3	C12H24O5Si	3-(triethoxysilyl)propyl prop-2-enoate
20246-63-3	C9H7F3N2O2S	no name
202483-62-3	C23H39NO2	2-(2-hexyl-decyloxy)-benzamide
203448-76-4	C12H19N	2-(4-methylpentan-2-yl)aniline
204255-06-1	C16H26N4O4	Ethyl (3R,4R,5S)-4-acetamido-5-azido-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylate
20485-39-6	C7H9NO3	ethyl 4-methyloxazole-5-carboxylate
2049-95-8	C11H16	tert-pentylbenzene
20566-35-2	C15H16Br4O7	2-(2-hydroxyethoxy)ethyl 2-hydroxypropyl 3,4,5,6-tetrabromophthalate
20769-85-1	C4H6Br2O	2-bromo-2-methylpropionyl bromide
20826-04-4	C6H4BrNO2	5-bromonicotinic acid
2082-79-3	C35H62O3	octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate
2084-69-7	C16H24	1,2,3,4-tetrahydro-1,1,2,4,4,7-hexamethylnaphthalene
2100-42-7	C8H9ClO2	1-chloro-2,5-dimethoxybenzene
21134-38-3	C7H14O5Si	(trimethoxysilyl)methyl prop-2-enoate
211515-46-7	C13H23ClO	1-(2-ethylbutyl)cyclohexanecarbonyl chloride
211915-06-9	C34H41N7O5	ß-Alanin,N-[[2-[[[4-[[[(hexyloxy)carbonyl]amino]iminomethyl]phenyl]amino]methyl]-1-methyl-1H-benzimidazol-5-yl]carbonyl]-N-2-pyridinyl-ethylester
212322-56-0	C18H22N4O3	N-(3-Amino-4-(methylamino)benzoyl)-N-2-pyridinyl-beta-alaninethylester
2125-23-7	C21H15N3O6	2,4,6-Tri(2,4-dihydroxyphenyl)-1,3,5-triazine
2135-17-3	C22H28F2O5	flumetasone
2136-89-2	C7H4Cl4	α,α,α,2-tetrachlorotoluene
2137-18-0	C20H28O3	gestonorone
213967-55-6	C15H17ClN6O2S	(E)-5-benzyl-1-(2-chloro-1,3-thiazol-5-ylmethyl)-3-methyl-N-nitro-1,3,5-triazinan-2-imine
2146-71-6	C14H26O2	vinyl laurate
21535-43-3	C15H14ClNO	N-[2-(Phenylmethyl)phenyl]-2-chloroacetamide
2163-42-0	C4H10O2	2-methyl-1,3-propanediol
21732-17-2	C3H4N4O2	1H-tetrazol-1-acetic acid
2186-92-7	C10H14O3	p-(dimethoxymethyl)anisole
218768-11-7	C15H14O3	(Z)-4-hydroxy-4-(6-methoxynaphthalen-2-yl)but-3-en-2-one
219715-34-1	C7H6F3NO	2-Methoxy-4-(trifluoromethyl)pyridine
21981-33-9	C4H5Cl5	1,1,1,3,3-pentachlorobutane
220410-74-2	C15H27NO9	1,4-dihydroxy-2,2,6,6-tetramethylpiperidinium 2-hydroxy-1,2,3-propanetricarboxylate

22094-93-5	C36H32Cl4N6O4	2,2'-[(2,2',5,5'-tetrachloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]
114266	C4H11ClO2Si	(Chloromethyl)dimethoxymethylsilane
2212-81-9	C20H34O4	[1,3-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide
221615-75-4	C15H15NO3S	1-(6-Methylpyridin-3-yl)-2-[4-(methylsulfonyl)phenyl]ethanone
2216-51-5	C10H20O	L-menthol
221667-31-8	C18H18N2O5S	Cyprosulfamide
222408-90-4	C14H17Cl2N3OS	2-[2-(1-chlorocyclopropyl)-3-(2-chlorophenyl)-2-hydroxypropyl]-1,2,4-triazolidine-3-thione
22252-43-3	C8H10N2O3S	(6R-trans)-7-amino-3-methyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
2234-82-4	C3H7ClMg	chloropropylmagnesium
224049-04-1	C11H5Cl2N3OS	3,4-dichloro-N-(2-cyanophenyl)isothiazole-5-carboxamide
2243-62-1	C10H10N2	1,5-naphthylenediamine
22673-19-4	C18H32O4Sn	dibutylbis(pentane-2,4-dionato-O,O')tin
22818-40-2	C8H9NO3	D-N-(4-hydroxyphenyl)glycine
22990-77-8	C6H14N2	piperidine-2-methylamine
23202-81-5	C9H16O4	methyl 5-deoxy-2,3-O-isopropylidene-β-D-ribofuranoside
23235-61-2	C12H26O5	2,2'-[oxybis(methylene)]bis[2-ethylpropane-1,3-diol]
236391-76-7	C15H26O4	2-[1-(3,3-Dimethylcyclohexyl)ethoxy]-2-oxoethyl propionate
2370-88-9	C4H16O4Si4	2,4,6,8-tetramethylcyclotetrasiloxane
23719-80-4	C3H5BrMg	Bromo(cyclopropyl)magnesium
23783-42-8	C9H20O5	3,6,9,12-tetraoxotridecanol
2380-86-1	C8H7NO	6-hydroxyindole
238098-26-5	C10H8F7N	RFA
2386-87-0	C14H20O4	7-oxabicyclo[4.1.0]hept-3-ylmethyl 7-oxabicyclo[4.1.0]heptane-3-carboxylate
23911-56-0	C11H10O2	Nerolione
23996-53-4	C6H7N3	Imidazole-1-propionitrile(8CI);1-(2-Cyanoethyl)imidazole
2402-79-1	C5HCl4N	2,3,5,6-tetrachloropyridine
2403-88-5	C9H19NO	2,2,6,6-tetramethylpiperidin-4-ol
2403-89-6	C10H21NO	1,2,2,6,6-pentamethylpiperidin-4-ol
24085-06-1	C13H14O5	3-Acetoxymethyl-4-acetoxyacetophenon
2409-55-4	C11H16O	2-tert-butyl-p-cresol
24131-07-5	C12H13NO2	2-phenyl-2-ethyl-2-cyanoacetic acid methyl ester
24155-42-8	C11H10Cl2N2O	α-(2,4-dichlorophenyl)-1H-imidazole-1-ethanol
2416-94-6	C9H12O	2,3,6-trimethylphenol
24199-46-0	C9H16O	6-methyloct-5-en-2-one
2420-17-9	C9H8N2O3	5-(4-hydroxyphenyl)imidazolidine-2,4-dione
2425-77-6	C16H34O	2-hexyldecan-1-ol
2425-79-8	C10H18O4	1,4-bis(2,3-epoxypropoxy)butane
24279-39-8	C7H4Cl2F3N	2,6-dichloro-4-trifluoromethylaniline

24280-93-1	C17H20O6	mycophenolic acid
24304-50-5	C16H20N2O4	N,N'-(2,5-dimethyl-1,4-phenylene)bis[3-oxobutyramide]
2431-50-7	C4H5Cl3	2,3,4-trichlorobut-1-ene
2432-99-7	C11H23NO2	11-aminoundecanoic acid
2436-29-5	C11H9NO3	3-(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)propanal
2436-90-0	C10H18	3,7-dimethylocta-1,6-diene
2437-25-4	C12H23N	dodecanenitrile
2439-35-2	C7H13NO2	2-(dimethylamino)ethyl acrylate
2440-22-4	C13H11N3O	2-(2H-benzotriazol-2-yl)-p-cresol
24468-13-1	C9H17ClO2	2-ethylhexyl chloroformate
24487-91-0	C9H9ClO2	3-methoxy-2-methylbenzoyl chloride
2451-62-9	C12H15N3O6	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione
24549-06-2	C9H13N	6-ethyl-2-toluidine
246035-38-1	C15H12N4O4S3	Methyl ({[(1Z)-1-(2-amino-1,3-thiazol-4-yl)-2-(1,3-benzothiazol-2-ylsulfanyl)-2-oxoethylidene]amino}oxy)acetate
24683-26-9	C12H13NO5S	ethyl 4-hydroxy-2-methyl-2H-1,2-benzothiazine-3-carboxylate 1,1-dioxide
24701-69-7	C9H12N2O4S	(6R,7R)-7-Amino-3-(methoxymethyl)-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
24731-73-5	C14H16N2O4	N,N'-1,4-phenylenebis[3-oxobutyramide]
24748-23-0	C12H24O6	methylethylketone peroxide trimer
247940-06-3	C24H31P	2-(DICYCLOHEXYLPHOSPHINO)BIPHENYL
24800-44-0	C9H20O4	[(methylethylene)bis(oxy)]dipropanol
24851-98-7	C13H22O3	methyl 3-oxo-2-pentylcyclopentaneacetate
24863-70-5	C13H20O3	METHYL (3-OXO-2-PENTYLCYCLOPENT-1-EN-1-YL)ACETATE
2487-90-3	C3H10O3Si	trimethoxysilane
2494-89-5	C8H11NO6S2	2-[(p-aminophenyl)sulphonyl]ethyl hydrogensulphate
2495-27-4	C20H38O2	hexadecyl methacrylate
25013-15-4	C9H10	vinyltoluene
25068-38-6	C18H21ClO3	reaction product: bisphenol-A-(epichlorhydrin); epoxy resin (number average molecular weight ≤ 700)
25103-09-7	C10H20O2S	isooctyl mercaptoacetate
25103-58-6	C12H26S	tert-dodecanethiol
25155-23-1	C24H27O4P	trixylyl phosphate
25155-25-3	C20H34O4	[1,3(or 1,4)-phenylenebis(1-methylethylidene)]bis[tert-butyl] peroxide
25167-67-3	C4H8	butene
25167-70-8	C8H16	2,4,4-trimethylpentene
2517-43-3	C5H12O2	3-methoxybutan-1-ol
252317-48-9	C28H28N2O	{(S)-1-[2-(2,3- Dihydro-benzofuran-5-yl)-ethyl]-pyrrolidin-3-yl}-diphenyl-acetonitrile
228004	C4H10ClO2PS	O,O-diethyl phosphorochloridothioate
25260-60-0	C8H12O4	(2Z)-but-2-ene-1,4-diyl diacetate

25265-71-8	C6H14O3	oxydipropanol
25265-77-4	C12H24O3	isobutyric acid, monoester with 2,2,4-trimethylpentane-1,3-diol
25265-78-5	C18H30	tetrapropylenebenzene
25307-17-9	C22H45NO2	2,2'-(octadec-9-enylimino)bisethanol
2530-83-8	C9H20O5Si	[3-(2,3-epoxypropoxy)propyl]trimethoxysilane
2530-85-0	C10H20O5Si	3-trimethoxysilylpropyl methacrylate
2530-87-2	C6H15ClO3Si	3-chloropropyltrimethoxysilane
25321-14-6	C7H6N2O4	dinitrotoluene
25321-41-9	C8H10O3S	xylenesulphonic acid
25339-53-1	C10H20	decene
25340-17-4	C10H14	diethylbenzene
232418	C15H10N2O2	methylenediphenyl diisocyanate
25376-45-8	C7H10N2	diaminotoluene
25377-72-4	C5H10	pentene
25377-82-6	C13H26	tridecene
25378-22-7	C12H24	dodecene
25383-06-6	C3H7O3P	cis-propenylphosphonic acid
25383-07-7	C11H18NO4P	(R)-α-phenylethylammonium (-)-(1R, 2S)-(1,2-epoxypropyl)phosphonate monohydrate
25485-88-5	C13H16O3	cyclohexyl 2-hydroxybenzoate
2549-53-3	C18H34O2	tetradecyl methacrylate
25498-49-1	C10H22O4	[2-(2-methoxymethylethoxy)methylethoxy]propanol
237563	C3H6Cl4Si	trichloro(3-chloropropyl)silane
2550-52-9	C16H30O	ISOMUSCONE
25513-64-8	C9H22N2	2,2,4(or 2,4,4)-trimethylhexane-1,6-diamine
25550-51-0	C9H12O3	hexahydromethylphthalic anhydride
2557-13-3	C9H7F3O2	Methyl, 3-Trifluoromethylbenzoate
25584-83-2	C6H10O3	acrylic acid, monoester with propane-1,2-diol
25586-42-9	C21H21O3P	tris(methylphenyl) phosphite
25634-93-9	C12H18O	2-methyl-5-phenylpentanol
25637-99-4	C12H18Br6	hexabromocyclododecane
2568-33-4	C5H12O2	3-methyl-1,3-butandiol
2568-90-3	C9H20O2	1,1'-[methylenebis(oxy)]dibutane
256-96-2	C14H11N	5H-dibenz[b,f]azepine
25713-60-4	C21H6Br9N3O3	2,4,6-tris(2,4,6-tribromophenoxy)-1,3,5-triazine
2579-20-6	C8H18N2	1,3-Cyclohexanedimethanamine
25869-00-5	C6FeN6H4N	ammonium iron(3+) hexakis(cyano-C)ferrate(4-)
25899-50-7	C5H7N	(Z)-pent-2-enenitrile
25953-19-9	C14H14N8O4S3	Cefazoline
2605-78-9	C10H23NO	octyldimethylamine oxide
2612-57-9	C7H3Cl2NO	2,4-dichlorophenyl isocyanate
26140-60-3	C18H14	terphenyl
26159-31-9	C14H14O3	(±)-2-(6-methoxy-2-naphthyl)propionic acid

26175-68-8	C8H10Cl2N2O2S	4-amino-2,5-dichloro-N,N-dimethylbenzenesulphonamide
26184-62-3	C5H12O	2-Pentanol, (2S)-
261953-36-0	C7H5IN2	6-iodo-1H-indazole
26218-04-2	C15H23NO2	2-ethylhexyl 4-aminobenzoate
26266-68-2	C8H14O	2-ethylhexenal
26272-90-2	C17H33ClO2	hexadecyl chloroformate
2629-68-7	C8H4Cl2F4	1,4-Bis-(chloro-difluoro-methyl)-benzene
26351-32-6	C21H40N2	(Z)-3-(9-octadecenylamino)propiononitrile
26364-65-8	C4H5N3S	2-Cyanimino-1,3-thiazolidine
26399-02-0	C26H50O2	2-ethylhexyl oleate
26401-35-4	C32H62O4	diisotridecyl adipate
271561	C11H14ClNO	p-[(2-chloroethyl)ethylamino]benzaldehyde
26447-85-8	C11H10O3S2	Di-2-thienylglycolic acid methyl ester
26471-62-5	C9H6N2O2	m-tolylidene diisocyanate
26472-00-4	C12H16	methylcyclopentadiene
2649-76-5	C24H34O3	3-ethoxypregna-3,5-diene-21,17α-carbolactone
26504-29-0	C15H14S3	Dibenzyl trithiocarbonate
265136-65-0	C16H18N2O5	Ethyl 3-amino-4-[2-(phthalimido)ethoxy]crotonate
26523-78-4	C45H69O3P	tris(nonylphenyl) phosphite
26576-46-5	C11H11N3O3	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide
2657-85-4	C13H13N3O	Benzamide, 4-amino-N-(3-aminophenyl)-
26586-02-7	C7H10O3	(E)-3-formylbut-2-enyl acetate
26760-64-5	C5H10	2-methylbutene
26761-45-5	C13H24O3	2,3-epoxypropyl neodecanoate
268567-32-4	C12H25O4PS2	3-[(diisoalkyloxyphosphorothioyl)thio]-2-methylalkanoic acid
2687-91-4	C6H11NO	1-ethylpyrrolidin-2-one
2687-94-7	C12H23NO	N-(n-octyl)-2-pyrrolidinone
26896-20-8	C10H20O2	neodecanoic acid
26896-48-0	C12H20O2	tricyclodecanedimethanol
26898-17-9	C21H20	dibenzyltoluene
26952-13-6	C14H28	tetradecene
26952-14-7	C16H32	hexadecene
26966-75-6	C7H10N2	3(or 4)-methylbenzene-1,2-diamine
2701-50-0	C24H30O4	17-acetoxy-1β,2β-methanopegna-4,6-diene-3,20-dione
27070-58-2	C18H36	octadecene
27076-30-8	C5H12N2O2	3-[(2-hydroxyethyl)amino]propionamide
27107-89-7	C38H74O6S3Sn	2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-octyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
27138-31-4	C20H22O5	oxydipropyl dibenzoate
27178-16-1	C26H50O4	diisodecyl adipate
27215-95-8	C9H18	nonene
27247-96-7	C8H17NO3	2-ethylhexyl nitrate

2725-22-6	C33H39N3O2	2-(4,6-bis-(2,4-dimethylphenyl)-1,3,5-triazin-2-yl)-5-(octyloxy)-phenol
27253-26-5	C34H58O4	diisotridecyl phthalate
2730-71-4	C22H25NO5S	thiocolchicine
27394-99-6	C4H6N2O	N-(1-cyanoethyl)formamide
27458-92-0	C13H28O	isotridecan-1-ol
27458-94-2	C9H20O	isononyl alcohol
27489-62-9	C6H13NO	trans-4-aminocyclohexan-1-ol
27614-71-7	C32H12Cl4CuN8	[tetrachloro-29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]copper
27624-67-5	C14H16N4O9S3	Polysubstituted-5-[4-[(2-sulfoxyl ethyl) sulfonyl]arylazo]benzenesulfonic acid
27665-39-0	C4H10O6S2	butane-1,4-disulfonic acid
317069	C5H12O3Si	trimethoxyvinylsilane
27776-01-8	C14H14	benzyltoluene
2778-42-9	C14H16N2O2	1,3-bis(1-isocyanato-1-methylethyl)benzene
322057	C24H48O4Sn	dibutyltin bis(2-ethylhexanoate)
27813-02-1	C7H12O3	methacrylic acid, monoester with propane-1,2-diol
324004	C22H28O3	17α-hydroxy-2-(hydroxymethylene)pregn-4-en-20-yn-3-one
27955-94-8	C20H18O3	4,4',4''-(ethan-1,1,1-triyl)triphenol
2807-30-9	C5H12O2	2-(propyloxy)ethanol
2809-21-4	C2H8O7P2	etidronic acid
2820-37-3	C5H8N2	DMP
282102-50-5	C26H31NO5S	Ethanamine, 2-[4-[(1Z)-1,2-diphenyl-1-butenyl]phenoxy]-N,N-dimethyl-, sulfate
28299-41-4	C14H14O	ditolyl ether
2833-30-9	C6H8O3	Ethoxyfuranon
2840-28-0	C7H6ClNO2	3-amino-4-chlorobenzoic acid
28416-82-2	C21H26F2O5	no name
28443-50-7	C6H6ClNO	2-amino-5-chlorophenol
28472-97-1	C29H56O4	diisodecyl azelate
28479-22-3	C8H6ClNO	3-chloro-p-tolyl isocyanate
2855-13-2	C10H22N2	3-aminomethyl-3,5,5-trimethylcyclohexylamine
28553-12-0	C26H42O4	di-''isononyl'' phthalate
2863-88-9	C20H28O2	3-Ethoxyestra-3,5-dien-17-one
2867-47-2	C8H15NO2	2-dimethylaminoethyl methacrylate
287471-30-1	C9H13Cl	(2E)-1-chloro-6,6-dimethyl-2-Hepten-4-yne
28768-32-3	C25H30N2O4	4,4'-methylenebis[N,N-bis(2,3-epoxypropyl)aniline]
287-92-3	C5H10	cyclopentane
288-32-4	C3H4N2	imidazole
28861-00-9	C13H18N2O5	Tyrosine, N-(aminocarbonyl)-3-methoxy-O,α-dimethyl-
28961-43-5	C21H32O9	Propylidynetrimethanol, ethoxylated, esters with acrylic acid
29091-09-6	C7HCl2F3N2O4	2,4-dichloro-1,3-dinitro-5-(trifluoromethyl)benzene
2909-38-8	C7H4ClNO	3-chlorophenyl isocyanate

2935-90-2	C4H8O2S	methyl 3-mercaptopropionate
294-62-2	C12H24	cyclododecane
294-90-6	C8H20N4	1,4,7,10-Tetraazacyclododecane
29518-11-4	C10H11NO2	4-Phenylmorpholin-3-on
2955-88-6	C6H13NO	2-pyrrolidin-1-ylethanol
29590-42-9	C11H20O2	isooctyl acrylate
29617-66-1	C3H5ClO2	(S)-2-chloropropionic acid
2963-69-1	C19H28O4	3 beta,7 alpha,15 alpha-Trihydroxy-5-androsten-17-one
29761-21-5	C22H31O4P	isodecyl diphenyl phosphate
29797-40-8	C7H6Cl2	dichloromethylbenzene
298-06-6	C4H11O2PS2	O,O-diethyl hydrogen phosphorodithioate
298692-41-8	C4H12N3O3P	isopropyl (diaminophosphoryl) carbamate
29911-27-1	C9H20O3	1-(1-methyl-2-propoxyethoxy)propan-2-ol
29911-28-2	C10H22O3	1-(2-butoxy-1-methylethoxy)propan-2-ol
299-35-4	C12H16N4OS2	3-(4-amino-2-methylpyrimidin-5-ylmethyl)-5-(2-hydroxyethyl)-4-methylthiazole-2(3H)-thione
29964-84-9	C14H26O2	isodecyl methacrylate
3006-82-4	C12H24O3	tert-butyl 2-ethylperoxyhexanoate
3009-97-0	C8H8N2	anilinoacetonitrile
30113-45-2	C13H29NO	3-(isodecyloxy)propylamine
302-23-8	C23H32O4	hydroxyprogesterone acetate
302776-68-7	C24H31NO4	Hexyl 2-[3-(diethylamino)-2-hydroxybenzoyl]benzoate
302964-24-5	C11H10ClN3OS	2-Amino-N-(2-chloro-6-methylphenyl)thiazole-5-carboxamide
30374-01-7	C11H22O2S	isooctyl 3-mercaptopropionate
30399-84-9	C18H36O2	isooctadecanoic acid
30414-53-0	C6H10O3	methyl 3-oxovalerate
304-59-6	C4H6O6Na	potassium sodium tartrate
3047-33-4	C3H3N3O3	1,3,5-triazine-2,4,6(1H,3H,5H)-trione
3071-32-7	C8H10O2	1-phenylethyl hydroperoxide
307-35-7	C8F18O2S	heptadecafluorooctanesulphonyl fluoride
431357	C19H26N2	N-(1,4-dimethylpentyl)-N'-phenylbenzene-1,4-diamine
3081-14-9	C20H36N2	N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine
3089-16-5	C20H10Cl2N2O2	4,11-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione
3089-17-6	C20H10Cl2N2O2	2,9-dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione
3091-25-6	C8H17Cl3Sn	trichlorooctylstannane
30989-05-0	C21H45BO12	tris[2-[2-(2-methoxyethoxy)ethoxy]ethyl] orthoborate
31024-26-7	C6H17NOSi	(3-aminopropyl)(methoxy)dimethylsilane
31027-31-3	C10H11NO	p-isopropylphenyl isocyanate
31127-80-7	C16H20I3N3O7	5-acetylamino-N,N'-bis(2,3-dihydroxypropyl)-2,4,6-triiodo-1,3-benzenecarboxamide
31251-41-9	C14H10ClNO	8-Chloro-5,6-dihydro-11H-benzo[5,6]cyclohepta[1,2-b]pyridin-11-one

31291-60-8	C14H22O	di-sec-butylphenol
31394-54-4	C7H16	isoheptane
31566-31-1	C21H42O4	stearic acid, monoester with glycerol
31570-04-4	C42H63O3P	tris(2,4-ditert-butylphenyl) phosphite
460029	C13H9NOS	Dibenzo[b,f][1,4]thiazepin-11(10H)-one
3173-72-6	C12H6N2O2	1,5-naphthylene diisocyanate
31775-20-9	C36H34Cl2N6O6	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-ethoxyphenyl)-3-oxobutyramide]
317815-81-9	C7H9NO4S2	Thiophenesulfonamide
319002-92-1	C11H22O3	Sclareolate
3195-24-2	C13H20O4	diethyl diallylmalonate
31981-44-9	C22H30O4	17-hydroxy-19-norpregn-4-ene-3,20-dione 17-acetate
3209-22-1	C6H3Cl2NO2	1,2-dichloro-3-nitrobenzene
3222-49-9	C7H7NO2	5-Methylnicotinic acid
32360-05-7	C22H42O2	octadecyl methacrylate
32539-83-6	C15H26O	3,4,5,6,7,8,9,10,11,12,13,14-dodecahydro-2H-cyclododeca[b]pyran
3266-23-7	C4H8O	2,3-epoxybutane
3268-49-3	C4H8OS	3-(methylthio)propionaldehyde
3282-30-2	C5H9ClO	pivaloyl chloride
3290-92-4	C18H26O6	propylidynetrimethyl trimethacrylate
329181-36-4	C8H21N3O7S2	(4Z)-3-ammoniomethyl-4-(methoxyimino)pyrrolidinium dimethanesulfonate
329216-67-3	C19H21N3OS	2-[4-(Dibenzo[b,f][1,4]thiazepin-11-yl)piperazin-1-yl] ethanol
512345	C9H18O2	3,5,5-trimethylhexanoic acid
33021-02-2	C8H18O	1-(1,1-dimethylethoxy)-2-methylpropane
330-54-1	C9H10Cl2N2O	diuron
3319-31-1	C33H54O6	tris(2-ethylhexyl) benzene-1,2,4-tricarboxylate
3320-83-0	C7H4ClNO	2-chlorophenyl isocyanate
3335-98-6	C14H11NO	Phenyloxindole
3349-36-8	C16H36O2Sn	dibutoxydibutylstannane
33511-66-9	C18H39NO3	Phytosphingosine
335153-21-4	C13H15NO6	2-(2-Formyl-4-nitrophenoxy)hexanoic acid
3356-88-5	C5H9NO3	3-(2-Hydroxyethyl)-1,3-oxazolidin-2-one
33703-08-1	C24H46O4	diisononyl adipate
3380-30-1	C12H8Cl2O2	DCCP
3380-34-5	C12H7Cl3O2	triclosan
3386-33-2	C18H37Cl	1-chlorooctadecane
33996-58-6	C8H14N2O2	2-(2-oxopyrrolidin-1-yl)butyramide
34090-76-1	C9H10O3	tetrahydro-4-methylphthalic anhydride
3409-21-0	C13H17NO	2-[2-(Dimethylamino)ethyl]-2,3-dihydro-1H-inden-1-one
342573-75-5	C8H16N2O4S	1-Ethyl-3-methylimidazolium ethylsulfate
3425-89-6	C9H10O3	1,2,3,6-tetrahydro-4-methylphthalic anhydride
344348-40-9	C15H20O	4-propionylcyclohexylbenzene

34494-24-1	C6H12N2O	Propanenitrile, 3-[(2-hydroxypropyl)amino
567040	C20H40	icos-1-ene
34590-94-8	C7H16O3	(2-methoxymethylethoxy)propanol
345-92-6	C13H8F2O	bis(4-fluorophenyl) ketone
34640-92-1	C8H17NO3	2,2-diethoxy-N,N-dimethylacetamide
3467-59-2	C10H13NO3	N-(2,5-dimethoxyphenyl)acetamide
34893-92-0	C7H3Cl2NO	1,3-dichloro-5-isocyanatobenzene
35000-38-5	C24H25O2P	tert-butyl (triphenylphosphoranylidene) acetate
35130-97-3	C9H17NO3S	(3-endo)-8-methyl-8-azabicyclo[3.2.1]oct-3-yl methanesulfonate
35176-06-8	C7H17NO3	2,2'-Iminodiethanol, propoxylated
35303-76-5	C8H12N2O2S	4-(2-aminoethyl)benzenesulphonamide
35410-28-7	C22H30O7S	11β,17,21-trihydroxypregna-1,4-diene-3,20-dione 21-methanesulphonate
3542-36-7	C16H34Cl2Sn	dichlorodioctylstannane
35435-21-3	C14H32O3Si	triethoxy(2,4,4-trimethylpentyl)silane
35453-19-1	C8H4I3NO4	5-amino-2,4,6-triiodoisophthalic acid
35480-52-5	C11H8F6O4	2,5-bis(2,2,2-trifluoroethoxy)benzoic acid
35687-90-2	C9H24NO4P	tripropylammonium dihydrogenphosphate
35884-66-3	C84H84NiO12P4	tetrakis(tritolyl phosphite)nickel
3590-84-9	C32H68Sn	tetraoctyltin
35958-64-6	C27H30O6	(3R,4R,5R)-4-benzyloxy-5-[(1R)-I ,2-dibenzyloxyethyl] tetrahydrofuran-2,3-diol
36130-02-6	C27H37FO5	6 alpha-Fluoro-11 beta-hydroxy-16 alpha-methyl-21-valeryloxy-1,4-pregnadiene-3,20-dione
361440-67-7	C11H18N2O3	Tert-butyl(1S,3S,5S)-3-carbamoyl-2-azabicyclo[3.1.0]hexane-2-carboxylate
36177-92-1	C13H28N2	N-butyl-2,2,6,6-tetramethylpiperidin-4-amine
3621-82-7	C7H3Cl2NO	2,6-dichlorobenzoxazole
3622-84-2	C10H15NO2S	N-butylbenzenesulphonamide
3648-20-2	C30H50O4	diundecyl phthalate
36567-04-1	C5H13NS	Alkylthioamin
36589-61-4	C4H10O6S2	disodium butane-1,4-disulfonate
366-18-7	C10H8N2	2,2'-bipyridyl
36635-56-0	C9H11NO3S	Tosyl MF
36653-82-4	C16H34O	hexadecan-1-ol
36687-82-8	C18H36N2O12	L-Propanaminium, 3-carboxy-2—hydroxy,N,N,N-trimethyl-(R)-salt with [R-(R*R*)]-2,3-dihydroxybutanedioic acid (2:1)
367-25-9	C6H5F2N	2,4-difluoroaniline
36727-29-4	C9H17ClO	3,5,5-trimethylhexanoyl chloride
36768-62-4	C9H20N2	2,2,6,6-tetramethyl-4-piperidylamine
3687-18-1	C3H9NO3S	3-aminopropane-1-sulphonic acid
3687-46-5	C28H54O2	decyl oleate
36878-20-3	C30H47N	bis(nonylphenyl)amine
368890-20-4	C15H12ClF2N3O2S	2-{[(4-chloro-3-methoxypyridin-2-yl)methyl]sulfanyl}-5-(difluoromethoxy)-1H-benzimidazole

371756-75-1	C44H46N12Na6O22S6	Hexasodium 2,2'-[vinylenebis[(3-sulfonato-4,1-phenylene)imino[6-[bis (2-hydroxypropyl)amino]-1,3,5-triazine-4,2-diyl]imino]]bis(benzene-1,4-disulfonate)
371771-07-2	C23H23F7N2O3S	N-(2-methylsulfinyl-1,1-dimethyl-ethyl)-N'-{2-methyl-4-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]phenyl}phthalamide
37208-53-0	C15H33NO6	2, 2', 2'' - Nitrilotriethanol, propoxylated
372-09-8	C3H3NO2	cyanoacetic acid
3724-43-4	C3H7Cl2N	Chloromethylene dimethylammonium chloride
3741-80-8	C18H17N3S4	N-(1,1-dimethylethyl)bis(2-benzothiazolesulfen)amide
3748-13-8	C12H14	m-bis(1-methylvinyl)benzene
3753-18-2	C16H18O2	4,4-bis(methoxymethyl)biphenyl
376348-77-5	C16H21F2NO2	4,4-Difluoro-N-[(1S)-3-hydroxy-1-phenylpropyl]cyclohexanecarboxamide
376348-78-6	C16H19F2NO2	4,4-Difluoro-N-[(1S)-3-oxo-1-phenylpropyl]cyclohexanecarboxamide
376608-71-8	C17H17F2NO3	trans-(1R,2S)-2-(3,4-difluorophenyl-cyclopropanaminium (2R)-2-hydroxy-2-phenylethanoate
376608-74-1	C17H27ClN4O4S	2-{[(3aR,4S,6R,6aS)-6-{[5-amino-6-chloro-2-(propylsulfanyl)-4,5-dihydropyrimidin-4-yl]amino}-2,2-dimethyltetrahydro-3aH-cyclopenta[d][1,3]dioxol-4-yl]oxy}ethanol
37763-23-8	C9H11NO3	methyl (R)-amino(4-hydroxyphenyl)acetate
37794-19-7	C10H9FO	6-fluoro-2-methylindan-1-one
378-44-9	C22H29FO5	betamethasone
37971-36-1	C7H11O9P	2-phosphonobutane-1,2,4-tricarboxylic acid
38051-10-4	C13H24Cl6O8P2	2,2-bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)
38083-17-9	C15H17ClN2O2	climbazole
380843-75-4	C26H29Cl2N5O3	4-[(2,4-Dichloro-5-methoxyphenyl)amino]-6-methoxy-7-[3-(4-methyl-1-piperazinyl)propoxy]-3-quinolinecarbonitrile
38089-93-9	C20H23ClN2O	8-chloro-11-(1-methylpiperidin-4-yl)-6,11-dihydro-5H-benzo[5,6]cyclohepta [1,2-b] pyridin-11-ol
38103-06-9	C31H20O8	4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride
381209-09-2	C13H24O2	1-(2-Ethyl-butyl)-cyclohexanecarboxylic acid
38223-29-9	C15H26O3	oxacyclohexadecane-2,13-dione
3845-76-9	C8H16N2O	N-[3-(dimethylamino)propyl]acrylamide
38585-74-9	C4H5NOS	5-thiazolylmethanol
38640-62-9	C16H20	bis(isopropyl)naphthalene
38720-66-0	C20H10Cl2N2O2	dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione
388606-32-4	C10H26N2Si2	1-Propanamine, 3-[(2 ,2-dimethyl-1-aza-2-silacyclopent-1-yl)dimethylsilyl]-
393-75-9	C7H2ClF3N2O4	4-chloro-3,5-dinitro-α,α,α-trifluorotoluene
394735-17-2	C9H17NO2	ethyl 2-amino-3-cyclobutylpropanoate
39515-51-0	C13H10O2	m-phenoxybenzaldehyde
39537-23-0	C8H15N3O4	(2S)-5-amino-2-{[(2S)-2-aminopropanoyl]amino}-5-oxopentanoic acid

39562-27-1	C12H11NO5	methyl 2-(2-nitrobenzylidene)acetoacetate
39605-45-3	C19H36ClN5	6-chloro-N,N,N',N'-tetrabutyl-1,3,5-triazine-2,4-diamine
39627-98-0	C14H14N2O	N-(2,6-dimethylphenyl)pyridine-2-carboxamide
39648-67-4	C20H13O4P	(R)-(-)-1,1'-Binaphthalene-2,2'-diyl hydrogen phosphate
39903-01-0	C5H5BrN2O	2-amino-5-bromopyridin-3-ol
399-95-1	C6H6FNO	4-amino-3-fluorophenol
400827-68-1	C36H28N4O4S3	Diphenylmethyl (6R,7R)-8-oxo-7-[(phenylacetyl)amino]-3-{[4-(pyridin-4-yl)-1,3-thiazol-2-yl]thio}-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate
40188-41-8	C10H19N	3,7-dimethyloctanenitrile
40292-82-8	C10H19ClO	neodecanoyl chloride
403848-04-4	C12H17NO3S2	N-ethyl-N-[(4S,6S)-6-methyl-7,7-dioxido-5,6-dihydro-4H-thieno[2,3-b]thiopyran-4-yl]acetamide
4062-46-8	C22H34O3	17β-hydroxy-1α-methyl-5-αandrostan-3-one acetate
40649-36-3	C9H16O	4-propylcyclohexanone
4067-16-7	C10H28N6	3,6,9,12-tetraazatetradecamethylenediamine
40722-73-4	C5H10Cl2NO2P	2-chloro-3-(2-chloroethyl)-1,3,2-oxazaphosphinane 2-oxide
4093-31-6	C11H12ClNO4	methyl 4-acetamido-5-chloro-o-anisate
4098-71-9	C12H18N2O2	3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate
41131-65-1	C15H17ClN2O4	N,N'-(2-chloro-5-methyl-1,4-phenylene)bis[3-oxobutyramide]
41198-08-7	C11H15BrClO3PS	O-(4-bromo-2-chlorophenyl) O-ethyl S-propyl phosphorothioate
41202-77-1	C10H12Cl2N2	1-(2,3-dichlorophenyl)piperazine
41263-74-5	C8H8N2O4	4-(Methylamino)-3-nitrobenzoic acid
4137-56-8	C16H22O7S	Methyl 2,3-O-(1-methylethylidene)-5-O-[(4-methylphenyl)sulfonyl]-β-D-ribofuranoside
41492-05-1	C10H13Br	1-Bromo-4-butylbenzene
41524-32-7	C36H48N2O8	(1R*,6S*)-6-(ethoxycarbonyl)-N,N-dimethyl-6-phenylcyclohex-2-en-1-aminium monooxalate
41672-81-5	C37H69NO5	trans-1-(1-oxohexadecyl)-4-[(1-oxohexadecyl)oxy]-L-proline
4170-30-3	C4H6O	crotonaldehyde
4186-71-4	C8H18IN	N-ethyl-N-methylpiperidinium iodide
4198-90-7	C9H9NO	4-Cyano-2,6-dimethylphenol
42036-65-7	C9H17NO	Dimethyl((2-oxocyclohexyl)methyl)ammonium chloride
42074-68-0	C19H14Cl2	1-chloro-2-(chlorodiphenylmethyl)benzene
42125-46-2	C11H19ClO2	4-tert-butylcyclohexyl chloroformate
42221-52-3	C7HCl5O	2,3,4,5-tetrachlorobenzoylchloride
4224-62-8	C6H11ClO2	6-chlorohexanoic acid
42399-49-5	C16H15NO3S	(2S-cis)-2,3-dihydro-3-hydroxy-2-(4-methoxyphenyl)-1,5-benzothiazepin-4(5H)-one
4245-76-5	C2H8N4O2	1-Methyl-2-nitroguanidine
42558-54-3	C7H12O3	methyl 4-methyl-3-oxopentanoate

868343	C16H28	Zyclen
42831-50-5	C5H5NO3	5-methylisoxazole-4-carboxylic acid
873943	C19H38N2O3	(carboxymethyl)dimethyl-3-[(1-oxododecyl)amino]propylammonium hydroxide
429659-01-8	C18H20N4O5	ethyl 3-((1-(4-methylamino-3-nitrophenyl)methanoyl)pyridin-2-yl-amino)propionate
42978-66-5	C15H24O6	(1-methyl-1,2-ethanediyl)bis[oxy(methyl-2,1-ethanediyl)] diacrylate
876403	C11H13NOS	2-n-butyl-benzo[d]isothiazol-3-one
43057-68-7	C14H16N2	2-Ethyl-2,3-dihydro-2-methyl-1H-perimidine
43170-88-3	C24H30N8O5	diethyl N-[4-[[(2,4-diamino-6-pteridinyl)methyl]methylamino]benzoyl]-L-glutamate
431-89-0	C3HF7	1,1,1,2,3,3,3-heptafluoropropane
433733-92-7	C10H12N2O5	(2S,3S,3aR,9aS)-3-hydroxy-2-(hydroxymethyl)-7-methyl-2,3,3a,9a-tertryhydro-6H-furo[2',3':4,5][1,3]oxazolo [3,2-a]pyrimidin-6-one
434-03-7	C21H28O2	ethisterone
434-22-0	C18H26O2	nandrolone
896982	C10H16O4	cyclohexanediacetic acid
438056-69-0	C10H12N2O2	4-(4-aminophenyl)morpholin-3-one
4394-85-8	C5H9NO2	N-Formylmorpholine
4404-43-7	C40H44N12O10S2	4,4'-bis[4-[bis(2-hydroxyethyl)amino]-6-anilino-1,3,5-triazin-2-yl]amino]stilbene-2,2'-disulphonic acid
4433-79-8	C12H14ClNO4	4'-chloro-2',5'-dimethoxyacetoacetanilide
4435-53-4	C7H14O3	3-methoxybutyl acetate
444065-11-6	C41H57N5O8	2-6-di-tert-butyl-4-methylcyclohexyl 5-{[bis(2-ethoxy-2-oxoethyl)carbamoyl]oxy}-2-(4-tert-butylphenyl)-6-cyano-1H-pyrrolo[1,2-b][1,2,4]triazole-7-carboxylate
932952	C6H10O2	3,4-dihydro-2-methoxy-2H-pyran
446292-04-2	C10H10N2O4	4-(4-Nitrophenyl)-morpholin-3-one
446292-07-5	C21H21N3O5	2-[(2R)-2-hydroxy-3-{[4-(3-oxomorpholin-4-yl)phenyl]amino}propyl]-1H-isoindole-1,3(2H)-dione
446292-08-6	C22H19N3O6	2-({(5S)-2-Oxo-3-[4-(3-oxomorpholin-4-yl)phenyl]-1,3-oxazolidin-5-yl}methyl)-1H-isoindole-1,3(2H)-dione
4463-59-6	C9H11BrO2	1-(2-bromoethoxy)-2-methoxybenzene
4488-57-7	C10H14	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indene
4511-42-6	C6H8O4	(3S-cis)-3,6-dimethyl-1,4-dioxane-2,5-dione
4531-49-1	C34H30Cl2N6O6	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methoxyphenyl)-3-oxobutyramide]
455-14-1	C7H6F3N	α,α,α-trifluoro-p-toluidine
4553-62-2	C6H8N2	2-methylglutaronitrile
456-04-2	C8H6ClFO	α-chloro-4-fluoroacetophenone
457-68-1	C13H10F2	1,1'-methylenebis[4-fluorobenzene]

461432-25-7	C29H33ClO10	(1S)-2,3,4,6-tetra-O-acetyl-1,5-anhydro-1-[4-chloro-3-(4-ethoxybenzyl)phenyl]-D-glucitol
462-06-6	C6H5F	fluorobenzene
4635-59-0	C4H6Cl2O	4-chlorobutyryl chloride
4635-87-4	C5H7N	pent-3-enenitrile
4637-24-5	C5H13NO2	1,1-dimethoxytrimethylamine
4707-49-7	C8H8O4	2,4-dihydroxy-3-methylbenzoic acid
1029713	C9H21N3O3	2,2',2''-(hexahydro-1,3,5-triazine-1,3,5-triyl)triethanol
473799-16-5	C14H15N3O2S	1-[(2-Propenylthio)carbonyl]-4-(2-methylphenyl)-5-amino-1H-pyrazol-3-one
474510-57-1	C21H24O4	2-hydroxy-1-(4-(4-(2-hydroxy-2-methylpropionyl) benzyl) phenyl)-2-methylpropan-1-one
4763-40-0	C15H30N2	3-(dodecylamino)propiononitrile
1047217	C5H10O4	2,2-bis(hydroxymethyl)propionic acid
477218-42-1	C18H32O3	Serenolide
477-29-2	C27H33NO11	colchicoside
482-89-3	C16H10N2O2	2-(1,3-dihydro-3-oxo-2H-indol-2-ylidene)-1,2-dihydro-3H-indol-3-one
486455-65-6	C21H41N3O3	(2S)-N, N'-dibutyl-2-(2-ethylhexanamido)pentanediamide
4866-00-6	C5H6N2O2	4-methyloxazole-5-carboxamide
488097-90-1	C11H17NO5	Ethyl (2S)-2-[(4S)-4-methyl-2,5-dioxo-1,3-oxazolidin-3-yl]pentanoate
4904-61-4	C12H18	cyclododeca-1,5,9-triene
494-19-9	C14H13N	10,11-dihydro-5H-dibenz[b,f]azepine
49562-28-9	C20H21ClO4	fenofibrate
49564-57-0	C9H14N2O3S	4-amino-5-methoxy-N,2-dimethylbenzenesulphonamide
49667-22-3	C8H9NO2	methylsalicylamide
49707-23-5	C7H13NO3	N-(2,2-dimethoxyethyl)prop-2-enamide
49708-81-8	C13H15ClO2	trans-4-(4-Chlorophenyl)cyclohexanecarboxylic acid
4979-32-2	C19H26N2S2	N,N-dicyclohexylbenzothiazole-2-sulphenamide
498-66-8	C7H10	8,9,10-trinorborn-2-ene
500011-86-9	C9H5BrClN3O2	3-bromo-1-(3-chloropyridin-2-yl)-1H-pyrazole-5-carboxylic acid
50-03-3	C23H32O6	hydrocortisone 21-acetate
501-53-1	C8H7ClO2	benzyl chloroformate
50-21-5	C3H6O3	lactic acid
50-23-7	C21H30O5	hydrocortisone
502421-44-5	C18H28N6O6	L-Valine, N-[(1,1-dimethylethoxy)carbonyl]-, 2-[(2-amino-1,6-dihydro-6-oxo-9H-purin-9-yl)methoxy]ethyl ester
502-44-3	C6H10O2	hexan-6-olide
50-24-8	C21H28O5	prednisolone
50-28-2	C18H24O2	estradiol
503-01-5	C9H19N	isometheptene
50372-61-7	C11H7Br2NO	(4,5-dibromo-1H-pyrrol-2-yl)(phenyl)methanone
504-02-9	C6H8O2	cyclohexane-1,3-dione

504-60-9	C5H8	penta-1,3-diene
504-63-2	C3H8O2	propane-1,3-diol
50-48-6	C20H23N	Amitryptiline
505-32-8	C20H40O	3,7,11,15-tetramethylhexadec-1-en-3-ol
5056-17-7	C10H12O2	(E,E,E)-2,7-dimethylocta-2,4,6-trienedial
505-65-7	C5H10O2	1,3-dioxepane
506-51-4	C24H50O	tetracosanol
50675-18-8	C6H10O2	Tetrahydro-2H-pyran-4-carbaldehyde
50892-62-1	C13H9ClN2O	8-chloro-5,10-dihydro-11H-dibenzo[b,e][1,4]diazepin-11-one
5089-70-3	C9H21ClO3Si	(3-chloropropyl)triethoxysilane
50910-55-9	C7H5Br2NO	2-amino-3,5-dibromobenzaldehyde
50940-49-3	C9H12O6	MAES
50977-10-1	C16H35NO	3-(isotridecyloxy)propylamine
51000-52-3	C12H22O2	vinyl neodecanoate
5102-83-0	C36H34Cl2N6O4	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]
51-03-6	C19H30O5	2-(2-butoxyethoxy)ethyl 6-propylpiperonyl ether
51076-95-0	C8H17ClO3	2-chloro-1,1,1-triethoxy-ethane
1175324	C7H11NO2	4-(1-oxo-2-propenyl)-morpholine
5124-30-1	C15H22N2O2	4,4'-methylenedicyclohexyl diisocyanate
5128-28-9	C6H2N4O6	4,6-dinitro-2,1,3-benzoxadiazole 1-oxide
5131-66-8	C7H16O2	1-butoxypropan-2-ol
513-35-9	C5H10	2-methylbut-2-ene
51336-95-9	C8H5ClF2O	2-Chloro-1-(3,4-difluorophenyl)ethanone
51368-55-9	C7H13BrO2	isopropyl 2-bromo-2-methylpropionate
513-85-9	C4H10O2	butane-2,3-diol
515851-08-8	C13H21Cl3N4	N4-[3-(1H-imidazol-1-yl)propyl]-2-methylbenzene-1,4-diamine trihydrochloride
51594-55-9	C3H5ClO	(R)-1-chloro-2,3-epoxypropane
517-23-7	C6H8O3	α-acetyl-γ-butyrolactone
518048-03-8	C16H19FN4O3	2-(1-amino-1-methylethyl)-N-(4-fluorobenzyl)-5-hydroxy-1-methyl-6-oxo-1,6-dihydropyrimidine-4-carboxamide
51997-51-4	C15H13NO2	4-(oxiran-2-ylmethoxy)-9H-carbazole
5205-93-6	C9H18N2O	N-[3-(dimethylamino)propyl]methacrylamide
5208-93-5	C15H24O	3-methyl-1-(2,6,6-trimethylcyclohex-1-en-1-yl)penta-1,4-dien-3-ol
521-18-6	C19H30O2	androstanolone
5216-25-1	C7H4Cl4	α,α,α,4-tetrachlorotoluene
52298-44-9	C14H16N2O4S	4-amino-2,5-dimethoxy-N-phenylbenzenesulphonamide
52299-25-9	C8HF18O2P	bis(nonafluorobutyl)phosphinic acid
5248-39-5	C6H10N4O	4-methoxy-N,6-dimethyl-1,3,5-triazin-2-ylamine
52589-39-6	C13H16O6	dimethyl 2,2'-[(4-methylbenzene-1,2-diyl)bis(oxy)]diacetate
52603-48-2	C7H5N3S	5-amino-3-methyl-2,4-thiophenedicarbonitrile

52688-08-1	C11H19NO2	no name
526-95-4	C6H12O7	D-gluconic acid
526-98-7	C6H10O7	L-xylo-hex-2-ulosonic acid
52722-86-8	C11H23NO2	4-hydroxy-2,2,6,6-tetramethylpiperidine-1-ethanol
1234986	C18H14N2O6S	calcium 3-hydroxy-4-[(4-methyl-2-sulphonatophenyl)azo]-2-naphthoate
52829-07-9	C28H52N2O4	bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate
52894-02-7	C24H51O3P	bis(2-ethylhexyl)octylphosphonate
52950-18-2	C8H7ClO3	(2R)-2-(2-chlorophenyl)-2-hydroxyethanoic acid
52950-19-3	C8H7ClO3	(S)-(+)-2-(2-Chlorophenyl)-2-hydroxyacetic acid
530-78-9	C14H10F3NO2	flufenamic acid
531-18-0	C9H18N6O6	1,3,5-triazine-2,4,6-triyltrinitrilohexamethanol
53-16-7	C18H22O2	estrone
53201-62-0	C20H14O6	Bis-4-(hydroxybenzoyl)hydrochinone
53207-58-2	C11H14OS	2-Methyl-1-[4-(methylthio)phenyl]-1-propanone
53306-54-0	C28H46O4	bis(2-propylheptyl) phthalate
5333-42-6	C20H42O	2-octyldodecan-1-ol
5333-84-6	C9H10O3	1,2,3,6-tetrahydro-3-methylphthalic anhydride
5343-44-2	C20H41NO	N,N-dibutyldodecanamide
5343-92-0	C5H12O2	pentane-1,2-diol
5344-48-9	C7H5NO7S	Potassium 2-carboxy-5-nitrobenzenesulfonate
53445-37-7	C9H16O4	2,2,4(or 2,4,4)-trimethyladipic acid
534-52-1	C7H6N2O5	2-methyl-4,6-dinitro-phenol, DNOC
1260545	C7H14N2	3-diethylaminopropiononitrile
53595-66-7	C4H4ClNO2S2	5-Chlorothiophene-2-Sulfonamide
53651-69-7	C6H12O3	propyl (2S)-2-hydroxypropanoate
536759-91-8	C22H20N4O6	ethyl 1-(4-methoxyphenyl)-6-(4-nitrophenyl)-7-oxo-4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-3-carboxylate
1267606	C8H16O4	Reaction mass of [cis-1,1,4,4-Tetramethoxy-2-butene + cis-1,1,4,4-Tetramethoxy-2-butene]
5372-81-6	C10H11NO4	dimethyl 2-aminoterephthalate
53-86-1	C19H16ClNO4	indometacin
5392-40-5	C10H16O	citral
5405-40-3	C6H10O3	(S)-2-Hydroxy-3,3-dimethyl-4-butanolide
540-84-1	C8H18	2,2,4-trimethylpentane
540-88-5	C6H12O2	tert-butyl acetate
540-97-6	C12H36O6Si6	dodecamethylcyclohexasiloxane
541-02-6	C10H30O5Si5	decamethylcyclopentasiloxane
541-05-9	C6H18O3Si3	hexamethylcyclotrisiloxane
541-41-3	C3H5ClO2	ethyl chloroformate
541-73-1	C6H4Cl2	1,3-dichlorobenzene
5417-35-6	C8H14O2	4,7-dihydro-2-isopropyl-1,3-dioxepin
5419-55-6	C9H21BO3	triisopropyl borate
54197-66-9	C9H9NO2	6-hydroxy-3,4-dihydroquinolin-2(1H)-one
5435-64-3	C9H18O	3,5,5-trimethylhexanal

54423-67-5	C11H20O2	vinyl neononanoate
54464-54-9	C16H26O	1-[1,6-dimethyl-3-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one
54527-65-0	C14H19NO3	2-(benzylmethylamino)ethyl acetoacetate
54549-24-5	C12H24O6	hexyl D-glucoside
1299990	C10H14O6	ethylene diacetoacetate
1300511	C10H9NO7S2	sodium hydrogen 4-amino-5-hydroxynaphthalene-2,7-disulphonate
54639-48-4	C28H24N2O5S	diphenylmethyl (6R,7R)-3-hydroxy-8-oxo-7-[(phenylacetyl)amino]-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate.
54660-00-3	C18H12N2O2	3,6-diphenyl-2,5-dihydropyrrolo[3,4-c]pyrrole-1,4-dione
5466-77-3	C18H26O3	2-ethylhexyl 4-methoxycinnamate
5468-75-7	C34H30Cl2N6O4	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxobutyramide]
54761-87-4	C19H18N2O2	2-benzoyl-1,2,3,6,7,11b-hexahydro-4H-pyrazino[2,1-a]isoquinolin-4-one
54811-38-0	C8H7IO2	5-iodo-2-methylbenzoic acid
54839-24-6	C7H14O3	2-ethoxy-1-methylethyl acetate
54914-85-1	C16H18O2	1,2-bis(3-methylphenoxy)ethane
54914-95-3	C7H9NO3S	sodium 2-amino-5-methylbenzenesulfonate
54982-83-1	C14H24O4	1,4-dioxacyclohexadecane-5,16-dione
5510-99-6	C14H22O	di-sec-butylphenol, mixed isomers
551-16-6	C8H12N2O3S	6-aminopenicillanic acid
5521-55-1	C6H6N2O2	5-methylpyrazine-2-carboxylic acid
552-30-7	C9H4O5	benzene-1,2,4-tricarboxylic acid 1,2-anhydride
55314-16-4	C10H12N2O	3-Dimethylamino-1-(pyrid-3-yl)-2-propen-1-one
553-86-6	C8H6O2	(3H)-benzofuran-2-one
554-00-7	C6H5Cl2N	2,4-dichloroaniline
554-52-9	C9H13NO2	4-(2-aminoethyl)-2-methoxyphenol
55-63-0	C3H5N3O9	glycerol trinitrate
556-52-5	C3H6O2	2,3-epoxypropan-1-ol
556-67-2	C8H24O4Si4	octamethylcyclotetrasiloxane
5567-15-7	C36H32Cl4N6O8	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-chloro-2,5-dimethoxyphenyl)-3-oxobutyramide]
556-82-1	C5H10O	3-methylbut-2-en-1-ol
5571-36-8	C20H26O3	cyclic 3-(1,2-ethanediylacetale)-estra-5(10),9(11)-diene-3,17-dione
557-20-0	C4H10Zn	diethylzinc
55818-57-0	C21H20O6	DGEBA diacrylate
558-30-5	C4H8O	2,2-dimethyloxirane
55934-93-5	C13H28O4	[(butoxymethylethoxy)methylethoxy]propan-1-ol
560-62-3	C19H26O3	9.alpha.-Hydroxyandrost-4-ene-3,17-dione
56107-04-1	C14H22O	3-(p-tert-butylphenyl)-2-methylpropanol

561-41-1	C24H29N3O	4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol [with â‰¥ 0.1% of Michler's ketone (EC No. 202-027-5) or Michler's base (EC No. 202-959-2)]
56358-17-9	C18H25N	N-(2-ethylhexyl)naphthalen-2-amine
56-35-9	C24H54OSn2	bis(tributyltin) oxide
563-78-0	C6H12	2,3-dimethylbut-1-ene
563-80-4	C5H10O	3-methylbutanone
5638-76-6	C8H12N2	betahistine
56519-71-2	C19H36O4	propane-1,3-diyl dioctanoate
56552-15-9	C8H14O5	4,4'-(oxy-(bismethylene))-bis-1,3-dioxolane
565-62-8	C6H10O	3-methylpent-3-en-2-one
5669-19-2	C10H10O2	2-Benzylacrylicacid
56706-10-6	C18H42O6S2Si2	4,4,13,13-tetraethoxy-3,14-dioxa-8,9-dithia-4,13-disilahexadecane
56718-71-9	C9H12O2	p-(2-methoxyethyl)phenol
56-81-5	C3H8O3	glycerol
56-84-8	C4H7NO4	aspartic acid
56-86-0	C5H9NO4	glutamic acid
56914-82-0	C4Cl3NOS	3,4-dichloroisothiazole-5-carbonyl chloride
5693-27-6	C9H6O3	1H-2-benzopyran-1,4(3H)-dione
56962-04-0	C6H4BrClO	3-Bromo-5-chlorophenol
56966-52-0	C12H8Cl3NO	5-chloro-2-(2,4-dichlorophenoxy)aniline
57043-35-3	C13H18O6	MAHP
57044-25-4	C3H6O2	R-2,3-epoxy-1-propanol
57-10-3	C16H32O2	palmitic acid
57-11-4	C18H36O2	stearic acid
57144-06-6	C20H28O2	3-methoxyandrosta-3,5-dien-17-one
57280-22-5	C7H12O3	4,4-dimethyl-3,5,8-trioxabicyclo[5.1.0]octane
57472-68-1	C12H18O5	oxybis(methyl-2,1-ethanediyl) diacrylate
574-93-6	C32H18N8	29H,31H-phthalocyanine
57-55-6	C3H8O2	propane-1,2-diol
57-57-8	C3H4O2	propiolactone
57583-34-3	C31H60O6S3Sn	2-ethylhexyl 10-ethyl-4-[[2-[(2-ethylhexyl)oxy]-2-oxoethyl]thio]-4-methyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
57583-35-4	C22H44O4S2Sn	2-ethylhexyl 10-ethyl-4,4-dimethyl-7-oxo-8-oxa-3,5-dithia-4-stannatetradecanoate
57583-54-7	C30H24O8P2	tetraphenyl m-phenylene bis(phosphate)
576-26-1	C8H10O	2,6-xylenol
57675-44-2	C60H110O6	Fatty acids, C16-18, even numbered and C18-unsatd. esters with Propylidynetrimethanol
57-83-0	C21H30O2	progesterone
5788-17-0	C5H8O3	methyl-3-methoxyacrylate
58-08-2	C8H10N4O2	caffeine
581076-60-0	C20H24N4O3	N-(4-Methyl-3-nitro-phenyl)-4-(4-methyl-piperazin-1-ylmethyl)-benzamide
58-22-0	C19H28O2	testosterone

584-84-9	C9H6N2O2	4-methyl-m-phenylene diisocyanate
585-07-9	C8H14O2	tert-butyl methacrylate
58-55-9	C7H8N4O2	theophylline
58670-89-6	C24H50O	2-decyltetradecanol
5873-54-1	C15H10N2O2	o-(p-isocyanatobenzyl)phenyl isocyanate
58861-48-6	C10H7FS	2-(4-fluorophenyl)thiophene
58-86-6	C5H10O5	xylose
58890-25-8	C27H36N4O2	3,3'-dicyclohexyl-1,1'-methylenebis(4,1-phenylene)diurea
590-19-2	C4H6	buta-1,2-diene
59084-08-1	C21H25NO2	Ethyl 1-benzyl-4-phenyl-4-piperidinecarboxylate
590-86-3	C5H10O	isovaleraldehyde
591-51-5	C6H5Li	phenyllithium
5922-69-0	C6H14N2O	N-[3-(dimethylamino)propyl]formamide
59227-88-2	C14H27NO	1-octylazepin-2-one
592-41-6	C6H12	hex-1-ene
5926-26-1	C4H11ClO3Si	(Chloromethyl)trimethoxysilane
59354-78-8	C9H18O2	neononanoic acid
5945-33-5	C39H34O8P2	(1-methylethylidene)di-4,1-phenylenetetraphenyl diphosphate
5958-24-7	C15H10Cl2N2O	Quinazoline, 6-chloro-2-(chloromethyl)-4-phenyl-, 3-oxide
59653-74-6	C12H15N3O6	1,3,5-tris[(2S and 2R)-2,3-epoxypropyl]-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione (Î²-TGIC)
59673-82-4	C15H12Cl2N2O3	methyl 2-amino-4-[[(2,5-dichlorophenyl)amino]carbonyl]benzoate
59721-67-4	C15H20O	4-cyclohexylpropiophenone
598-56-1	C4H11N	ethyldimethylamine
598-78-7	C3H5ClO2	2-chloropropionic acid
5989-27-5	C10H16	(R)-p-mentha-1,8-diene
599-04-2	C6H10O3	α-hydroxy-β,β-dimethyl-γ-butyrolactone
5994-61-6	C5H10NO7P	N-(carboxymethyl)-N-(phosphonomethyl)glycine
599-64-4	C15H16O	4-(α,α-dimethylbenzyl)phenol
600-00-0	C6H11BrO2	ethyl 2-bromo-2-methylpropionate
60-00-4	C10H16N2O8	edetic acid
60-09-3	C12H11N3	4-aminoazobenzene
60-29-7	C4H10O	diethyl ether
603-35-0	C18H15P	triphenylphosphine
605-50-5	C18H26O4	diisopentyl phthalate
6065-63-0	C13H24O4	diethyl dipropylmalonate
60728-43-0	C29H23Cl3N6O8	3,3'-((2-chloro-5-methylbenzene-1,4-diyl)bis(imino(1,3-dioxobutane-1,2-diyl)diazene-2,1-diyl))bis(4-chlorobenzoic acid)
60-80-0	C11H12N2O	phenazone
60811-21-4	C6H3BrClF	4-bromo-2-chlorofluorobenzene
608-27-5	C6H5Cl2N	2,3-dichloroaniline
609-15-4	C6H9ClO3	ethyl 2-chloroacetoacetate

61010-04-6	C8H9ClO2	2-chloro-3-(hydroxymethylene)cyclohex-1-ene-1-carbaldehyde
6104-30-9	C6H14N4O2	N,N''-(isobutylidene)diurea
611-06-3	C6H3Cl2NO2	1,3-dichloro-4-nitrobenzene
611-19-8	C7H6Cl2	α,2-dichlorotoluene
611-20-1	C7H5NO	salicylonitrile
6112-76-1	C5H6N4S	1,7-dihydro-6H-purine-6-thione hydrate (1:1)
611-70-1	C10H12O	isobutyrophenone
61203-94-9	C15H22	4-trans-Propylcyclohexylbenzene
61260-55-7	C24H50N4	N,N'-bis(2,2,6,6-tetramethylpiperidin-4-yl)hexane-1,6-diamine
61320-65-8	C8H8N2O2S	methyl 5-amino-4-cyano-3-methylthiophene-2-carboxylate
61337-89-1	C17H21N3O	1-[3-(Hydroxymethyl)pyridin-2-yl)-4-methyl-2-phenylpiperazine
613-62-7	C17H14O	2-(phenylmethoxy)naphthalene
614-45-9	C11H14O3	tert-butyl perbenzoate
615-16-7	C7H6N2O	2-hydroxybenzimidazole
6156-18-9	C5H12S2	2,2-Bis(methylthio)propane
61571-06-0	C6H10OS	tetrahydrothiopyran-3-carboxaldehyde
616-30-8	C3H9NO2	3-aminopropane-1,2-diol
616-38-6	C3H6O3	dimethyl carbonate
616-45-5	C4H7NO	2-pyrrolidone
6166-86-5	C5H20O5Si5	2,4,6,8,10-pentamethylcyclopentasiloxane
61718-80-7	C13H15F3O2	5-methoxy-4'-(trifluoromethyl)valerophenone
6172-80-1	C5H13O2P	butyl methylphosphinate
617-48-1	C4H6O5	DL-malic acid
61788-32-7	C18H22	Terphenyl, hydrogenated
61788-44-1	C10H10O	Phenol, styrenated
61832-41-5	C4H8N2O2S	N-methyl-1-(methylthio)-2-nitrovinylamine
6195-20-6	C19H30ClNO2	dodecyl 3-amino-4-chlorobenzoate
6197-30-4	C24H27NO2	octocrilene
62037-80-3	C6H4F11NO3	Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate
62211-93-2	C11H16O7	1,2,3-Triacetyl-5-deoxy-D-ribose
62285-89-6	C28H32ClO2P	[(2E)-3-(5,5-dimethyl-1,3-dioxan-2-yl)-2-butenyl]triphenylphosphonium chloride
623-03-0	C7H4ClN	4-chlorobenzonitrile
623-36-9	C6H10O	2-methylpent-2-enal
623-53-0	C4H8O3	Ethyl methyl carbonate
623-84-7	C7H12O4	propane-1,2-diyl diacetate
624-48-6	C6H8O4	dimethyl maleate
6246-48-6	C10H19N	(2E)-3,7-dimethylocta-2,6-dien-1-amine
62478-82-4	C9H22N2	N,N-diethyl-N',N'-dimethylpropan-1,3-diamine
624-86-2	C2H7NO	O-ethylhydroxylamine
62-53-3	C6H7N	aniline
625-45-6	C3H6O3	methoxyacetic acid

6259-76-3	C13H18O3	hexyl salicylate
626-43-7	C6H5Cl2N	3,5-dichloroaniline
62756-44-9	C6H8FNO	Fluoronicomethanol
627-93-0	C8H14O4	dimethyl adipate
6283-86-9	C11H22O3	2-ethylhexyl lactate
62889-66-1	C19H41NO2	1,1'-(tridecylimino)bis-2-propanol
6289-46-9	C10H12O6	dimethyl 2,5-dioxocyclohexane-1,4-dicarboxylate
629-11-8	C6H14O2	hexane-1,6-diol
6291-89-0	C8H11N3O3	1-Phenylguanidine hemicarbonate
629-50-5	C13H28	tridecane
629-59-4	C14H30	tetradecane
629-73-2	C16H32	hexadec-1-ene
629-82-3	C16H34O	dioctyl ether
629-96-9	C20H42O	icosan-1-ol
63-05-8	C19H26O2	androst-4-ene-3,17-dione
63187-91-7	C13H24O3	2-hydroxymethyl-9-methyl-6-(1-methylethyl)-1,4-dioxaspiro[4.5]decane
632-79-1	C8Br4O3	tetrabromophthalic anhydride
6330-25-2	C4H6N2O	2-cyano-N-methylacetamide
6331-96-0	C6H5Cl2NO3S	2-amino-4,5-dichlorobenzenesulfonic acid
6334-25-4	C14H28N2O6	N,N,N',N',-tetrakis(2-hydroxyethyl)hexanediamide
634-55-9	C7H9NO3	ethyl 2-cyano-3-oxobutanoate
6358-30-1	C34H22Cl2N4O2	8,18-dichloro-5,15-diethyl-5,15-dihydrodiindolo[3,2-b:3',2'-m]triphenodioxazine
6358-31-2	C18H18N4O6	2-[(2-methoxy-4-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide
6358-37-8	C34H30Cl2N6O4	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(4-methylphenyl)-3-oxobutyramide]
6358-64-1	C8H10ClNO2	4-chloro-2,5-dimethoxyaniline
6358-85-6	C32H26Cl2N6O4	2,2'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[3-oxo-N-phenylbutyramide]
636-30-6	C6H4Cl3N	2,4,5-trichloroaniline
6364-17-6	C13H14N2	2,3-dihydro-2,2-dimethyl-1H-perimidine
63675-73-0	C16H16O3S	Beta Ketosulfide
637-92-3	C6H14O	2-ethoxy-2-methylpropane
6386-38-5	C18H28O3	methyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate
63968-64-9	C15H22O5	(3R,5aS,6R,8aS,9R,12S,12aR)-3,6,9-trimethyloctahydro-3,12-epoxypyrano[4,3-j][1,2]benzodioxepin-10(3H)-one
641571-11-1	C11H10F3N3	3-(4-Methyl-1H-imidazol-1-yl)-5-(trifluoromethyl)aniline
6419-19-8	C3H12NO9P3	nitrilotrimethylenetris(phosphonic acid)
6422-86-2	C24H38O4	bis(2-ethylhexyl) terephthalate
64354-92-3	C13H25NO	3-(isodecyloxy)propiononitrile
64485-90-1	C25H21N3O3S	(2Z)-(Methoxyimino)[2-(tritylamino)-1,3-thiazol-4-yl]acetic acid
645-62-5	C8H14O	2-ethylhex-2-enal

646-06-0	C3H6O2	1,3-dioxolane
64-67-5	C4H10O4S	diethyl sulphate
64744-50-9	C9H15NO	3,3-pentamethylene-4-butyrolactam
64838-55-7	C11H17NO4S	(S)-1-[3-(acetylthio)-2-methyl-1-oxopropyl]-L-proline
6485-55-8	C6H13NO	cis-2,6-dimethylmorpholine
64-86-8	C22H25NO6	colchicine
65181-78-4	C38H32N2	N,N'-diphenyl-N,N'-bis(3-methylphenyl)-(1,1'-diphenyl)-4,4'-diamine
652-37-9	C9H10N4O4	theophyllin-7-ylacetic acid
652-67-5	C6H10O4	1,4:3,6-dianhydro-D-glucitol
6535-46-2	C24H16Cl3N3O2	3-hydroxy-N-(o-tolyl)-4-[(2,4,5-trichlorophenyl)azo]naphthalene-2-carboxamide
65405-84-7	C14H24O	α,2,2,6-tetramethylcyclohexene-1-butyraldehyde
65-45-2	C7H7NO2	salicylamide
654-70-6	C12H8N2O	4-amino-2-(trifluoromethyl)benzonitrile
65-85-0	C7H6O2	benzoic acid
65855-02-9	C12H14N2O3	1-benzyl-5-ethoxyimidazolidine-2,4-dione
65962-45-0	C17H34N2	3,3’,5,5’-tetramethyl-4,4’-diaminodicyclohexylmethane
66063-15-8	C12H16ClN	4-chloro-N-cyclopentylbenzylamine
6607-34-7	C10H16O5	2,3,7,8-tetrahydro-2,5,8-benzotrioxacycloundecine-1,9-dione
6607-41-6	C26H19NO3	3,3-Bis(4-hydroxyphenyl)-2-phenylisoindolin-1-one
661-19-8	C22H46O	docosan-1-ol
6613-44-1	C9H9ClO	3,5-dimethylbenzoyl chloride
66309-83-9	C11H12O	2,3-Dihydro-2,6-dimethyl-1H-inden-1-one
66356-53-4	C10H18N2OS	5-[[(2-aminoethyl)thio]methyl]-N,N-dimethyl-2-furfurylamine
6642-31-5	C6H9N3O2	6-amino-1,3-dimethyluracil
666816-98-4	C10H9BrN4O2	8-Bromo-7-but-2-inyl-3-methyl-3,7-dihydro-purin-2,6-dione
66682-07-3	C7H2Cl6	1,2,3-trichloro-5-(trichloromethyl)benzene
66742-57-2	C14H11FO2	4-(3-Fluorbenzyloxy)benzaldehyd
6683-19-8	C73H108O12	pentaerythritol tetrakis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate)
669005-94-1	C28H23F3N6	4-Methyl-2,6-bis-p-tolylamino-5-(2-trifluoromethyl-phenylazo)-nicotinonitrile
6731-36-8	C17H34O4	di-tert-butyl 3,3,5-trimethylcyclohexylidene diperoxide
67330-25-0	C18H18F3NO2	butyl 2-{[3-(trifluoromethyl)phenyl]amino}benzoate
67-43-6	C14H23N3O10	N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid)
6746-94-7	C5H6	Ethynyl cyclopropane
674-82-8	C4H4O2	but-3-en-3-olide
67-52-7	C4H4N2O3	barbituric acid
67567-23-1	C16H32O6	ethyl 3,3-bis[(1,1-dimethylpropyl)peroxy]butyrate
67-63-0	C3H8O	propan-2-ol
67-64-1	C3H6O	acetone

1776823	C12H8ClNO2S	1-(4-chlorophenyl)sulfanyl-2-nitrobenzene
67843-74-7	C3H5ClO	(S)-Epichlorohydrin
6786-83-0	C33H33N3O	Î±,Î±-Bis[4-(dimethylamino)phenyl]-4 (phenylamino)naphthalene-1-methanol (C.I. Solvent Blue 4) [with â‰¥ 0.1% of Michler's ketone (EC No. 202-027-5) or Michler's base (EC No. 202-959-2)]
67881-98-5	C11H22NO6P	2-(Methacryloyloxyethyl)-2'-((trimethylammonium)ethyl)phosphate
67911-21-1	C7H8O3	(1R,5S)-6,6-Dimethyl-3-oxabicyclo[3.1.0]hexane-2,4-dione
6807-17-6	C18H22O2	4,4-isobutylethylidenediphenol
68-12-2	C3H7NO	N,N-dimethylformamide
682-09-7	C12H22O3	2,2-bis(allyloxymethyl)butan-1-ol
68-22-4	C20H26O2	norethisterone
68-26-8	C20H30O	retinol
683-18-1	C8H18Cl2Sn	dibutyltin dichloride
68412-54-4	C19H32O3	2-{2-[4-(2,4,5-trimethylhexan-3-yl)phenoxy]polyethoxy}ethanol
6842-62-2	C12H8Cl2O	1-chloro-3-(4-chlorophenoxy) benzene
6846-50-0	C16H30O4	1-isopropyl-2,2-dimethyltrimethylene diisobutyrate
68479-04-9	C19H42N2O	1,3-Propanediamine, N-[3-(tridecyloxy)propyl]-, branched
68479-06-1	C16H31NO	Propanenitrile, 3-(tridecyloxy)-, branched and linear
68479-98-1	C11H18N2	diethylmethylbenzenediamine
6850-63-1	C8H17N	2,6-dimethylcyclohexylamine
685-88-1	C7H11FO4	diethyl fluoromalonate
6864-37-5	C15H30N2	2,2'-dimethyl-4,4'-methylenebis(cyclohexylamine)
68684-63-9	C22H20O	Ethanamine, 2-(4-(1,2-diphenyl-1-butenyl)phenoxy)-N,N-dimethyl-, (Z)-, 2-hydroxy- 1,2,3-propanetricarboxylate (1:1)
1816263	C14H17NO2	Methyl 1,3,3-trimethyl-2-methylidene-2,3-dihydro-1H-indole-5-carboxylate
687-47-8	C5H10O3	ethyl (S)-2-hydroxypropionate
68860-54-8	C14H28O3	1,1-dimethylpropyl 3,5,5-trimethylperoxyhexanoate
688-84-6	C12H22O2	2-ethylhexyl methacrylate
68909-95-5	C16H35NO	3-(tridecyloxy)propylamine, branched and linear
68937-40-6	C30H39O4P	Phenol, isobutylenated, phosphate (3:1)
68937-41-7	C27H33O4P	Phenol, isopropylated, phosphate (3:1)
689-67-8	C13H22O	6,10-dimethylundeca-5,9-dien-2-one
69011-06-9	C8H4O6Pb3	[phthalato(2-)]dioxotrilead
69045-82-5	C6H3F4N	2-Fluoro-6-trifluoromethylpyridine
69045-84-7	C6H2Cl2F3N	2,3-dichloro-5-trifluoromethylpyridine
69098-08-4	C12H16O4	3-(4-methoxy phenyl)-3-methoxy propionic acid methyl ester
6915-15-7	C4H6O5	malic acid
69184-17-4	C8H7Cl2FN2O3	methyl O-(4-amino-3,5-dichloro-6-fluoropyridin-2-yloxy)acetate

693-23-2	C12H22O4	dodecanedioic acid
693-36-7	C42H82O4S	dioctadecyl 3,3'-thiodipropionate
693-98-1	C4H6N2	2-methylimidazole
6940-53-0	C8H8ClNO4	1-chloro-2,5-dimethoxy-4-nitrobenzene
69555-14-2	C17H17NO2	Ethyl 2-(diphenylmethyleneamino)acetate
696-23-1	C4H5N3O2	2-methyl-4-nitroimidazole
6962-44-3	C10H13NO2	N-(2-methoxy-5-methylphenyl)acetamide
6969-71-7	C6H5N3O	1,2,4-triazolo[4,3-a]pyridin-3(2H)-one
69-72-7	C7H6O3	Acetyl salycilic acid metabolite: Salicylic acid
69739-16-8	C20H20N6O7S4	(6R,7R)-7-{[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-(methoxyimino)acetyl]amino}-3-({[5-(carboxymethyl)-4-methyl-1,3-thiazol-2-yl]sulfanyl}methyl)-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
69788-75-6	C13H17ClO4	4-chlorobutyl veratrate
698-29-3	C6H6N4	4-amino-2-methylpyrimidine-5-carbonitrile
69901-75-3	C16H21NO4	(2S)-[[(benzyloxy)carbonyl]amino](cyclohexyl)acetic acid
699-83-2	C8H8O3	2',6'-dihydroxyacetophenone
700-13-0	C9H12O2	2,3,5-trimethylhydroquinone
1872907	C10H15NO	3-cyano-3,5,5-trimethylcyclohexanone
704-10-9	C8H5Cl2FO	1-(2,4-dichloro-5-fluorophenyl)ethanone
70445-33-9	C11H24O3	3-(2-ethylhexyloxy)propane-1,2-diol
1880366	C3H10ClNO3S	(2R)-2-amino-3-sulfanyl-propanoic acid hydrochloride monohydrate
705283-58-5	C11H14BrNO2	N-benzyl-2-bromo-3-methoxypropanamide
70693-64-0	C14H17N5O2S	5-nitro-2-(2-methyl-4-(diethylamino)phenylazo)thiazole
7069-42-3	C23H34O2	retinyl propionate
7085-19-0	C10H11ClO3	mecoprop (MCPP)
7085-85-0	C6H7NO2	ethyl 2-cyanoacrylate
70918-00-2	C13H16N2O3	2,3-Dihydro-1,4-benzodioxin-2-yl(piperazin-1-yl)methanone
70918-74-0	C13H17ClN2O3	1-(1,4-benzodioxan-2-ylcarbonyl)piperazine hydrochloride
71048-82-3	C13H20O	[1α(E),2β]-1-(2,6,6-trimethylcyclohex-3-en-1-yl)but-2-en-1-one
71-23-8	C3H8O	propan-1-ol
712-50-5	C13H16O	cyclohexyl phenyl ketone
71-36-3	C4H10O	butan-1-ol
1913545	C16H20Cl2N6	2,6-dichloro-4,8-dipiperidinopyrimido[5,4-d]pyrimidine
71-41-0	C5H12O	pentan-1-ol
71420-85-4	C10H11N6NaO6S3	sodium (6R-trans)-7-amino-8-oxo-3-[[[1-(sulfomethyl)-1H-tetrazol-5-yl]thio]methyl]-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate monohydrate
71-43-2	C6H6	benzene
71617-10-2	C15H20O3	isopentyl p-methoxycinnamate
7173-62-8	C21H44N2	(Z)-N-9-octadecenylpropane-1,3-diamine

71839-12-8	C12H17NO2	Methyl 4-(butylamino)benzoate
71868-10-5	C15H21NO2S	2-methyl-1-(4-methylthiophenyl)-2-morpholinopropan-1-one
718-71-8	C13H15NO2	Ethyl 2-cyano-2-phenylbutanoate
7195-44-0	C14H14O6	bis(2,3-epoxypropyl) terephthalate
7212-44-4	C15H26O	3,7,11-trimethyldodeca-1,6,10-trien-3-ol,mixed isomers
72217-12-0	C5H6N4O3S	(5-Amino-[1,2,4]thiadiazol-3-yl)-methoxyimino-acetic acid
7226-23-5	C6H12N2O	tetrahydro-1,3-dimethyl-1H-pyrimidin-2-on; dimethylpropyleenureum
72291-30-6	C6H9NO2	2-cyano-2-methyl-propanoic acid methyl ester
72621-59-1	C10H11N3O3S	N-[(2-methyl-5-nitrophenyl)carbamothioyl]acetamide
72684-95-8	C9H9NO3	4-hydroxy-3,5-dimethoxybenzonitrile
72714-62-6	C10H14Cl3F3O2	methyl 4,6,6-trichloro-7,7,7-trifluoro-3,3-dimethylheptanoate
72869-86-4	C23H38N2O8	7,7,9(or 7,9,9)-trimethyl-4,13-dioxo-3,14-dioxa-5,12-diazahexadecane-1,16-diyl bismethacrylate
72955-94-3	C31H32N2O4	1-{benzyl[2-(2-methoxyphenoxy)ethyl]amino}-3-(9H-carbazol-4-yloxy)propan-2-ol
7299-99-2	C37H68O8	2,2-bis[[(2-ethyl-1-oxohexyl)oxy]methyl]propane-1,3-diyl bis(2-ethylhexanoate)
7319-16-6	C4H8O	(E)-1-methoxyprop-1-ene
732-26-3	C18H30O	2,4,6-tri-tert-butylphenol
7327-60-8	C6H6N4	nitrilotriacetonitrile
73344-75-9	C11H15NO2	(3,4-Dimethoxy-bicyclo[4.2.0]octa-1,3,5-trien-7-yl)-methylamine
73573-88-3	C23H34O5	(1S,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxotetrahydro-2H-pyran-2-yl]ethyl}-7-methyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl(2S)-2-methylbutanoate
7357-67-7	C7H14ClNO	4-(3-chloropropyl)morpholine
73754-27-5	C45H71NO6	4-[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionyloxy]-1-[2-[3-(3,5-di-tert-butyl-4-hydrophenyl)propionyloxy]ethyl]-2,2,6,6-tetramethylpiperidine
7378-99-6	C10H23N	dimethyl(octyl)amine
7381-13-7	C20H24N2O4	1,1'-(1,3-Phenylenedicarbonyl)diazepan-2-one
7384-80-7	C10H14O	2-methyl-3-phenylpropanol
7396-58-9	C21H45N	N-methyldidecylamine
7397-46-8	C5H13BO	Demb
7397-62-8	C6H12O3	butyl glycollate
74149-72-7	C20H20N2O7	Methyl 4-[4-(4-methoxybenzoylamino)-3-nitrophenyl]-3-methyl-4-oxo-butyrate
74351-78-3	C30H26Cl2N6O8	3,3'-((2,5-dimethylbenzene-1,4-diyl)bis(imino(1,3-dioxobutane-1,2-diyl)diazene-2,1-diyl))bis(4-chlorobenzoic acid)
74441-06-8	C14H13N3O2	4-amino-N-[4-(aminocarbonyl)phenyl]benzamide
74638-76-9	C4H11N4O	2,4-Diamino pyrimidine-3-oxide
7473-98-5	C10H12O2	2-hydroxy-2-methylpropiophenone
74805-60-0	C10H8N2O2	(5Z)-5-benzylideneimidazolidine-2,4-dione
74-85-1	C2H4	ethyleen

74860-00-7	C23H16N2O2	2-(11H-dibenzo[b,e]azepin-6-ylmethyl)-1H-isoindole-1,3(2H)-dione
74-98-6	C3H8	propane
75028-24-9	C6H8N4O3S	methyl (2Z)-2-[5-(dichlorophosphorylamino)-1,2,4-thiadiazol-3-yl]-2-ethoxyimino-acetate
75-21-8	C2H4O	ethyleenoxide
75-26-3	C3H7Br	2-bromopropane
75-28-5	C4H10	isobutane
75-29-6	C3H7Cl	2-chloropropane
75302-98-6	C25H26ClNO6	(tert-Butoxycarbonyl)methyl 2-[1-[(4-chlorophenyl)carbonyl]-5-methoxy-2-methylindol-3-yl]acetate
75-31-0	C3H9N	isopropylamine
75-33-2	C3H8S	propane-2-thiol
7534-94-3	C14H22O2	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl methacrylate
754-12-1	C3H2F4	2,3,3,3-Tetrafluoropropene
7541-49-3	C20H40O	PHYTOL
75490-39-0	C13H17N	2,2,4-trimethyl-4-phenyl-butane-nitrile
75-50-3	C3H9N	trimethylamine
75-55-8	C3H7N	2-methylaziridine
75-56-9	C3H6O	methyloxirane
756-13-8	C6F12O	3-Pentanone, 1,1,1,2,2,4,5,5-nonafluoro-4-(trifluoromethyl)-
75-64-9	C4H11N	tert-butylamine
75-65-0	C4H10O	2-methylpropan-2-ol
75-66-1	C4H10S	2-methylpropane-2-thiol
756-79-6	C3H9O3P	dimethyl methylphosphonate
7575-23-7	C17H28O8S4	pentaerythritol tetrakis(3-mercaptopropionate)
75-76-3	C4H12Si	tetramethylsilane
75-77-4	C3H9ClSi	chlorotrimethylsilane
757-86-8	C5H11O4PS2	methyl [(dimethoxyphosphinothioyl)thio]acetate
7585-39-9	C42H70O35	cycloheptapentylose
75-86-5	C4H7NO	2-hydroxy-2-methylpropionitrile
75-91-2	C4H10O2	tert-butyl hydroperoxide
75-98-9	C5H10O2	pivalic acid
759-94-4	C9H19NOS	EPTC
760-23-6	C4H6Cl2	3,4-dichlorobut-1-ene
760-67-8	C8H15ClO	2-ethylhexanoyl chloride
76114-73-3	C8H13NO2	2-propynyl butylcarbamate
761-65-9	C9H19NO	N,N-dibutylformamide
763-32-6	C5H10O	3-methylbut-3-en-1-ol
763-69-9	C7H14O3	ethyl 3-ethoxypropionate
7646-67-5	C5H9NO2	N-(2-hydroxyethyl)prop-2-enamide
7659-86-1	C10H20O2S	2-ethylhexyl mercaptoacetate
766-05-2	C7H11N	cyclohexanecarbonitrile
76-72-2	C14H26O4	diethyl ethyl(1-methylbutyl)malonate

76-74-4	C11H18N2O3	pentobarbital
76-75-5	C11H18N2O2S	5-ethyl-5-(1-methylbutyl)-2-thiobarbituric acid
76801-93-9	C14H18I3N3O6	Iohexol Intermediate
7680-73-1	C6H8N	1-methylpyridinium chloride
76823-93-3	C8H11N5S2	3-(2-(diaminomethyleneamino)thiazol-4-yl)methylthio)propiononitrile
7695-91-2	C31H52O3	3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-yl acetate
770-35-4	C9H12O2	1-phenoxypropan-2-ol
77-09-8	C20H14O4	phenolphthalein
77168-63-9	C8H6N2S2	4-(4-pyridyl)-3H-thiazole-2-thione
77402-03-0	C7H11NO4	methyl acrylamidomethoxyacetate (containing ≥ 0,1 % acrylamid)
77402-05-2	C6H9NO4	methyl acrylamidoglycolate (containing ≥ 0,1 % acrylamide)
7747-35-5	C7H13NO2	7a-ethyldihydro-1H,3H,5H-oxazolo[3,4-c]oxazole
77497-97-3	C24H25NO5S	(S)-3-benzyloxycarbonyl-1,2,3,4-tetrahydro-isoquinolinium 4-methylbenzenesulfonate
77-58-7	C32H64O4Sn	dibutyltin dilaurate
776-04-5	C7H4ClF3O2S	2-(trifluoromethyl)benzenesulfonyl chloride
77-71-4	C5H8N2O2	5,5-dimethylhydantoin
77-73-6	C10H12	3a,4,7,7a-tetrahydro-4,7-methanoindene
77745-66-5	C39H81O3P	triisotridecyl phosphite
77-75-8	C6H10O	methylpentynol
7786-67-6	C10H18O	5-methyl-2-(1-methylvinyl)cyclohexan-1-ol
778-94-9	C8H3F3N2O2	2-nitro-4-(trifluoromethyl)benzonitrile
77-90-7	C20H34O8	tributyl O-acetylcitrate
77-92-9	C6H8O7	citric acid
77-99-6	C6H14O3	propylidynetrimethanol
78-00-2	C8H20Pb	tetraethyllead
78-04-6	C12H20O4Sn	dibutyltin maleate
78-10-4	C8H20O4Si	tetraethyl orthosilicate
78-11-5	C5H8N4O12	pentaerithrityl tetranitrate
78-26-2	C7H16O2	2-methyl-2-propylpropane-1,3-diol
78-40-0	C6H15O4P	triethyl phosphate
78418-01-6	C15H20O4	2-Hydroxy-5-(1-oxooctyl)benzoic acid
78-42-2	C24H51O4P	tris(2-ethylhexyl) phosphate
78-51-3	C18H39O7P	tris(2-butoxyethyl) phosphate
78531-61-0	C17H24O	4-(trans-4-propylcyclohexyl)acetophenone
78-59-1	C9H14O	3,5,5-trimethylcyclohex-2-enone
78629-20-6	C9H14O	6,6-dimethylhept-1-en-4-yn-3-ol
78-63-7	C16H34O4	di-tert-butyl 1,1,4,4-tetramethyltetramethylene diperoxide
78-67-1	C8H12N4	2,2'-dimethyl-2,2'-azodipropiononitrile
78-69-3	C10H22O	3,7-dimethyloctan-3-ol
78-70-6	C10H18O	linalool

787582-75-6	C26H21F7O2	2-{4'-[Difluoro(3,4,5-trifluorophenoxy)methyl]-3',5'-difluoro-[1,1'-biphenyl]-4-yl)}5-ethyltetrahydro-2H-pyran
78-78-4	C5H12	2-methylbutane
78-79-5	C5H8	isoprene
78-83-1	C4H10O	2-methylpropan-1-ol
78-84-2	C4H8O	isobutyraldehyde
78850-37-0	C18H23NO10	methyl (3aR,4R,7aR)-2-methyl-4-(1S,2R,3-triacetoxypropyl)-3a,7a-dihydro-4H-pyrano[3,4-d]oxazole-6-carboxylate
78-87-5	C3H6Cl2	1,2-dichloropropane
78-88-6	C3H4Cl2	2,3-dichloropropene
78-90-0	C3H10N2	propylenediamine
78-92-2	C4H10O	butan-2-ol
78-93-3	C4H8O	butanone
78-95-5	C3H5ClO	chloroacetone
78-96-6	C3H9NO	1-aminopropan-2-ol
78-97-7	C3H5NO	lactonitrile
79-06-1	C3H5NO	acrylamide
79-08-3	C2H3BrO2	Bromic acid
79-09-4	C3H6O2	propionic acid
79-10-7	C3H4O2	acrylic acid
791-28-6	C18H15OP	triphenylphosphine oxide
79-16-3	C3H7NO	N-methylacetamide
79185-77-6	C13H25NO2	7a-ethyl-3,5-bis(1-methylethyl)-2,3,4,5-tetrahydrooxazolo[3,4-c]-2,3,4,5-tetrahydrooxazole
79-20-9	C3H6O2	methyl acetate
79-31-2	C4H8O2	isobutyric acid
793-24-8	C18H24N2	N-1,3-dimethylbutyl-N'-phenyl-p-phenylenediamine
79-33-4	C3H6O3	l-(+)-lactic acid
79349-82-9	C9H10N2O3S	(6R,7R)-7-Amino-8-oxo-3-vinyl-5-thia-1-aza-bicyclo[4,2,0]oct-2-ene-2-carboxylic acid
79-39-0	C4H7NO	methacrylamide
79-41-4	C4H6O2	methacrylic acid
79-44-7	C3H6ClNO	dimethylcarbamoyl chloride
79456-26-1	C6H4ClF3N2	3-chloro-5-trifluoromethyl-2-pyridylamine
79-46-9	C3H7NO2	2-nitropropane
79-74-3	C16H26O2	2,5-di-tert-pentylhydroquinone
79-77-6	C13H20O	(E)-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-buten-2-one
79-81-2	C36H60O2	retinyl palmitate
79-92-5	C10H16	camphene
79944-37-9	C7H15NO3	trans-(5RS,6SR)-6-amino-2,2-dimethyl-1,3-dioxepan-5-ol
79-94-7	C15H12Br4O2	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol
79992-76-0	C12H22MgO4	Magnesium bis(2-ethylbutanoate)
8000-41-7	C10H18O	Terpineol

80012-43-7	C16H15N3	9,13b-Dihydro-1H-dibenz(c,f)imidazo(1,5a)azepin-3-amin
80-05-7	C15H16O2	4,4'-isopropylidenediphenol
80-07-9	C12H8Cl2O2S	bis(4-chlorophenyl) sulphone
80-09-1	C12H10O4S	4,4'-sulphonyldiphenol
80-15-9	C9H12O2	α,α-dimethylbenzyl hydroperoxide
80286-58-4	C15H22O2	2-[(1R,4R,4aS,8aR)-4,7-dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-1-yl]prop-2-enoic acid
80-43-3	C18H22O2	bis(α,α-dimethylbenzyl) peroxide
2246493	C20H30O2	Rosin
80-53-5	C10H20O2	p-menthane-1,8-diol
80-54-6	C14H20O	2-(4-tert-butylbenzyl)propionaldehyde
80-56-8	C10H16	pin-2(3)-ene
80-62-6	C5H8O2	methyl methacrylate
80675-49-6	C18H18N4O6	Butanamide, 2-[2-(2-methoxy-5-nitrophenyl)diazenyl]-N-(2-methoxyphenyl)-3-oxo-
80793-17-5	C8H5F13	1,1,1,2,2,3,3,4,4,5,5,6,6-Tridecafluoro octane
81-11-8	C14H14N2O6S2	4,4'-diaminostilbene-2,2'-disulphonic acid
81-19-6	C7H4Cl4	α,α,2,6-tetrachlorotoluene
81541-12-0	C22H26O6	1-(2,6-bis(4-tolyl)-1,3-dioxano(5,4-d)-1,3-dioxan-4-yl)ethane-1,2-diol
816431-72-8	C15H12ClNO5S	4-[(2-methoxybenzoyl)sulfamoyl]benzoyl chloride
81653-77-2	C11H13NO2S	(4S)-4-(phenylsulfanyl)-L-proline
818-08-6	C8H18OSn	dibutyltin oxide
81-81-2	C19H16O4	warfarin
81-84-5	C12H6O3	naphthalene-1,8-dicarboxylic anhydride
818-61-1	C5H8O3	2-hydroxyethyl acrylate
81936-33-6	C15H22O	4-(4-trans-propylcylohexyl)phenol
821-06-7	C4H6Br2	(E)-1,4-dibromobut-2-ene
822-06-0	C8H12N2O2	hexamethylene diisocyanate
82324-60-5	C6H6N2O5S	Reaction mass of ammonium 4-amino-3-nitrobenzenesulfonate and sodium 4-amino-3-nitrobenzenesulfonate
82410-32-0	C9H15N5O4	2-amino-9-{[(1,3-dihydroxypropan-2-yl)oxy]methyl}-6,9-dihydro-1H-purin-6-one
82413-20-5	C26H29NO2	(E)-3-[1-[4-[2-(Dimethylamino)ethoxy]phenyl]-2-phenylbut-1-enyl]phenol
82419-35-0	C13H9F2NO4	8,9-Difluoro-3-methyl-6-oxo-2,3-dihydro-6H-1-oxa-3a-aza-phenalene-5-carboxylic acid
82469-79-2	C28H50O8	1,2,3-propanetricarboxylic acid, 2-(1-oxobutoxy)-, trihexyl ester
824-80-6	C6H5FO2S	Sodium 4-fluorobenzenesulfinate
82530-64-1	C7H12Cl2O2	4-Chlorobutyl 3-chloropropanoate
82543-09-7	C25H36O4	7 beta-Hydroxy-15 beta,16 beta-methylene-3 beta-pivaloyloxy-5-androsten-17-one
82543-14-4	C25H36O4	5-Hydroxy-15 beta,16 beta-methylene-3 beta-pivaloyloxy-5 beta-androst-6-en-17-one
82543-15-5	C20H28O3	3 beta,5 beta-Dihydroxy-15 beta,16 beta-methylene-5 beta-androst-6-en-17-one
82543-16-6	C21H30O3	3 beta,5-Dihydroxy-6 beta,7 beta;15 beta,16 beta-dimethylene-5 beta-androstan-17-one

82543-17-7	C24H34O4	21a-Homo-6 alpha,7 alpha,15 alpha,16 alpha-tetrahydro-bis-3' H-cyclopropa[1',2':6,7;1'',2'':15,16]-5 beta,17 alpha-pregn-20-yne-3 beta,5,17,21a-tetrol
826-36-8	C9H17NO	2,2,6,6-tetramethyl-4-piperidone
82654-98-6	C12H18O3	4-(butoxymethyl)-2-methoxyphenol
826-81-3	C10H9NO	2-methylquinolin-8-ol
82832-73-3	C15H26O	(1's,4'r)-4'-Propyl-[1,1'-bi(cyclohexan)]-4-one
830-13-7	C12H22O	cyclododecanone
830322-14-0	C11H22O	reaction mass of cis 4-(3-methylbutyl)cyclohexanol and trans 4-(3-methylbutyl)cyclohexanol
83066-88-0	C15H12F3NO4	(2R)-2-(4-{[5-(trifluoromethyl)pyridin-2-yl]oxy}phenoxy)propanoic acid
832088-69-3	C32H35NO3	4-(4-(4-(hydroxydiphenylmethyl)-1-piperidinyl)-1-butynyl)-α,α-dimethylbenzeneacetic acid
83261-15-8	C7H13ClO2	isobutyl (S)-2-chloropropionate
83-32-9	C12H10	acenaphthene
834-12-8	C9H17N5S	ametryn
83857-96-9	C8H11ClN2O	2-butyl-4-chloro-5-formylimidazole
838-88-0	C15H18N2	4,4'-methylenedi-o-toluidine
83929-47-9	C15H10Cl2N2O5	methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-nitrobenzoate
839-90-7	C9H15N3O6	tris(2-hydroxyethyl)-1,3,5-triazinetrione
84023-60-9	C15H12BrNO3	5-benzoyl-7-bromo-2,3-dihydro-1H-Pyrrolizine-1-carboxylic acid
846023-24-3	C10H8Cl2N2O2	2-cyano-N-(2,4-dichloro-5-methoxyphenyl)acetamide
846023-54-9	C15H23N3O4	1-(3-(2-methoxy-5-nitrophenoxy)propyl)-4-methylpiperazine
84632-65-5	C18H10Cl2N2O2	CROMOPHTAL DPP RED BP
846-48-0	C19H26O2	boldenone
84-65-1	C14H8O2	anthraquinone
84-66-2	C12H14O4	diethyl phthalate
84-69-5	C16H22O4	diisobutyl phthalate
84713-17-7	C9H14N2	2,2,4(or 2,4,4)-trimethylhexanedinitrile
84-74-2	C16H22O4	dibutyl phthalate
84793-24-8	C16H19NO5	N-[1-(S)-ethoxycarbonyl-3-phenylpropyl] L-alanyl-N-carboxyanhydride
84852-15-3	C15H24O	Phenol, 4-nonyl-, branched
84852-53-9	C14H4Br10	1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]
84896-44-6	C40H80O4S2Sn	diisotridecyl 3,3'-[(dibutylstannylene)bis(thio)]dipropionate
849793-87-9	C7H8ClNO4S2	ethyl [(5-chlorothiophen-2-yl)sulfonyl]carbamate
851976-50-6	C20H13F6N3O2S	N-{1-cyano-2-[5-cyano-2-(trifluoromethyl)phenoxy]-1-methylethyl}-4-[(trifluoromethyl)thio]benzamide
85390-93-8	C19H28O4	3 beta,7 beta,15 alpha-Trihydroxy-5-androsten-17-one
85390-94-9	C29H44O6	7 beta-Hydroxy-3 beta,15 alpha-dipivaloyloxy-5-androsten-17-one
853950-77-3	C14H12N4O3S	(R)-2-{[(3-methyl-4-nitropyridine-2-yl)methyl]sulfinyl}-1H-benzimidazole
85-40-5	C8H9NO2	1,2,3,6-tetrahydrophthalimide

85-41-6	C8H5NO2	phthalimide
85-42-7	C8H10O3	cyclohexane-1,2-dicarboxylic anhydride
85-43-8	C8H8O3	1,2,3,6-tetrahydrophthalic anhydride
85-44-9	C8H4O3	phthalic anhydride
85491-26-5	C14H13ClF2Si	(chloromethyl)bis(4-fluorophenyl)methylsilane
85507-79-5	C30H50O4	diundecyl phthalate, branched and linear
855425-38-6	C13H23N	1-(2-Ethylbutyl)cyclohexanecarbonitrile
85-68-7	C19H20O4	benzyl butyl phthalate
85909-49-5	C16H32	isohexadecene
859-18-7	C18H34N2O6S	Lincomycin
85954-11-6	C22H26O4	2,2'-((3,3',5,5'-tetramethyl-(1,1'-biphenyl)-4,4'-diyl)-bis(oxymethylene))-bis-oxirane
860035-07-0	C8H14O4S	1-{[(methylsulphanyl)carbonyl]oxy}ethyl 2-methylpropanoate
86087-23-2	C4H8O2	(S)-tetrahydrofuran-3-ol
86089-17-0	C13H29N	tridecylamine, branched and linear
86357-14-4	C15H19N5O7	Acetamide,N-[9-[[2-(acetyloxy)-1-[(acetyloxy)methyl]ethoxy]methyl]-6,9-dihydro-6-oxo-1H-purin-2-yl]-
86386-77-8	C11H9F2N3O	1-{[2-(2,4-Difluorophenyl)oxiran-2-yl]methyl}-1H-1,2,4-triazole monomethanesulfonate
86393-34-2	C7H2Cl3FO	2,4-Dichlor-5-fluor-benzoylchlorid
86604-75-3	C9H13Cl2NO	Sulfo-6
86604-79-7	C8H10N2O3	4-nitro-2,3,5-trimethylpyridine, 1-oxide
86-73-7	C13H10	fluorene
86-74-8	C12H9N	carbazole
868-77-9	C6H10O3	2-hydroxyethyl methacrylate
86978-24-7	C13H18N2O4S	(2Z)-2-{2-[(tert-Butoxycarbonyl)amino]-1,3-thiazol-4-yl}pent-2-enoic acid
87010-29-5	C6H11NO3	3-(3-hydroxypropyl)oxazolidin-2-one
87135-01-1	C12H30O6Si2	3,3,10,10-tetramethoxy-2,11-dioxa-3,10-disiladodecane
871-78-3	C6H12N2O2	N,N'-ethylenedi(diacetamide)
872-05-9	C10H20	dec-1-ene
872-36-6	C3H2O3	vinylene carbonate
872-50-4	C5H9NO	1-methyl-2-pyrrolidone
872728-82-0	C10H9N3O4	Oxa-Acid
87305-03-1	C8H9Br3O2	(1R,4R,5S)-6,6-dimethyl-4-(tribromomethyl)-3-oxabicyclo[3.1.0]hexan-2-one
87-33-2	C6H8N2O8	isosorbide dinitrate
873-32-5	C7H4ClN	2-chlorobenzonitrile
87333-22-0	C6H10ClNO3	Methyl 2-(acetylamino)-3-chloropropionate
873888-84-7	C14H18O3	(4Z)-hept-4-en-2-yl salicylate
873-94-9	C9H16O	3,3,5-trimethylcyclohexan-1-one
87-41-2	C8H6O2	phthalide
874649-82-8	C11H11FO3	Methyl 6-fluorochroman-2-carboxylate
874819-71-3	C6H9N4O3P	N-(2-nitrophenyl)phosphoric triamide
875-74-1	C8H9NO2	D-(-)-α-phenylglycine

87-59-2	C8H11N	2,3-xylidine
87-60-5	C7H8ClN	3-chloro-o-toluidine
87-61-6	C6H3Cl3	1,2,3-trichlorobenzene
87-62-7	C8H11N	2,6-xylidine
87-69-4	C4H6O6	(+)-tartaric acid
877179-03-8	C14H10Cl2FNO	N-(3',4'-dichloro-5-fluorobiphenyl-2-yl)acetamide
877179-04-9	C12H8Cl2FN	3',4'-dichloro-5-fluorobiphenyl-2-amine
877397-65-4	C8H7Cl2FO	(S)-1-(2,6-Dichloro-3-fluorophenyl)ethanol
877399-00-3	C13H10BrCl2FN2O	(R)-5-bromo-3-(1-(2,6-dichloro-3-fluorophenyl)ethoxy)pyridin-2-amine
877670-90-1	C18H17N3O5	2-{[1-[(2-Methoxyphenyl)amino]-1,3-dioxobutan-2-yl]azo}benzoic acid
879671-67-7	C13H14ClNO	2-(1-hydroxy-1-phenylethyl)pyridinium chloride
88110-89-8	C11H15N5O5	2-[(2-amino-6-oxo-1,6-dihydro-9H-purin-9-yl)methoxy]-3-hydroxypropyl acetate
88-12-0	C6H9NO	1-vinyl-2-pyrrolidone
88122-99-0	C48H66N6O6	tris(2-ethylhexyl)-4,4',4''-(1,3,5-triazine-2,4,6-triyltriimino)tribenzoate
88150-62-3	C28H27ClN2O7	3-ethyl 5-methyl 4-(2-chlorophenyl)-1,4-dihydro-2-[2-(1,3-dihydro-1,3-dioxo-(2H)isoindol-2-yl)-ethoxymethyl]-6-methyl-3,5-pyridinedicarboxylate
883794-93-2	C18H36N2O6S2Si2	Bis(2,8,9-trioxa-5-aza-1-silabicyclo(3.3.3)undecane-1-propane)disulfide
88-44-8	C7H9NO3S	4-aminotoluene-3-sulphonic acid
88-60-8	C11H16O	6-tert-butyl-m-cresol
88-66-4	C7H5Cl3	1-chloro-2-(dichloromethyl)benzene
887148-70-1	C20H13F6N3O2S	N-{(1R)-1-cyano-2-[5-cyano-2-(trifluoromethyl)phenoxy]-1-methylethyl}-4-[(trifluoromethyl)thio]benzamide
88-72-2	C7H7NO2	2-nitrotoluene
88-73-3	C6H4ClNO2	1-chloro-2-nitrobenzene
88-74-4	C6H6N2O2	2-nitroaniline
88805-65-6	C9H12O4	ethyl 3-hydroxy-5-oxo-3-cyclohexene-1-carboxylate
88-85-7	C10H12N2O5	dinoseb
88-99-3	C8H6O4	phthalic acid
89-05-4	C10H6O8	benzene-1,2,4,5-tetracarboxylic acid
89281-73-2	C6H10Cl2O3	[(1-3 Dichlopropan-2-yl)oxy]methyl acetate
89331-94-2	C35H36N2O3	6'-(dibutylamino)-3'-methyl-2'-(phenylamino)spiro[isobenzofuran-1(3H),9-(9H)-xanthen]-3-one
89392-03-0	C13H13N3O4	phenyl N-(4,6-dimethoxypyrimidin-2-yl)carbamate
89-39-4	C8H9NO4	1,4-dimethoxy-2-nitrobenzene
89402-43-7	C5H2ClF2N	5-chloro-2,3-difluoropyridine
895525-72-1	C11H10F3NO3	({[2-(trifluoromethyl)phenyl]carbonyl}amino)methyl acetate
89604-91-1	C12H9N5O2S3	S-1,3-Benzothiazol-2-yl (2Z)-(5-amino-1,2,4-thiadiazol-3-yl)(methoxyimino)ethanethioate
89604-92-2	C20H22N4O4S3	2-mercaptobenzothiazolyl-(Z)-(2-aminothiazol-4-yl)-2-(tert-butoxycarbonyl) isopropoxyiminoacetate

		2,2-di(tetrahydrofuryl)propane
89686-69-1	C11H20O2	or
		2,2'-propane-2,2-diylditetrahydrofuran
89-72-5	C10H14O	2-sec-butylphenol
89-78-1	C10H20O	menthol
89786-04-9	C10H12N4O5S	(2S,3S,5R)-3-methyl-7-oxo-3-(1H-1,2,3-triazol-1-ylmethyl)-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid 4,4-dioxide
89-79-2	C10H18O	isopulegol
89-83-8	C10H14O	thymol
898566-17-1	C18H14FIS	2-(4-fluorophenyl)-5-(5-iodo-2-methylbenzyl)thiophene
89-87-2	C8H9NO2	4-nitro-m-xylene
89878-14-8	C9H14BN	3-(diethylboryl)pyridine
89-98-5	C7H5ClO	2-chlorobenzaldehyde
90-04-0	C7H9NO	o-anisidine
9004-77-7	C6H14O2	Polyethylene glycol butyl ether
90-05-1	C7H8O2	guaiacol
90-12-0	C11H10	1-methylnaphthalene
901-44-0	C19H24O4	2,2'-isopropylidenebis(p-phenyleneoxy)diethanol
90-30-2	C16H13N	N-1-naphthylaniline
90315-82-5	C12H16O3	(R)-(−)-2-hydroxy-4-phenylbutyric acid ethyl esther
90356-78-8	C18H14F4N2O2S	N-[4-Cyano-3-(trifluoromethyl)phenyl]-3-(4-fluorophenylsulfanyl)-2-hydroxy-2-methylpropionamide
90-43-7	C12H10O	biphenyl-2-ol
90480-88-9	C9H12O	Phenol, isopropylated
9051-49-4	C22H48O12	Pentaerythritol, propoxylated
90657-55-9	C11H20ClNO2	trans-4-cyclohexyl-L-proline monohydrochloride
90-72-2	C15H27N3O	2,4,6-tris(dimethylaminomethyl)phenol
90-80-2	C6H10O6	D-glucono-1,5-lactone
908145-87-9	C20H27NO6	Diethyl N-[4-(4-oxobutyl)benzoyl]-L-glutamate
91-15-6	C8H4N2	phthalonitrile
91-17-8	C10H18	decahydronaphthalene
91-20-3	C10H8	naphthalene
91-22-5	C9H7N	quinoline
91273-04-0	C19H38N4	1-(N,N-bis(2-ethylhexyl)aminomethyl)-1,2,4-triazole
91-57-6	C11H10	2-methylnaphthalene
91-68-9	C10H15NO	3-diethylaminophenol
916975-92-3	C11H8F3N3O2	4-methyl-1-[3-nitro-5-(trifluoromethyl)phenyl]-1H-imidazole
917392-54-2	C18H16N4O2	4-Methyl-3-(4-pyridin-3-yl-pyrimidin-2-ylamino)-benzoic acid methyl ester
91-76-9	C9H9N5	6-phenyl-1,3,5-triazine-2,4-diyldiamine
919-30-2	C9H23NO3Si	3-aminopropyltriethoxysilane
919-31-3	C9H19NO3Si	3-(triethoxysilyl)propiononitrile
91-97-4	C16H12N2O2	3,3'-dimethylbiphenyl-4,4'-diyl diisocyanate

919-94-8	C7H16O	2-ethoxy-2-methylbutane
920-36-5	C4H9Li	ISOBUTYLLITHIUM
92096-37-2	C29H26N2O7S2	diphenylmethyl (6R,7R)-3-[(methylsulfonyl)oxy]-8-oxo-7-[(phenylacetyl)amino]-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate
921-03-9	C3H3Cl3O	1,1,3-trichloroacetone
92-15-9	C11H13NO3	2'-methoxyacetoacetanilide
922165-31-9	C20H36O8	Bis[2-(2-ethoxyethoxy)ethyl] cyclohexane-1,4-dicarboxylate
92339-11-2	C35H44I6N6O15	5-(Acetyl-(3-(acetyl-(3,5-bis(2,3-dihydroxypropylcarbamoyl)-2,4,6-triiodophenyl)amino)-2- hydroxypropyl)amino)-N,N'-bis(2,3-dihydroxypropyl)-2,4,6-triiodobenzene-1,3-dicarboxamide; 5,5'-((2-Hydroxytrimethylene)bis(acetylimino))bis(N,N'-bis(2,3-dihydroxypropyl)-2,4,6- triiodoisophthalamide);
924-42-5	C4H7NO2	N-(hydroxymethyl)acrylamide
924-88-9	C10H18O4	diisopropyl succinate
92-52-4	C12H10	biphenyl
92-54-6	C10H14N2	N-phenylpiperazine
926-57-8	C4H6Cl2	1,3-dichlorobut-2-ene
92671-67-5	C14H19NO4	1,5-dihydro-3-isopropyl-8-methyl-[1,3]dioxepino[5,6-c]pyridin-9-yl acetate
92700-68-0	C15H22N2O4	benzyl {5-[N-acetyl(hydroxy)amino]pentyl}carbamate
92-70-6	C11H8O3	3-hydroxy-2-naphthoic acid
92-74-0	C19H17NO3	2'-ethoxy-3-hydroxy-2-naphthanilide
92761-26-7	C28H34O8S2	(E-E)-3,3'-(1,4-phenylenedimethylidene)bis(2-oxobornane-10-sulfonic acid)
92-84-2	C12H9NS	phenothiazine
92878-95-0	C10H12ClNO4	2-(3-chloropropoxy)-1-methoxy-4-nitrobenzene
929-06-6	C4H11NO2	2-(2-aminoethoxy)ethanol
92952-81-3	C9H12N2O4	4-[(3-hydroxypropyl)amino]-3-nitrophenol
930-28-9	C5H9Cl	chlorocyclopentane
931419-77-1	C21H41NO4	3-(2-(2-Hydroxyethoxy)ethylimino)-2,2-dimethylpropyl dodecanoate
931-87-3	C8H14	(Z)-cyclooctene
932742-30-8	C44H82N2O4	3-({5-[3-(Dodecanoyloxy)-2,2-dimethylpropylideneamino]-1,3,3-trimethylcyclohexyl}methylimino}-2,2-dimethylpropyl docecanoate
933999-84-9	C12H22O4	1,6-bis(2,3-epoxypropoxy)hexane
93413-62-8	C16H25NO2	4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol
93413-69-5	C17H28ClNO2	Venlafaxine, 1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol
936-49-2	C9H10N2	2-phenyl-2-imidazoline
93-68-5	C11H13NO2	2'-methylacetoacetanilide
93-70-9	C10H10ClNO2	2'-chloroacetoacetanilide

938063-63-9	C10H18O3S	Methyl 3-[(2,2-dimethylbutanoyl)thio]propanoate
93839-21-5	C14H11N3O4	N-[4-(aminocarbonyl)phenyl]-4-nitrobenzamide
93-84-5	C7H5N3O3	1,3-dihydro-5-nitro-2H-benzimidazol-2-one
939-97-9	C11H14O	4-tert-butylbenzaldehyde
94-04-2	C10H18O2	vinyl 2-ethylhexanoate
94050-90-5	C9H10O4	(R)-2-(4-hydroxyphenoxy)propanoic acid
941-69-5	C10H7NO2	N-phenylmaleimide
94213-23-7	C9H7Cl2N5	(Z)-[cyano(2,3-dichlorophenyl)methylene]carbazamidine
94-28-0	C22H42O6	2,2'-ethylenedioxydiethyl bis(2-ethylhexanoate)
94317-64-3	C4H14N3PS	N-(n-butyl)-thiophosphoric triamide
943516-53-8	C14H15NO2	3-benzyl-6,6-dimethyl-3-azabicyclo[3.1.0]hexane-2,4-dione
94-36-0	C14H10O4	dibenzoyl peroxide
94361-26-9	C13H15ClO	2-(4-chlorophenyl)-2-(1-cyclopropylethyl)-oxirane
947-04-6	C12H23NO	dodecane-12-lactam
94-71-3	C8H10O2	2-ethoxyphenol
947-19-3	C13H16O2	hydroxycyclohexyl phenyl ketone
95-02-3	C6H10N4	4-amino-2-methylpyrimidine-5-methylamine
950782-86-2	C16H20FN5	N-[(1R,2S)-2,6-dimethyl-2,3-dihydro-1H-inden-1-yl]-6-[(1RS)-1-fluoroethyl]-1,3,5-triazine-2,4-diamine
95-16-9	C7H5NS	benzothiazole
95235-30-6	C15H16O4S	4-(4-isopropoxyphenylsulfonyl)phenol
95-23-8	C7H7N3O	5-amino-1,3-dihydro-2H-benzimidazol-2-one
95-31-8	C11H14N2S2	N-tert-butylbenzothiazole-2-sulphenamide
95-33-0	C13H16N2S2	N-cyclohexylbenzothiazole-2-sulfenamide
95-38-5	C22H42N2O	2-(2-heptadec-8-enyl-2-imidazolin-1-yl)ethanol
95-47-6	C8H10	o-xylene
95-48-7	C7H8O	o-cresol
95-49-8	C7H7Cl	2-chlorotoluene
95-50-1	C6H4Cl2	1,2-dichlorobenzene
95-51-2	C6H6ClN	2-chloroaniline
95-53-4	C7H9N	o-toluidine
95-54-5	C6H8N2	o-phenylenediamine
95-55-6	C6H7NO	2-aminophenol
95-57-8	C6H5ClO	2-Chlorophenol
956317-36-5	C10H9N3O2	5-methyl-2-(2H-1,2,3-triazol-2-yl)benzoic acid
95-63-6	C9H12	1,2,4-trimethylbenzene
95-68-1	C8H11N	2,4-xylidine
95709-82-3	C13H9Cl3N2O2	N-(4-amino-5-chloro-2-hydroxyphenyl)-3,4-dichlorobenzamide
95709-83-4	C13H7Cl3N2O4	3,4-dichloro-N-(5-chloro-2-hydroxy-4-nitrophenyl)benzamide
95-74-9	C7H8ClN	3-chloro-p-toluidine
95-76-1	C6H5Cl2N	3,4-dichloroaniline
95-80-7	C7H10N2	4-methyl-m-phenylenediamine
95-82-9	C6H5Cl2N	2,5-dichloroaniline

95-92-1	C6H10O4	diethyl oxalate
95962-14-4	C15H24O	2-(2-(4-methyl-3-cyclohexen-1-yl)propyl)cyclopentanone
959624-24-9	C16H16O3	6-(HYDROXYMETHYL)-4-PHENYL-3,4-DIHYDRO-2H-CHROMEN-2-OL
95-96-5	C6H8O4	dilactide
96-09-3	C8H8O	(epoxyethyl)benzene
96-12-8	C3H5Br2Cl	1,2-dibromo-3-chloropropane
96-17-3	C5H10O	2-methylbutyraldehyde
96-18-4	C3H5Cl3	1,2,3-trichloropropane
96-20-8	C4H11NO	2-aminobutan-1-ol
96-22-0	C5H10O	pentan-3-one
96-23-1	C3H6Cl2O	1,3-dichloropropan-2-ol
96240-10-7	C5H10N4O	4-amino-2,4-dihydro-5-(1-methylethyl)-3H-1,2,4-triazol-3-one
96-24-2	C3H7ClO2	3-chloropropane-1,2-diol
96-26-4	C3H6O3	1,3-dihydroxyacetone
96-29-7	C4H9NO	butanone oxime
96-31-1	C3H8N2O	1,3-dimethylurea
96-33-3	C4H6O2	methyl acrylate
96-34-4	C3H5ClO2	methyl chloroacetate
96-45-7	C3H6N2S	imidazolidine-2-thione
96478-09-0	C18H17N3O3	2-(2-hydroxy-5-(2-(methacryloyloxy)ethyl)phenyl)-2H-benzotriazole
96-48-0	C4H6O2	γ-butyrolactone
96-49-1	C3H4O3	ethylene carbonate
96-69-5	C22H30O2S	6,6'-di-tert-butyl-4,4'-thiodi-m-cresol
96702-03-3	C6H10N2O2	(S)-2-methyl-3,4,5,6-tetrahydropyrimidine-4-carboxylic acid
96-76-4	C14H22O	2,4-di-tert-butylphenol
97-00-7	C6H3ClN2O4	1-chloro-2,4-dinitrobenzene
97042-18-7	C15H14O4S	BPS-MAE
97-36-9	C12H15NO2	2',4'-dimethylacetoacetanilide
97-52-9	C7H8N2O3	4-nitro-o-anisidine
97-63-2	C6H10O2	ethyl methacrylate
97-65-4	C5H6O4	itaconic acid
976-70-5	C22H30O3	3-oxopregn-4-ene-21,17α-carbolactone
97-72-3	C8H14O3	isobutyric anhydride
97-77-8	C10H20N2S4	disulfiram
97-86-9	C8H14O2	isobutyl methacrylate
97-88-1	C8H14O2	butyl methacrylate
97888-41-0	C14H14KNO4S2	potassium-N-(4-toluenesulfonyl)-4-toluenesulfonamide
97-93-8	C6H15Al	triethylaluminium
97963-62-7	C8H6F2N2OS	5-(difluoromethoxy)-1,3-dihydrobenzimidazole-2-thione
98-00-0	C5H6O2	furfuryl alcohol
98-01-1	C5H4O2	2-furaldehyde

980-26-7	C22H16N2O2	5,12-dihydro-2,9-dimethylquino[2,3-b]acridine-7,14-dione
98-07-7	C7H5Cl3	α,α,α-trichlorotoluene
98-09-9	C6H5ClO2S	benzenesulphonyl chloride
98-10-2	C6H7NO2S	Benzenesulfonamide
98-11-3	C6H6O3S	benzenesulphonic acid
98-13-5	C6H5Cl3Si	trichloro(phenyl)silane
98-16-8	C7H6F3N	α,α,α-trifluoro-m-toluidine
98-17-9	C7H5F3O	α,α,α-trifluoro-m-cresol
98210-99-2	C18H10Cl2N4O8S2	4,11-Triphenodioxazinedisulfonic acid, 3,10-diamino-6,13-dichloro-
98-29-3	C10H14O2	4-tert-butylpyrocatechol
98-44-2	C6H7NO6S2	2-aminobenzene-1,4-disulphonic acid
98-51-1	C11H16	4-tert-butyltoluene
98-53-3	C10H18O	4-tert-butylcyclohexanone
98-54-4	C10H14O	4-tert-butylphenol
98-56-6	C7H4ClF3	4-chloro-α,α,α-trifluorotoluene
98-67-9	C6H6O4S	4-hydroxybenzenesulphonic acid
98730-04-2	C11H11Cl2NO2	2,2-dichloro-1-(3-methyl-2,3-dihydro-4H-1,4-benzoxazin-4-yl)ethanone
98-73-7	C11H14O2	4-tert-butylbenzoic acid
98-82-8	C9H12	cumene
98-83-9	C9H10	2-phenylpropene
98-85-1	C8H10O	1-phenylethanol
98-86-2	C8H8O	acetophenone
98-87-3	C7H6Cl2	α,α-dichlorotoluene
98-88-4	C7H5ClO	benzoyl chloride
98-94-2	C8H17N	cyclohexyldimethylamine
98-95-3	C6H5NO2	nitrobenzene
98967-40-9	C12H9F2N5O2S	2',6'-difluoro-5-methyl[1,2,4]triazolo[1,5-a]pyrimidine-2-sulfoanilide
99-08-1	C7H7NO2	3-nitrotoluene
99189-60-3	C10H17NO3	1,1-cyclohexanediacetic acid monoamide
99199-60-7	C10H9FO3	6-Fluorochromane-2-carboxylic acid
99305-42-7	C23H42N2O4	4,4'-Methylenebis(N-butoxycarbonylcyclohexanamine)
994-05-8	C6H14O	2-methoxy-2-methylbutane
99-54-7	C6H3Cl2NO2	1,2-dichloro-4-nitrobenzene
99-55-8	C7H8N2O2	5-nitro-o-toluidine
99-57-0	C6H6N2O3	2-amino-4-nitrophenol
99591-74-9	C2H4O6S2	1,5,2,4-dioxadithiane 2,2,4,4-tetraoxide
99607-70-2	C18H22ClNO3	CLOQUINTOCEET_MEXYL, heptan-2-yl [(5-chloroquinolin-8-yl)oxy]acetate
99627-05-1	C6H3F3O	3,4,5-trifluorophenol
99-63-8	C8H4Cl2O2	isophthaloyl dichloride
99-66-1	C8H16O2	Valproic acid
99-76-3	C8H8O3	methyl 4-hydroxybenzoate

99817-36-4	C8H7Cl2NO3	2,4-dichloro-3-ethyl-6-nitrophenol
99817-37-5	C8H9Cl2NO	2,4-dichloro-3-ethyl-6-aminophenol
99-87-6	C10H14	p-cymene
99-88-7	C9H13N	4-isopropylaniline
99-96-7	C7H6O3	4-hydroxybenzoic acid
99-99-0	C7H7NO2	4-nitrotoluene
999-97-3	C6H19NSi2	1,1,1,3,3,3-hexamethyldisilazane
no CAS	C19H16ClNO4	Indometacin
no CAS	C11H22O	4-cyclohexyl-2-methyl-2-butanol
no CAS		4-(3,4-dichlorophenylazo)-2,6-di-sec-butyl-phenol
no CAS		4-(4-nitrophenylazo)-2,6-di-sec-butyl-phenol
no CAS		benzyl-2-hydroxydodecyldimethylammonium benzoate

REACH 100-1000 tons

100-01-6	C6H6N2O2	4-nitroaniline
100-06-1	C9H10O2	4'-methoxyacetophenone
100-18-5	C12H18	1,4-diisopropylbenzene
1003-03-8	C5H11N	cyclopentylamine
100-39-0	C7H7Br	α-bromotoluene
100-43-6	C7H7N	4-vinylpyridine
100-50-5	C7H10O	cyclohex-3-ene-1-carbaldehyde
100-64-1	C6H11NO	cyclohexanone oxime
10081-67-1	C30H31N	4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline
10094-45-8	C40H79NO	(Z)-N-octadecyldocos-13-enamide
100-99-2	C12H27Al	triisobutylaluminium
101012-97-9	C26H55N	Tridecanamine, N-tridecyl-, branched and linear
101-20-2	C13H9Cl3N2O	triclocarban
101-41-7	C9H10O2	methyl phenylacetate
10175-31-2	C9H12ClN	1-(2-chlorophenyl)-N,N-dimethylmethanamine
10191-60-3	C4H6N2S2	S,S-dimethyl cyanoimidodithiocarbonate
101-96-2	C14H24N2	N,N'-di-sec-butyl-p-phenylenediamine
102-08-9	C15H16N2S	1,3-diphenyl-2-thiourea
10217-34-2	C14H28O4Si	Y-4036
102-20-5	C16H16O2	phenethyl phenylacetate
102229-10-7	C8H20O2Si	2-[tert-butyl(dimethyl)silyl]oxyethanol
1025-15-6	C12H15N3O3	1,3,5-triallyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione
102-54-5	C10H10Fe	ferrocene
10254-57-6	C19H38N2S4	4,4'-methylene bis(dibutyldithiocarbamate)
10257-32-6	C5H10O5	D-Ribopyranose
10257-33-7	C5H10O5	D-Ribopyranose
102-69-2	C9H21N	tripropylamine
102-81-8	C10H23NO	2-dibutylaminoethanol
1030385-16-0	C18H20FNO2	(1R)-2-(benzylamino)-1-[(2S)-6-fluoro-3,4-dihydro-2H-chromen-2-yl]ethanol

103-24-2	C25H48O4	bis(2-ethylhexyl) azelate
103-26-4	C10H10O2	methyl cinnamate
103300-89-6	C13H20F3N3O4	N-(N6-trifluoroacetyl-L-lysyl)-L-proline
10339-55-6	C11H20O	3,7-dimethylnona-1,6-dien-3-ol
10341-03-4	C32H60O4	ditetradecyl fumarate
103-45-7	C10H12O2	phenethyl acetate
103-49-1	C14H15N	dibenzylamine
1035-69-4	C19H24O2	Deltaandrost-4,9(11)-diene-3,17-dione
103-60-6	C12H16O3	2-phenoxyethyl isobutyrate
103-67-3	C8H11N	benzyl(methyl)amine
103-69-5	C8H11N	N-ethylaniline
1037184-07-8	C14H19Cl2NO	Hexanamide, 2,6-dichloro-N-(2,6-dimethylphenyl)-
103-71-9	C7H5NO	phenyl isocyanate
103-73-1	C8H10O	phenetole
103-82-2	C8H8O2	phenylacetic acid
103-90-2	C8H9NO2	Paracetamol (Acetaminophen)
103-95-7	C13H18O	3-p-cumenyl-2-methylpropionaldehyde
10411-92-4	C12H22O2	cis-4-tert-butylcyclohexyl acetate
10416-59-8	C8H21NOSi2	trimethylsilyl N-trimethylsilylacetamidate
104-23-4	C12H11N3O3S	4'-aminoazobenzene-4-sulphonic acid
104358-16-9	C16H28O	4'-trans-propyl-1,1'-bicyclohexyl-4-trans-carboxaldehyde
104372-31-8	C10H15NO3S	11,11-dimethyl-5-oxa-3-thia-4-azatetracyclo[6.2.1.01,6.04,6]undecane-3,3-dione
104-38-1	C10H14O4	2,2'-p-phenylenedioxydiethanol
104-54-1	C9H10O	cinnamyl alcohol
104-55-2	C9H8O	cinnamaldehyde
104-61-0	C9H16O2	nonan-4-olide
104-66-5	C14H14O2	1,2-diphenoxyethane
104-67-6	C11H20O2	undecan-4-olide
104-68-7	C10H14O3	2-(2-phenoxyethoxy)ethanol
104-78-9	C7H18N2	3-aminopropyldiethylamine
104-90-5	C8H11N	5-ethyl-2-methylpyridine
104-92-7	C7H7BrO	4-bromoanisole
105-05-5	C10H14	1,4-diethylbenzene
10508-09-5	C10H22O2	di-tert-pentyl peroxide
105112-76-3	C24H20N2O2	3,3'-[biphenyl-4,4'-diylbis(oxy)]dianiline
105-13-5	C8H10O2	4-methoxybenzyl alcohol
105-55-5	C5H12N2S	1,3-diethyl-2-thiourea
105-58-8	C5H10O3	diethyl carbonate
10563-26-5	C8H22N4	N,N'-bis(3-aminopropyl)ethylenediamine
10563-29-8	C8H21N3	N'-(3-aminopropyl)-N,N-dimethylpropane-1,3-diamine
105-67-9	C8H10O	2,4-xylenol
105-83-9	C7H19N3	N,N-bis(3-aminopropyl)methylamine
105-87-3	C12H20O2	geranyl acetate

10591-84-1	C16H16N2S4	N,N'-dimethyldiphenylthiuram disulphide
105-95-3	C15H26O4	1,4-dioxacycloheptadecane-5,17-dione
10595-60-5	C16H33N3	N,N'-bis(1,3-dimethylbutylidene)-2,2'-iminobis(ethylamine)
105-99-7	C14H26O4	dibutyl adipate
106006-84-2	C10H15N3OS	(S)-2-Amino-6-propionylamino-4,5,6,7-tetrahydrobenzothiazole
106-02-5	C15H28O2	pentadecan-15-olide
106-09-2	C16H34N2O2	N-[2-[(2-hydroxyethyl)amino]ethyl]dodecanamide
106092-09-5	C7H11N3S	(S)-2,6-Diamino-4,5,6,7-tetrahydrobenzothiazole
106-20-7	C16H35N	bis(2-ethylhexyl)amine
106-21-8	C10H22O	3,7-dimethyloctan-1-ol
106-25-2	C10H18O	nerol
106-26-3	C10H16O	(Z)-3,7-dimethylocta-2,6-dienal
106410-46-2	C17H24N2O6	4-[(5-{[(benzyloxy)carbonyl]amino}pentyl)(hydroxy)amino]-4-oxobutanoic acid
106483-59-4	C15H17N3O6S	3-[(2-amino-4,5-dimethoxyphenyl)diazenyl]-4-methoxybenzenesulfonic acid (free acid) 3-[(E)-(2-ammonio-4,5-dimethoxyphenyl)diazenyl]-4-methoxybenzenesulfonate (inner salt)
106-48-9	C6H5ClO	4-chlorophenol
106-51-4	C6H4O2	p-benzoquinone
106-58-1	C6H14N2	1,4-dimethylpiperazine
106-70-7	C7H14O2	methyl hexanoate
1067-25-0	C6H16O3Si	trimethoxypropylsilane
1068-55-9	C3H7ClMg	chloro(1-methylethyl)magnesium
106904-09-0	C9H9ClO4S	2-chloro-3-methyl-4-(methylsulfonyl) benzoic acid
106-95-6	C3H5Br	3-bromopropene
1070-00-4	C24H51Al	trioctylaluminium
1070-10-6	C8H18O	titanium tetrakis(2-ethylhexanolate)
107-11-9	C3H7N	allylamine
1071-93-8	C6H14N4O2	adipohydrazide
107-20-0	C2H3ClO	chloroacetaldehyde
1072-15-7	C9H20O4S	sodium nonyl sulphate
1072-63-5	C5H6N2	1-vinylimidazole
1072957-71-1	C18H15Cl2F2N3O	N-[9-(dichloromethylidene)-1,2,3,4-tetrahydro-1,4-methanonaphthalen-5-yl]-3-(difluoromethyl)-1-methyl-1H-pyrazole-4-carboxamide
107-51-7	C8H24O2Si3	octamethyltrisiloxane
107551-67-7	C13H18O3	3-(3-tert-butyl-4-hydroxyphenyl)propionic acid
107-56-2	C6H15O2PS2	O,O-diisopropyl hydrogen dithiophosphate
107-58-4	C7H13NO	N-tert-butylacrylamide
107-66-4	C8H19O4P	dibutyl hydrogen phosphate
1076-97-7	C8H12O4	cyclohexane-1,4-dicarboxylic acid
107-85-7	C5H13N	isopentylamine
107869-45-4	C10H15NO2S	(1R,7S)-10,10-Dimethyl-3-thia-4-azatricyclo[5.2.1.0(1,5)]dec-4-ene 3,3-dioxide

107-87-9	C5H10O	pentan-2-one
107934-68-9	C25H18Cl2N2	4,4'-(9H-fluoren-9-ylidene)bis(2-chloroaniline)
107-93-7	C4H6O2	trans-crotonic acid
1079-66-9	C12H10ClP	chlorodiphenylphosphine
108-12-3	C5H9ClO	isovaleryl chloride
108-16-7	C5H13NO	1-(dimethylamino)propan-2-ol
108-23-6	C4H7ClO2	isopropyl chloroformate
108-26-9	C4H6N2O	2,4-dihydro-5-methyl-3H-pyrazol-3-one
1083057-14-0	C17H20N2O2	Benzoic acid, 3-(6-amino-3-methyl-2-pyridinyl)-, 1,1-dimethylethyl ester
108313-21-9	C54H60N4O2	[Name not available]
108-42-9	C6H6ClN	3-chloroaniline
108-69-0	C8H11N	3,5-xylidine
109-01-3	C5H12N2	1-methylpiperazine
109-02-4	C5H11NO	4-methylmorpholine
109113-72-6	C10H9ClN2	Quinazoline
109-13-7	C8H16O3	tert-butyl peroxyisobutyrate
109-16-0	C14H22O6	2,2'-ethylenedioxydiethyl dimethacrylate
1091-93-6	C19H28O2	3-methoxyestra-2,5(10)-dien-17β-ol
109-43-3	C18H34O4	dibutyl sebacate
109-54-6	C5H12ClN	3-chloropropyl(dimethyl)amine
109-63-7	C4H10O	diethyl ether--boron trifluoride
109-65-9	C4H9Br	1-bromobutane
109-74-0	C4H7N	butyronitrile
109-76-2	C3H10N2	trimethylenediamine
110-02-1	C4H4S	thiophene
110-03-2	C8H18O2	2,5-dimethylhexane-2,5-diol
110-31-6	C38H72N2O2	N,N'-ethane-1,2-diylbisoleamide
1103234-56-5	C10H11F2NO4S	2,6-difluoro-3-[(propylsulfonyl)amino]benzoic acid
110-33-8	C18H34O4	dihexyl adipate
1103-38-4	C20H14N2O4S	barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate]
110-41-8	C12H24O	2-methylundecanal
110-44-1	C6H8O2	hexa-2,4-dienoic acid
110-53-2	C5H11Br	1-bromopentane
110-59-8	C5H9N	valeronitrile
110-61-2	C4H4N2	succinonitrile
110-73-6	C4H11NO	2-ethylaminoethanol
110-76-9	C4H11NO	2-ethoxyethylamine
110-87-2	C5H8O	3,4-dihydro-2H-pyran
110-89-4	C5H11N	piperidine
110-93-0	C8H14O	6-methylhept-5-en-2-one
110-95-2	C7H18N2	N,N,N',N'-tetramethyltrimethylenediamine
111-01-3	C30H62	2,6,10,15,19,23-hexamethyltetracosane
111-02-4	C30H50	2,6,10,15,19,23-hexamethyltetracosa-2,6,10,14,18,22-hexaene

111-05-7	C21H41NO2	N-(2-hydroxypropyl)oleamide
111-18-2	C10H24N2	N,N,N',N'-tetramethylhexamethylenediamine
111-21-7	C10H18O6	2,2'-[ethane-1,2-diylbis(oxy)]bisethyl diacetate
1112-39-6	C4H12O2Si	dimethoxydimethylsilane
111-44-4	C4H8Cl2O	bis(2-chloroethyl) ether
111-49-9	C6H13N	perhydroazepine
111-55-7	C6H10O4	ethylene di(acetate)
1115-70-4	C4H11N5	metformin hydrochloride
111-57-9	C20H41NO2	N-(2-hydroxyethyl)stearamide
1116-73-0	C18H39Al	trihexylaluminium
1117-31-3	C8H14O4	1,3-butylene diacetate
111-75-1	C6H15NO	2-butylaminoethanol
1117-86-8	C8H18O2	octane-1,2-diol
111-83-1	C8H17Br	1-bromooctane
111850-25-0	C43H58O3	4,4',4''-(1-methylpropan-1-yl-3-ylidene)tris(2-cyclohexyl-5-methylphenol)
1118-84-9	C7H10O3	allyl acetoacetate
1118-92-9	C10H21NO	N,N-dimethyloctanamide
1119-34-2	C6H14N4O2	(+)-L-arginine hydrochloride
111974-73-3	C19H15NO2S	carbamic acid, [2-(phenylthio)phenyl]-, phenyl ester
1119-97-7	C17H39NO	tetradonium bromide
1120-48-5	C16H35N	dioctylamine
112-11-8	C21H40O2	isopropyl oleate
112-13-0	C10H19ClO	decanoyl chloride
112-15-2	C8H16O4	2-(2-ethoxyethoxy)ethyl acetate
112-29-8	C10H21Br	1-bromodecane
112-31-2	C10H20O	decanal
1123-25-7	C8H14O2	1-methylcyclohexane-1-carboxylic acid
112-33-4	C7H17NO3	2-[2-(3-aminopropoxy)ethoxy]ethanol
112-36-7	C8H18O3	bis(2-ethoxyethyl) ether
112-45-8	C11H20O	undec-10-enal
1125-21-9	C9H12O2	2,6,6-trimethylcyclohex-2-ene-1,4-dione
112-54-9	C12H24O	dodecanal
112-59-4	C10H22O3	2-(2-hexyloxyethoxy)ethanol
112-60-7	C8H18O5	3,6,9-trioxaundecane-1,11-diol
112-64-1	C14H27ClO	myristoyl chloride
112-73-2	C12H26O3	bis(2-butoxyethyl) ether
112-77-6	C18H33ClO	oleoyl chloride
112-82-3	C16H33Br	1-bromohexadecane
1129-42-6	C6H12N4O2	6-methyl-2-oxoperhydropyrimidin-4-ylurea
112-95-8	C20H42	icosane
112-96-9	C19H37NO	octadecyl isocyanate

1132935-63-7	C26H27N3O5S	N-{6-[3-tert-butyl-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-2-methoxyphenyl]naphthalen-2-yl}methanesulfonamide
1132940-53-4	C15H17IN2O3	1-(3-tert-Butyl-5-iodo-4-methoxyphenyl)pyrimidine-2,4(1H,3H)-dione
113479-65-5	C16H18Cl2N2O4S	5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-amino-3-(chloromethyl)-8-oxo-, (4-methoxyphenyl)methyl ester, hydrochloride,(1:1), (6R,7R)
113889-23-9	C14H20O2	Reaction mass of 3a, 4, 5, 6, 7, 7a-hexahydro-1H-4, 7-methanoinden-5-yl butyrate and 3a, 4, 5, 6, 7, 7a-hexahydro-1H-4, 7-methanoinden-6-yl butyrate
1141-23-7	C11H12ClNO3	5-amino-3-(4-chlorophenyl)-5-oxopentanoic acid
1141487-54-8	C12H24O	5-cyclohexyl-2-methylpentan-1-ol
114-49-8	C17H21NO4	hyoscine hydrobromide
115-18-4	C5H10O	2-methylbut-3-en-2-ol
115241-16-2	C7H13NO6	6-deoxy-6-formamido-L-sorbose
115-46-8	C18H21NO	azacyclonol
115-70-8	C5H13NO2	2-amino-2-ethylpropanediol
116-11-0	C4H8O	isopropenyl methyl ether
116-16-5	C3Cl6O	hexachloroacetone
116313-85-0	C7H5NO5	3,4-dihydroxy-5-nitrobenzaldehyde
116-53-0	C5H10O2	2-methylbutyric acid
116-75-6	C32H30N2O2	1,4-bis(mesitylamino)anthraquinone
1170-02-1	C16H16N2O4	ethylenediamine-N,N'-bis((2-hydroxyphenyl)acetic acid)
1174931-74-8	C25H36O3S2	Estr-4-ene-3,11,17-trione 3-(ethylene dithioketal) 17-(2,2-dimethylpropane-1,3-diyl ketal)
117-61-3	C12H12N2O6S2	benzidine-2,2'-disulphonic acid
117-69-1	C20H14N4O10S2	4-[(6-amino-1-hydroxy-3-sulpho-2-naphthyl)azo]-3-hydroxy-7-nitronaphthalene-1-sulphonic acid
117-96-4	C11H9I3N2O4	3,5-diacetamido-2,4,6-triiodobenzoic acid
1182822-31-6	C16H25NO3	Carbonic acid, 5-amino-2,4-bis(1,1-dimethylethyl)phenyl methyl este
118289-55-7	C10H9Cl2NO	6-chloro-5-(2-chloroethyl)-1,3-dihydroindol-2-one
118-41-2	C10H12O5	3,4,5-trimethoxybenzoic acid
118-56-9	C16H22O3	homosalate
118-58-1	C14H12O3	benzyl salicylate
118-60-5	C15H22O3	2-ethylhexyl salicylate
118-69-4	C7H6Cl2	2,6-dichlorotoluene
1187-93-5	C3F6O	trifluoro(trifluoromethoxy)ethylene
118800-30-9	C2H8N2O	2-[2-[2-[2-(1-methyl-2-prop-2-enoyloxy-ethoxy)ethoxymethyl]-2-[2-(2-prop-2-enoyloxypropoxy)ethoxymethyl]butoxy]ethoxy]propyl prop-2-enoate
118-82-1	C29H44O2	2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol
118-83-2	C7H3ClF3NO2	5-chloro-α,α,α-trifluoro-2-nitrotoluene
118-88-7	C7H9NO3S	4-aminotoluene-2-sulphonic acid
1189-08-8	C12H18O4	1-methyltrimethylene dimethacrylate
118-92-3	C7H7NO2	anthranilic acid

118969-29-2	C14H10N2Na2O5S	3-[(2E)-2-benzylidenehydrazino]-4-sulfonatobenzoate, disodium salt
1191-16-8	C7H12O2	3-methyl-2-butenyl acetate
119-17-5	C10H10N2O4S	m-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)benzenesulphonic acid
119302-24-8	C29H48N2O4	Androstan-3,17-diol,2-(4-morpholinyl)-16-(1-pyrrolidinyl)-, 17-acetate (2α,3α,5α,16α,17β)-
1194-65-6	C7H3Cl2N	DICHLOBENIL
119-60-8	C13H22O	dicyclohexyl ketone
119-70-0	C12H13N3O3S	5-amino-2-(p-aminoanilino)benzenesulphonic acid
119-79-9	C10H9NO3S	5-aminonaphthalene-2-sulphonic acid
119-80-2	C14H10O4S2	2,2'-dithiodi(benzoic acid)
120-00-3	C17H20N2O3	4'-amino-2',5'-diethoxybenzanilide
120-20-7	C10H15NO2	3,4-dimethoxyphenethylamine
120-35-4	C14H14N2O2	3-amino-4-methoxybenzanilide
12036-37-2	C24H30N6O17P2	Flamtard S
120-40-1	C16H33NO3	N,N-bis(2-hydroxyethyl)dodecanamide
120-47-8	C9H10O3	ethyl 4-hydroxybenzoate
120-51-4	C14H12O2	benzyl benzoate
120-57-0	C8H6O3	piperonal
120570-77-6	C6H10O5	2,2'-oxybis-ethanol diformate
1207339-61-4	C13H15NO4S	2-({[3-(methylsulfanyl)phenyl]carbamoyl}oxy)ethyl prop-2-enoate
120807-02-5	C13H15NO6S	cis-1-benzoyl-4-[(4-methylsulfonyl)oxy]-L-proline
120-93-4	C3H6N2O	2-imidazolidone
1210-35-1	C15H12O	dibenzo(b,f)cycloheptan-1-one
121-30-2	C6H8ClN3O4S2	4-amino-6-chlorobenzene-1,3-disulphonamide
121315-20-6	C11H16N2O7S2	2-({2-[(3-aminobenzoyl)amino]ethyl}sulfonyl)ethyl hydrogen sulfate
121-32-4	C8H8O3	3-ethoxy-4-hydroxybenzaldehyde
121-43-7	C3H9BO3	trimethyl borate
121-45-9	C3H9O3P	trimethyl phosphite
121-47-1	C6H7NO3S	3-aminobenzenesulphonic acid
121-57-3	C6H6O3S	sulphanilic acid
121-60-8	C8H8ClNO3S	N-acetylsulphanilyl chloride
121627-17-6	C46H44O8P2	6,6'-[(3,3'-di-tert-butyl-5,5'-dimethoxybiphenyl-2,2'-diyl)bis(oxy)]bis(dibenzo[d,f][1,3,2]dioxaphosphepine)
121-69-7	C8H11N	N,N-dimethylaniline
1217271-49-2	C24H46N4O2	1,6-Bis[2,2-dimethyl-3-(N-morpholino)-propylideneamino]-hexane
121776-33-8	C11H13Cl2NO3	3-(dichloroacetyl)-5-(2-furyl)-2,2-dimethyloxazolidine, 2,2-dichloro-1-[5-(2-furyl)-2,2-dimethyl-oxazolidin-3-yl]ethanone
121-82-4	C3H6N6O6	perhydro-1,3,5-trinitro-1,3,5-triazine
121-88-0	C6H6N2O3	2-amino-5-nitrophenol
121-97-1	C10H12O2	p-methoxypropiophenone
122-00-9	C9H10O	4'-methylacetophenone
122-01-0	C7H4Cl2O	4-chlorobenzoyl chloride

122-03-2	C10H12O	4-isopropylbenzaldehyde
12225-06-8	C32H24N6O5	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide
12225-08-0	C27H24N6O7S	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2,5-dimethoxy-4-[(methylamino)sulphonyl]phenyl]azo]naphthalene-2-carboxamide
12225-18-2	C26H27ClN4O8S	N-(4-chloro-2,5-dimethoxyphenyl)-2-[[2,5-dimethoxy-4-[(phenylamino)sulphonyl]phenyl]azo]-3-oxobutyramide
122-32-7	C57H104O6	1,2,3-propanetriyl trioleate
12236-62-3	C17H13ClN6O5	2-[(4-chloro-2-nitrophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide
12236-64-5	C26H20ClN5O4	N-[4-(acetylamino)phenyl]-4-[[5-(aminocarbonyl)-2-chlorophenyl]azo]-3-hydroxynaphthalene-2-carboxamide
122-57-6	C10H10O	4-phenylbutenone
122584-18-3	C17H18BrNO4	N-[2-bromo-5-hydroxy-4-methoxyphenyl)methyl]-N-[2-(4-hydroxyphenyl)ethyl]formamide
122-62-3	C26H50O4	bis(2-ethylhexyl) sebacate
122-63-4	C10H12O2	benzyl propionate
12286-66-7	C17H16N4O7S	calcium bis[4-[[1-[[(2-methylphenyl)amino]carbonyl]-2-oxopropyl]azo]-3-nitrobenzenesulphonate]
123-04-6	C8H17Cl	3-(chloromethyl)heptane
123-11-5	C8H8O2	anisaldehyde
123-15-9	C6H12O	2-methylvaleraldehyde
123-17-1	C12H26O	2,6,8-trimethylnonan-4-ol
123-26-2	C38H76N2O4	N,N'-ethane-1,2-diylbis(12-hydroxyoctadecan-1-amide)
123-28-4	C30H58O4S	didodecyl 3,3'-thiodipropionate
123-56-8	C4H5NO2	succinimide
123599-82-6	C19H29O5P	SQ 28449
123-68-2	C9H16O2	allyl hexanoate
123-75-1	C4H9N	pyrrolidine
1238449-42-7	C21H42O3	Carbonic acid, bis (2-propylheptyl) ester
12389-75-2	C14H23N3O10	sodium hydrogen [N,N-bis[2-[bis(carboxymethyl)amino]ethyl]glycinato(5-)]ferrate(2-)
123-93-3	C4H6O4S	thiodi(acetic acid)
124-12-9	C8H15N	octanenitrile
124-19-6	C9H18O	nonanal
124-26-5	C18H37NO	stearamide
125109-84-4	C13H16O	3-(3-(prop-1-en-2-yl)phenyl)butanal
12542-30-2	C13H16O2	hexahydro-4,7-methano-1H-indenyl acrylate
125-65-5	C22H34O5	pleuromulin
126-13-6	C40H62O19	sucrose di(acetate) hexaisobutyrate
126-71-6	C12H27O4P	triisobutyl phosphate
126-86-3	C14H26O2	2,4,7,9-tetramethyldec-5-yne-4,7-diol

126-92-1	C8H18O4S	sodium etasulfate
126-96-5	C2H4O2	sodium hydrogen di(acetate)
126-97-6	C2H7NO	(2-hydroxyethyl)ammonium mercaptoacetate
127337-60-4	C9H10Cl2F3NO	2-(chloromethyl)-3-methyl-4-(2,2,2-trifluoroethoxy)pyridine hydrochloride (1:1)
127-39-9	C12H22O7S	sodium 1,2-diisobutoxycarbonylethanesulphonate
127-52-6	C6H6ClNO2S	sodium N-chlorobenzenesulphonamide
127-63-9	C12H10O2S	diphenyl sulphone
127-68-4	C6H5NO5S	sodium 3-nitrobenzenesulphonate
12788-93-1	C4H11O4P	Phosphoric acid, butyl ester
127-91-3,18172-67-3	C10H16	pin-2(10)-ene
127946-77-4	C4H7ClN2	1-cyanocyclopropanaminium chloride
128-03-0	C5H11NS2	potassium dimethyldithiocarbamate
128-08-5	C4H4BrNO2	N-bromosuccinimide
128119-70-0	C14H26O2	Reaction mass of 2-methyl-3-{[(2R)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl]oxy}propan-1-ol and 2-methyl-3-{[(2S)-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl]oxy}propan-1-ol
128-42-7	C14H10N2O10S2	4,4'-dinitrostilbene-2,2'-disulphonic acid
128-80-3	C28H22N2O2	1,4-bis(p-tolylamino)anthraquinone
129050-23-3	C11H11FO2	(+)-(S,S)-6-fluoro-3,4-dihydro-2-(2-oxiranyl)-2H-1-benzopyran
129050-26-6	C11H11FO2	(-)-(R,S)-6-fluoro-3,4-dihydro-2-(2-oxiranyl)-2H-1-benzopyran
129050-27-7	C18H20FNO2	(1S)-2-(benzylamino)-1-[(2R)-6-fluoro-3,4-dihydro-2H-chromen-2-yl]ethanol
129499-78-1	C12H18O11	L-Ascorbic acid 2-glucoside
130-00-7	C11H7NO	benz[cd]indol-2(1H)-one
13001-46-2	C5H10OS2	potassium O-isobutyl dithiocarbonate
13007-85-7	C7H14O8	sodium D-glycero-D-gulo-heptonate
130-13-2	C10H9NO3S	sodium 4-aminonaphthalene-1-sulphonate
13014-18-1	C7H3Cl5	2,4-dichloro-1-(trichloromethyl)benzene
130-17-6	C14H12N2O3S2	2-(4-aminophenyl)-6-methylbenzothiazole-7-sulphonic acid
130-26-7	C9H5ClINO	clioquinol
13040-19-2	C18H34O3	zinc diricinoleate
13043-55-5	C16H32	2-hexyl-1-decene
13052-09-0	C24H46O6	1,1,4,4-tetramethylbutane-1,4-diyl bis(2-ethylperoxyhexanoate)
1307233-94-8	C20H21ClN4O3	3-[(2-chloromethyl-1-methyl-1H-benzimidazole-5-carbonyl)-pyridine-2-yl-amino]-propionic acid ethyl ester
131-57-7	C14H12O3	oxybenzone
13170-23-5	C12H24O6Si	diacetoxydi-tert-butoxysilane
13188-60-8	C12H22O4	dodecanedioic acid, compound with hexane-1,6-diamine (1:1)
13189-00-9	C4H6O2	zinc methacrylate
1320-51-0	C3H8N2O2	(hydroxyethyl)urea

1324-76-1	C37H29N3O3S	[[4-[[4-(anilino)phenyl][4-(phenylimino)-2,5-cyclohexadien-1-ylidene]methyl]phenyl]amino]benzenesulphonic acid
132-57-0	C10H8O4S	7-hydroxynaphthalene-1-sulphonic acid
13290-96-5	C10H9NO6	dimethyl 5-nitroisophthalate
1329-99-3	C10H16	Reaction mass of 1-Methyl-4-(1-methylethenyl)cyclohexene and 1-Methyl-4-(1-methylethylidene)-cyclohexene and 1-methyl-4-(propan-2-yl)cyclohexa-1,3-diene
1330-61-6	C13H24O2	isodecyl acrylate
1330-86-5	C22H42O4	diisooctyl adipate
133-14-2	C14H6Cl4O4	bis(2,4-dichlorobenzoyl) peroxide
1333-07-9	C7H9NO2S	toluenesulphonamide
13360-63-9	C6H15N	butyl(ethyl)amine
13360-78-6	C8H19PS2	sodium diisobutyldithiophosphinate
133745-75-2	C12H10FNO4S2	N-Fluoro-N-(phenylsulfonyl)benzenesulfonamide
1338-39-2	C18H34O6	sorbitan laurate
1338-41-6	C24H46O6	sorbitan stearate
133-91-5	C7H4I2O3	3,5-diiodosalicylic acid
13393-93-6	C20H36O	tetradecahydro-7-isopropyl-1,4a-dimethylphenanthren-1-methanol
133978-15-1	C12H19NO2	2-Propenoic acid, 2-cyano-, 1-methylheptyl ester
13402-02-3	C19H36O2	hexadecyl acrylate
134-03-2	C6H8O6	sodium ascorbate
13419-15-3	C18H36O2	(octadecanoato-O)oxoaluminium
13423-15-9	C5H10O	tetrahydro-3-methylfuran
134283-49-1	C8H9NO3	4-[(1E)-(hydroxyimino)methyl]-2-methoxyphenol
134605-64-4	C20H18ClF3N2O6	(2-allyloxy-1,1-dimethyl-2-oxo-ethyl) 2-chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidin-1-yl]benzoate
134701-20-5	C24H42O	2,4-dimethyl-6-(1-methyl-pentadecyl)phenol
13472-08-7	C10H16N4	2,2'-azobis[2-methylbutyronitrile]
134-81-6	C14H10O2	benzil
13501-76-3	C8H19ClO2Si	(3-chloropropyl)diethoxymethylsilane
13515-40-7	C17H15ClN4O5	2-[(4-chloro-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide
135302-13-5	C4H7N3O2	5-methoxy-4-methyl-2,4-dihydro-3H-1,2,4-triazol-3-one
135-37-5	C6H11NO5	disodium 2-hydroxyethyliminodi(acetate)
13560-89-9	C18H17Cl7	1,6,7,8,9,14,15,16,17,17,18,18-dodecachloropentacyclo[12.2.1.16,9.02,13.05,10]octadeca-7,15-diene
135-62-6	C18H15NO3	3-hydroxy-2'-methoxy-2-naphthanilide
135-63-7	C18H14ClNO2	5'-chloro-3-hydroxy-2'-methyl-2-naphthanilide
13586-84-0	C18H36O2	stearic acid, cobalt salt
13595-25-0	C24H26O2	4,4'-(1,3-fenyleenbis(1-methylethylideen))bisphenol
136239-66-2	C10H12F2O	1-butoxy-2,3-difluorobenzene
13641-96-8	C6H7NO3	2-Isocyanatoethyl acrylate

136-51-6	C8H16O2	calcium bis(2-ethylhexanoate)
136-53-8	C8H16O2	zinc bis(2-ethylhexanoate)
13676-54-5	C21H14N2O4	1,1'-(methylenedi-p-phenylene)bismaleimide
13683-89-1	C8H9NO3	methyl (3-hydroxyphenyl)-carbamate
13732-62-2	C7H8O3S	morpholinium toluene-4-sulphonate
13734-41-3	C10H19NO4	N-[(tert-butoxy)carbonyl]-L-valine
13749-61-6	C7H13NO	N-isopropylmethacrylamide
137-51-9	C6H7NO6S2	4-aminobenzene-1,3-disulphonic acid
137658-79-8	C36H45N3O4	2-(4,6-bis(2,4-dimethylphenyl)-1,3,5-triazin-2-yl)-5-(3-((2-ethylhexyl)oxy)-2-hydroxypropoxy)phenol
138-24-9	C9H15NO	N,N,N-trimethylanilinium chloride
138-59-0	C7H10O5	(3R,4S,5R)-3,4,5-trihydroxycyclohex-1-enecarboxylic acid
139007-06-0	C14H21NO	(E)-2-Ethoxy-N-(2-methyl-1-phenylpropylidene)ethylamine
13927-71-4	C9H19NS2	bis(dibutyldithiocarbamato-S,S')copper
139481-58-6	C26H24N6O3	ethyl 1-((2'-(1H-tetrazol-5-yl)-[1,1'-biphenyl]-4-yl)methyl)-2-ethoxy-1H-benzo[d]imidazole-7-carboxylate
139-89-9	C10H18N2O7	trisodium 2-(carboxylatomethyl(2-hydroxyethyl)amino)ethyliminodi(acetate)
14025-15-1	C10H16N2O8	disodium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,N',O,O',ON,ON']cuprate(2-)
14025-21-9	C10H16N2O8	disodium [[N,N'-ethylenediylbis[N-(carboxylatomethyl)glycinato]](4-)-N,N',O,O',ON,ON']zincate(2-)
14064-10-9	C7H11ClO4	diethyl chloromalonate
14073-97-3	C10H18O	L-menthan-3-one
140-89-6	C3H6OS2	potassium O-ethyl dithiocarbonate
140-90-9	C3H6OS2	sodium O-ethyl dithiocarbonate
141-17-3	C22H42O8	bis(2-(2-butoxyethoxy)ethyl) adipate
141-18-4	C18H34O6	bis(2-butoxyethyl) adipate
141-62-8	C10H30O3Si4	decamethyltetrasiloxane
141-63-9	C12H36O4Si5	dodecamethylpentasiloxane
141-75-3	C4H7ClO	butyryl chloride
141-98-0	C6H13NOS	O-isopropyl ethylthiocarbamate
14205-39-1	C5H9NO2	methyl 3-aminocrotonate
142-18-7	C15H30O4	2,3-dihydroxypropyl laurate
142-31-4	C8H18O4S	sodium octyl sulphate
14234-82-3	C12H20O4	diisobutyl maleate
142-62-1	C6H12O2	hexanoic acid
142-72-3	C2H4O2	magnesium di(acetate)
142-87-0	C10H22O4S	sodium decyl sulphate
142-88-1	C4H10N2	piperazine adipate
142-92-7	C8H16O	hexyl acetate
142-96-1	C8H18O	dibutyl ether
14320-04-8	C32H16N8Zn	[29H,31H-phthalocyaninato(2-)-N29,N30,N31,N32]zinc

143-24-8	C10H22O5	bis(2-(2-methoxyethoxy)ethyl) ether
14338-82-0	C13H24O4S2	dibutyl methylenedithiodi(acetate)
14352-61-5	C9H16O2	methyl cyclohexylacetate
14367-46-5	C12H19NO	N-ethyl-p-methoxy-α-methylphenethylamine
143782-23-4	C9H3F3N2S	4-isothiocyanato-2-(trifluoromethyl)benzonitrile
144-15-0	C32H58O8	tris(2-ethylhexyl) 2-(acetyloxy)propane-1,2,3-tricarboxylate
144163-97-3	C11H8N2O5S	(4-Nitrophenyl) thiazol-5-ylmethyl carbonate
144-19-4	C8H18O2	2,2,4-trimethylpentane-1,3-diol
14442-94-5	C35H63NO2	3-(3,5-di-tert-butyl-4-hydroxyphenyl)-N-octadecylpropanamide
144689-93-0	C12H20N2O3	ethyl 4-(2-hydroxypropan-2-yl)-2-propyl-1H-imidazole-5-carboxylate
144690-92-6	C48H44N6O6	(5-methyl-2-oxo-1,3-dioxol-4-yl)methyl 4-(2-hydroxypropan-2-yl)-2-propyl-1-{[2'-(1-trityl-1H-tetrazol-5-yl)biphenyl-4-yl]methyl}-1H-imidazole-5-carboxylate
144702-27-2	C33H29N5	4’-(2-Propyl-4-methyl-6-(1-methylbenzimidazolyl-2-yl)-benzimidazol-1-ylmethyl)biphenyl-2-carbonitril
1448-36-8	C25H42O5	methyl cholate
1450-14-2	C6H18Si2	hexamethyldisilane
14531-84-1	C18H24O2	17B-hydroxyestra-4,6-diene-3-one
1453-58-3	C4H6N2	3-methylpyrazole
1455-42-1	C15H28O6	3,9-bis(1,1-dimethyl-2-hydroxy ethyl-2,4,8,10-tetraoxa spiro [5,5] undecane
14559-13-8	C8H10O2S	Methyl 4,5-dimethyl-3-thiophenecarboxylate
1458-18-0	C6H5Cl2N3O2	methyl 3-amino-5,6-dichloropyrazine-2-carboxylate
14593-46-5	C5H12O	sodium 2-methylbutan-2-olate
1459-93-4	C10H10O4	dimethyl isophthalate
14666-78-5	C6H10O6	diethyl peroxydicarbonate
147118-40-9	C23H30FN3O6S	(3R,5S,6E)-methyl-7-(4-(4-fluorophenyl)-6-isopropyl-2-(N-methylmethylsulfonamido)pyrimidin-5-yl)-3,5-dihydroxyhept-6-enoate
147126-62-3	C14H24O4S	(1R,2S,5R)-2-Isopropyl-5-methylcyclohexyl (2R,5R)-5-hydroxy-1,3-oxathiolane-2-carboxylate
147-85-3	C5H9NO2	L-proline
1480-96-2	C5H5FN2O2	5-fluoro-2-methoxypyrimidin-4(3H)-one
14814-09-6	C9H22O3SSi	3-(triethoxysilyl)propanethiol
148-24-3	C9H7NO	quinolin-8-ol
1484-84-0	C7H15NO	2-piperidin-2-ylethanol
14858-73-2	C17H34O3	bis(2-ethylhexyl) carbonate
14882-18-9	C7H5BiO4	bismuth oxide salicylate
14901-07-6	C13H20O	4-(2,6,6-trimethylcyclohex-1-ene-1-yl)-but-3-ene-2-one
149021-58-9	C13H24O2	2-Propylheptyl acrylate
149-74-6	C7H8Cl2Si	dichloro(methyl)(phenyl)silane
149968-48-9	C27H54N2O	13-DOCOSENAMIDE, N-[3-(DIMETHYLAMINO)PROPYL]-, (13Z)-
150-13-0	C7H7NO2	4-aminobenzoic acid

150-84-5	C12H22O2	citronellyl acetate
15086-94-9	C20H8Br4O5	2-(3,6-dihydroxy-2,4,5,7-tetrabromoxanthen-9-yl)-benzoic acid
151262-57-6	C10H11FO5S	3-[(4-Fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanoic acid
15206-55-0	C9H8O3	methyl benzoylformate
15217-42-2	C6H5N3	sodium 1H-benzotriazolide
1522-41-4	C6H9FO3	Ethyl 2-fluoro-3-oxobutanoate
15267-95-5	C7H17ClO3Si	(chloromethyl)triethoxysilane
15307-86-5	C14H11Cl2NO2	Diclofenac
15396-00-6	C7H15NO4Si	3-(trimethoxysilyl)propyl isocyanate
154477-55-1	C33H39NO4	Methyl 2-[4-[4-[4-[hydroxy(diphenyl)methyl]piperidin-1-yl]butanoyl]phenyl]-2-methylpropanoate
15458-48-7	C10H13NO3	1,2,3,6,-tetrahydro-N-(2-hydroxyethyl)phthalimide
15471-17-7	C8H11NO3S	1-(3-sulphonatopropyl)pyridinium
15520-10-2	C6H16N2	2-methylpentane-1,5-diamine
15520-11-3	C22H38O6	bis(4-tert-butylcyclohexyl) peroxydicarbonate
15535-79-2	C18H36O2SSn	2,2-dioctyl-1,3,2-oxathiastannolan-5-one
1561-92-8	C4H8O3S	sodium 2-methylprop-2-ene-1-sulphonate
15647-08-2	C20H27O3P	2-ethylhexyl diphenyl phosphite
156732-13-7	C32H32N2O	5-amino-[2S-di(methylphenyl)amino]-1,6-diphenyl-4Z-hexen-3-one
1569-69-3	C6H12S	cyclohexanethiol
15721-78-5	C28H43N	bis(4-(1,1,3,3-tetramethylbutyl)phenyl)amine
15793-73-4	C34H28Cl2N8O2	4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[2,4-dihydro-5-methyl-2-(p-tolyl)-3H-pyrazol-3-one]
15821-13-3	C11H10N2O	2-methylquinoline-4-carboxamide
1583-59-1	C7H4F2O2	2,2-difluoro-1,3-benzodioxole
15854-73-6	C13H11NO3	1-methoxy-2-nitro-4-phenylbenzene
15875-13-5	C18H42N6	N,N,N',N',N'',N''-hexamethyl-1,3,5-triazine-1,3,5(2H,4H,6H)-tripropanamine
15894-70-9	C10H18N8	N,N'''-1,6-hexanediylbis[N'-cyanoguanidine]
15956-58-8	C8H16O2	2-ethylhexanoic acid, manganese salt
15968-01-1	C8H6O4	disodium phthalate
15993-42-7	C18H17ClN4O6	N-(5-chloro-2-methoxyphenyl)-2-[(2-methoxy-4-nitrophenyl)azo]-3-oxobutyramide
1599-67-3	C22H44	docos-1-ene
16029-98-4	C3H9ISi	iodotrimethylsilane
16039-53-5	C3H6O3	zinc dilactate
16096-31-4	C12H22O4	1,6-bis(2,3-epoxypropoxy)hexane
1609-86-5	C5H9NO	tert-butyl isocyanate
16111-62-9	C18H34O6	bis(2-ethylhexyl) peroxydicarbonate
161462-35-7	C14H13F3O2S	1-cyclo-propyl-3-(2-methylthio-4-trifluoromethylphenyl)-1,3-propanedione
16251-77-7	C10H12O	3-phenylbutyraldehyde
16260-09-6	C34H67NO	(Z)-N-octadec-9-enylhexadecan-1-amide

162691-59-0	C21H32O5	5-[3-(1-ethoxyethoxy)-3-methyl-4-penten-1-ynyl]-2,4,6,6-tetramethyl-5,6,7,7a-tetrahydro-1,3-benzodioxol-5-ol
16298-03-6	C6H7N3O2	methyl 3-aminopyrazinecarboxylate
16397-70-9	C15H21NO4	p-Nitrobenzoic acid-2-ethylhexylester
16409-43-1	C10H18O	Reaction mass of (2S-cis)-tetrahydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran and Tetrahydro-4-methyl-2-(2-methylpropen-1-yl)pyran (2R,4R) and Tetrahydro-4-methyl-2-(2-methylpropen-1-yl)pyran (2S,4S) and (2R-cis)-tetrahydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran
16415-12-6	C19H42O3Si	hexadecyltrimethoxysilane
16485-10-2	C9H19NO4	panthenol , DL-form
165101-57-5	C14H29NO	N-Butyl-2-(1-ethylpentyl)-1,3-oxazolidine
165115-73-1	C12H14F2O2	2-[2-(2,4-difluorophenyl)prop-2-en-1-yl]propane-1,3-diol
165253-31-6	C5H11NO	N-(tetrahydrofuran-3-ylmethyl)amine
1655-07-8	C9H14O3	ethyl 2-oxocyclohexanecarboxylate
166524-64-7	C5H7FN4O	5-Fluoro-4-hydrazino-2-methoxypyrimidine
166524-74-9	C12H8F2N8O2S2	2,2-Dithiobis-8-fluoro-5-methoxy-[1,2,4]-triazolo-[1,5-c]pyrimidine
16712-64-4	C11H8O3	6-hydroxy-2-naphthoic acid
1678-25-7	C12H11NO2S	N-phenylbenzenesulphonamide
16851-82-4	C10H9NO2S	1-phenylsulfonylpyrrole
16881-77-9	C3H10O2Si	dimethoxymethylsilane
16935-34-5	C6H10N2O2	5-Isopropyl-imidazolidine-2,4-dione
1694-31-1	C8H14O3	3,3-dimethylbutyryl chloride
16958-92-2	C32H62O4	bis(tridecyl) adipate
170222-39-6	C27H22N6O6	RED RA 10463
1704-62-7	C6H15NO2	2-[2-(dimethylamino)ethoxy]ethanol
1709-70-2	C54H78O3	3,3',3'',5,5',5''-hexa-tert-butyl-α,α',α''-(mesitylene-2,4,6-triyl)tri-p-cresol
171599-84-1	C28H19ClN11Na5O19S6	pentasodium 7-(4-(4-(5-amino-4-sulfonato-2-(4-((2-(sulfonatoethoxy)sulfonyl)phenylazo)phenylamino)-6-chloro-1,3,5-triazin-2-yl)amino-2-ureidophenylazo)naphtalene-1,3,6-trisulfonate
17183-98-1	C24H30Cl2O4	17-Acetoxy-6-chloro-1 alpha-chloromethyl-4,6-pregnadiene-3,20-dione
171850-30-9	C10H5Cl2NO3	5,7-dichloro-4-hydroxyquinoline-3-carboxylic acid
1719-58-0	C4H9ClSi	chlorodimethylvinylsilane
172529-93-0	C12H14ClN5O4	1,3-dimethyl 2-[2-(2-amino-6-chloro-9H-purin-9-yl)ethyl]propanedioate
17261-28-8	C19H15O2P	2-diphenylphosphinobenzoic acid
173194-95-1	C10H9BO3	(6-hydroxynaphthalen-2-yl)boronic acid
17392-83-5	C4H8O3	methyl (R)-lactate
1739-84-0	C5H8N2	1,2-dimethylimidazole
17438-89-0	C20H40	1-DECENE, DIMER
1746-23-2	C12H16	p-tert-butylstyrene
17462-58-7	C5H9ClO2	sec-butyl chloroformate

175217-23-9	C10H16O2SSi	4,5-dimethyl-2-(trimethylsilyl)-3-thiophenecarboxylic acid
17526-94-2	C13H20N4O2	N,N''-(4-methyl-m-phenylene)bis[N',N'-dimethylurea]
17527-29-6	C11H7F13O2	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl acrylate
1760-24-3	C8H22N2O3Si	N-(3-(trimethoxysilyl)propyl)ethylenediamine
17636-10-1	C3H8O3S2	sodium 3-mercaptopropanesulphonate
17637-11-5	C18H12O7	tartaric anhydride dibenzoate
17671-27-1	C44H88O2	docosyl docosanoate
17673-56-2	C40H76O2	(Z)-octadec-9-enyl (Z)-docos-13-enoate
17696-64-9	C6H11ClO2	Chloro-acetic acid sec-butyl ester
17766-26-6	C3H3N3S3	1,3,5-triazine-2,4,6(1H,3H,5H)-trithione
178452-66-9	C63H83N27O17S4	3-(2,4-bis(4-((5-(4,6-bis(2-aminopropylamino)-1,3,5-triazin-2-ylamino)-4-hydroxy-2,7-disulfonaphthalen-3-yl)azo)phenylamino)-1,3,5-triazin-6-ylamino)propyldiethylammonium lactate
17865-07-5	C9H16O6Si	propyltriacetoxysilane
178671-58-4	C69H48N4O8	3-{[2-cyano-2-(diphenylmethylidene)acetyl]oxy}-2,2-bis({[2-cyano-2-(diphenylmethylidene)acetyl]oxy}methyl)propyl 2-cyano-3,3-diphenylprop-2-enoate
17913-76-7	C14H30O2	[Name not available]
17927-72-9	C16H28O6Ti	bis(pentane-2,4-dionato-O,O')bis(propan-2-olato)titanium
17928-28-8	C10H31O3Si4	1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]trisiloxane
179688-26-7	C15H21NO8	Ethyl 4,5-bis(2-methoxyethoxy)-2-nitrobenzoate
1798-60-3	C9H10O2	(R)-1-hydroxy-1-phenylacetone
18016-43-8	C18H34O2	oleic acid, compound with N-(2-aminoethyl)ethane-1,2-diamine
18063-03-1	C7H5F2NO	2,6-difluorobenzamide
1809-19-4	C8H19O3P	dibutyl phosphonate
18109-80-3	C18H29NO3	butamirate
18127-01-0	C13H18O	3-(4-tert-butylphenyl)propionaldehyde
181525-38-2	C11H12N2O3	9-HYDROXY-3-(2-HYDROXYETHYL)-2-METHYL-4H-PYRIDO[1,2-A]PYRIMIDIN-4-ONE
18156-74-6	C6H12N2Si	N-(trimethylsilyl)imidazole
18171-19-2	C6H15ClO2Si	(3-chloropropyl)dimethoxymethylsilane
181997-71-7	C10H11ClOS	2-Chloro-3-methyl-4-methylthioacetophenone
181997-72-8	C10H11ClO3S	1-(2-Chloro-4-methanesulphonyl-3-methyl-phenyl)ethanone
182061-89-8	C25H26N9Na3O12S3	TRISODIUM 1-[[[[4-[4-[BIS-(2-HYDROXYETHYL)AMINO]-6- [(2-SULFONATOETHYL)AMINO]]-1,3,5-TRIAZIN-2-YL]AMINO]-2-SULPHONATOPHENYL]AZO]-2-AMINO-8-HYDROXY-6-NAPHTHALENE SULFONATE
18282-59-2	C6H3BrCl2	4-bromo-1,2-dichlorobenzene
182918-16-7	C33H23N3O2	4-(4,6-Bis((biphenyl-4-yl)-1,3,5-triazine-2-yl)-1,3-benzodiole
18297-63-7	C7H20N2OSi2	1,3-bis(trimethylsilyl)urea
18299-85-9	C25H48O2	docosyl acrylate
1830-54-2	C7H10O5	dimethyl 3-oxoglutarate

18328-90-0	C6H13N	N-ethylmethacrylamine
183322-16-9	C15H22O6	Ethyl 3,4-bis(2-methoxyethoxy)benzoate
18361-03-0	C8H6O6S	2,3-Dihydro-thieno[3,4-b][1,4]dioxin-5,7-dicarboxylic acid
18395-30-7	C7H18O3Si	trimethoxy(2-methylpropyl)silane
1843-03-4	C37H52O3	4,4',4''-(1-methylpropanyl-3-ylidene)tris[6-tert-butyl-m-cresol]
1852-04-6	C11H20O4	undecanedioic acid
18559-94-9	C13H21NO3	salbutamol
18626-98-7	C14H22O	o-(1-methylheptyl)phenol
18637-00-8	C9H13ClN2O	2-ethoxybenzenecarboximidamide hydrochloride
18755-43-6	C5H13O3P	dimethyl propylphosphonate
187592-70-7	C9H9Cl2F3O2	(1R,4R,5S)- 4-(1,1-Dichloro-2,2,2-trifluoroethyl)-6,6-dimethyl-3-oxabicyclo[3.1.0]hexan-2-one
1879-09-0	C13H20O	6-tert-butyl-2,4-xylenol
188199-50-0	C16H28O2	Belambre
1885-14-9	C7H5ClO2	phenyl chloroformate
188570-78-7	C10H16O2	(3Z)-Hex-3-en-1-yl cyclopropanecarboxylate
1888-87-5	C4H9AlCl2	dichloroisobutylaluminium
188907-52-0	C18H17N3O9S3	4-amino-3-[[4-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]-1-naphthalene sulfonic acid
1889-67-4	C18H22	1,1'-(1,1,2,2-tetramethylethylene)dibenzene
18917-91-4	C3H6O3	aluminium trilactate
18936-17-9	C5H9N	2-methylbutyronitrile
1897-52-5	C7H3F2N	2,6-difluorobenzonitrile
189956-45-4	C11H8N4O	4-[(4-HYDROXYPYRIMIDIN-2-YL)AMINO]BENZONITRILE
19035-79-1	C16H35O4P	potassium hexadecyl hydrogen phosphate
19147-16-1	C6H10O4	dipotassium adipate
1917-64-2	C7H8O3	5-(methoxymethyl)-2-furaldehyde
19186-97-1	C15H24Br9O4P	tris[3-bromo-2,2-bis(bromomethyl)propyl] phosphate
19223-55-3	C20H44N2O6S	(2-hydroxy-3-sulphopropyl)dimethyl[3-[(1-oxododecyl)amino]propyl]ammonium hydroxide
19234-20-9	C7H14O3	2-(1-methylethoxy)ethyl acetate
19321-40-5	C77H140O8	pentaerythritol tetraoleate
19372-44-2	C10H14CaO4	bis(pentane-2,4-dionato)calcium
19444-21-4	C7H12O3	2-hydroxy-2-methyl-propionic acid allyl ester
194602-23-8	C14H20N2O5S	2-ethoxy-5-(4-methyl-1-piperazinylsulfonyl)benzoic acid
1948-33-0	C10H14O2	2-tert-butylhydroquinone
1955-46-0	C9H7NO6	methyl 5-nitrohydrogen.isophthalate
19694-10-1	C7H7ClN2O	3-amino-4-chlorobenzamide
19708-81-7	C3H6OS2	O,S-dimethyl carbonodithioate
1975-78-6	C10H19N	decanenitrile
19766-89-3	C8H16O2	sodium 2-ethylhexanoate
197706-50-6	C11H11FO2	(-)-(R,R)-6-fluoro-3,4-dihydro-2-(2-oxiranyl)-2H-1-benzopyran

197706-51-7	C11H11FO2	(+)-(S,R)-6-fluoro-3,4-dihydro-2-(2-oxiranyl)-2H-1-benzopyran
19780-11-1	C16H26O3	3-(2-dodecenyl)succinic anhydride
19794-93-5	C20H23ClN4O	trazodone
19894-99-6	C10H16O	[1R-(1α,2β,4β,6α)]-2,2,7-trimethyl-3-oxatricyclo[4.1.1.02,4]octane
199119-58-9	C14H13F3N5NaO6S	sodium (4,6-dimethoxypyrimidin-2-yl)carbamoyl-[[3-(2,2,2-trifluoroethoxy)-2-pyridyl]sulfonyl]azanide
1999-85-5	C12H18O2	α,α,α',α'-tetramethyl-m-xylene-α,α'-diol
20120-33-6	C6H14NO5P	dimethyl [3-[(hydroxymethyl)amino]-3-oxopropyl]phosphonate
201214-53-1	C11H12INO4	methyl 4-(acetylamino)-5-iodo-2-methoxybenzoate
201733-56-4	C10H20B2O4	5,5,5',5'-tetramethyl-2,2'-Bi-1,3,2-dioxaborinane
20193-20-8	C5H13N	N-ethylpropylamine
2022-85-7	C4H4FN3O	flucytosine
20262-58-2	C20H19N3O11S3	disodium 6-acetamido-4-hydroxy-3-[[4-[[2-(sulphonatooxy)ethyl]sulphonyl]phenyl]azo]naphthalene-2-sulphonate
20292-08-4	C20H40O2	2-ethylhexyl laurate
20298-69-5	C12H22O2	cis-2-tert-butylcyclohexyl acetate
2031-67-6	C7H18O3Si	triethoxy(methyl)silane
203313-47-7	C19H27NO4	methyl cis-1-{[(2,5-dimethylphenyl)acetyl]amino}-4-methoxycyclohexanecarboxylate
2033-24-1	C6H8O4	2,2-dimethyl-1,3-dioxane-4,6-dione
2043-57-4	C8H4F13I	1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-8-iodooctane
2044-56-6	C12H26O4S	lithium dodecyl sulphate
2044-64-6	C6H11NO2	N,N-dimethyl-3-oxobutyramide
2050-46-6	C10H14O2	1,2-diethoxybenzene
2051-49-2	C12H22O3	hexanoic anhydride
2052-25-7	C16H12N2O6S	sodium 3-[(1,5-dihydroxy-2-naphthyl)azo]-4-hydroxybenzenesulphonate
20749-68-2	C18H6Cl4N2O	8,9,10,11-tetrachloro-12H-phthaloperin-12-one
2082-81-7	C12H18O4	tetramethylene dimethacrylate
20846-91-7	C10H16N2O8	N,N'-1,2-ethanediylbis-L-aspartic acid
208711-58-4	C9H9NO2	1-benzofuran-3(2H)-one O-methyloxime
20893-30-5	C6H5NS	2-thienylacetonitrile
21049-70-7	C3H9NO	2-(methylamino)ethanol, compound with sulphur dioxide
21145-77-7	C18H26O	1-(5,6,7,8-tetrahydro-3,5,5,6,8,8-hexamethyl-2-naphthyl)ethan-1-one
2123-24-2	C6H11NO	hexahydro-2H-azepin-2-one, sodium salt
212652-59-0	C25H22FN8Na3O13S4	Trisodium 3-amino-4-[4-[4-(2-(2-ethenylsulfonylethoxy)ethylamino)-6-fluoro-1,3,5-triazine-2-ylamino]-2-sulfophenylazo]-5-hydroxynaphthalene-2,7-disulfonate
21282-97-3	C10H14O5	2-[(2-methyl-1-oxoallyl)oxy]ethyl acetoacetate
213265-81-7	C10H5Cl2FN2O	4-chloro-6-(2-chlorophenoxy)-5-fluoropyrimidine

21331-43-1	C13H10N2S	4-(2-naphthyl)-1,3-thiazol-2-amine
2144-53-8	C12H9F13O2	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl methacrylate
21524-36-7	C15H25N	2,4,6-tri(propan-2-yl)aniline
21542-96-1	C24H51N	N,N-dimethyldocosylamine
2156-97-0	C15H28O2	dodecyl acrylate
2162-73-4	C17H22N2O2	2,4,6-triisopropyl-m-phenylene diisocyanate
2162-74-5	C25H34N2	bis(2,6-diisopropylphenyl)carbodiimide
2163-00-0	C6H12Cl2	1,6-dichlorohexane
21643-42-5	C17H32O2	tetradecyl acrylate
21700-31-2	C3H3Cl5	1,1,1,2,3-Pentachlorpropane
2182-55-0	C8H14O	(vinyloxy)cyclohexane
21850-44-2	C21H20Br8O2	1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]
21862-63-5	C10H20O	trans-4-tert-butylcyclohexanol
21890-09-5	C16H28	2-methyl-2,3,4,5,6,7,8,9,10,11,12,13-dodecahydro-1H-cyclopenta[12]annulene
21890-10-8	C16H28O2	3-methylcyclopentadecane-1,5-dione
22038-86-4	C9H13NO	(R)-1-(4-METHOXYPHENYL)ETHYLAMINE
22047-49-0	C26H52O2	2-ethylhexyl stearate
2210-24-4	C9H9NO	N-phenylprop-2-enamide
2210-79-9	C10H12O2	2,3-epoxypropyl o-tolyl ether
2215-35-2	C12H27O2PS2	zinc O,O,O',O'-tetrakis(1,3-dimethylbutyl) bis(phosphorodithioate)
2217-40-5	C10H13N	1,2,3,4-tetrahydro-1-naphthylamine
22174-70-5	C17H36O2	3,3'-[methylenebis(oxymethylene)]bisheptane
22235-81-0	C19H27NO3	endo-(±)-8-aza-8-isopropylbicyclo[3.2.1]oct-3-yl (hydroxymethyl)phenylacetate
2224-33-1	C14H27N3O3Si	butan-2-one O,O',O''-(vinylsilylidyne)trioxime
2226-96-2	C9H18NO2	4-hydroxy-2,2,6,6-tetramethylpiperidinoxyl
22288-43-3	C16H32O3	1,1,3,3-tetramethylbutyl 2-ethylperoxyhexanoate
22326-31-4	C8H6O7S	5-sulphoisophthalic acid
22327-32-8	C10H14O	(1R,6S)- 4,7,7-trimethylbicyclo[4.1.0]hept-3-en-2-one
2234-16-4	C8H6Cl2O	1-(2,4-dichlorophenyl)ethan-1-one
2235-00-9	C8H13NO	1-vinylhexahydro-2H-azepin-2-one
2235-46-3	C8H15NO2	N,N-diethyl-3-oxobutyramide
22393-85-7	C32H62O2	tetradecyl oleate
22464-99-9	C8H16O2	2-ethylhexanoic acid, zirconium salt
224785-90-4	C23H34N6O4S	2-{2-ethoxy-5-[(4-ethylpiperazin-1-yl)sulfonyl]phenyl}-5-methyl-7-propylimidazo[5,1-f][1,2,4]triazin-4(1H)-one
2253-52-3	C8H19O2PS2	O,O-diisobutyl hydrogen dithiophosphate
2269-22-9	C4H10O	aluminium tri-sec-butanolate
227197-72-0	C7H4ClNO	6-Chlorobenzoxazole
22722-98-1	C6H15AlO4	sodium dihydridobis(2-methoxyethanolato)aluminate(1-)
2280-49-1	C13H10Cl3NO2S2	N-phenyl-N-[(trichloromethyl)thio]benzenesulphonamide

22871-58-5	C10H9I3N2O4	3-amino-5-[[(2-hydroxyethyl)amino]carbonyl]-2,4,6-triiodo-benzoic acid
22984-54-9	C13H27N3O3Si	butan-2-one O,O',O''-(methylsilylidyne)trioxime
2306-88-9	C16H32O2	octyl octanoate
2312-35-8	C19H26O4S	propargite
23128-74-7	C40H64N2O4	N,N'-hexane-1,6-diylbis[3-(3,5-di-tert-butyl-4-hydroxyphenylpropionamide]
23175-18-0	C17H21NO2	2-[benzyl(2-hydroxyethyl)amino]-1-phenylethanol
153954	C20H12O5	2-(6-hydroxy-3-oxo-(3H)-xanthen-9-yl)benzoic acid
23357-46-2	C10H13N	1-Naphthalenamine, 1,2,3,4-tetrahydro-, (1R)-
23357-52-0	C10H13N	1-Naphthalenamine, 1,2,3,4-tetrahydro-, (1S)-
23386-52-9	C16H26O7S	sodium 1,4-dicyclohexyl sulphonatosuccinate
23410-40-4	C9H24N2O2Si	N-[3-(dimethoxymethylsilyl)-2-methylpropyl]ethylenediamine
2356-53-8	C3Cl2F6O	1,2-dichloro-1,1,2-trifluoro-2-(trifluoromethoxy)ethane
23588-51-4	C9H17NO2	2,2-dimethyl-3-(morpholin-4-yl)propanal
2362-14-3	C20H24O2	4,4'-cyclohexylidenedi-o-cresol
23680-84-4	C10H10ClN3O2	2-chloro-6,7-dimethoxyquinazolin-4-amine
2372-45-4	C4H10O	sodium butanolate
23727-15-3	C10H16O	(S)-2,2,3-trimethylcyclopent-3-ene-1-acetaldehyde
2372-82-9	C18H41N3	N-(3-aminopropyl)-N-dodecylpropaan-1,3-diamine
2373-38-8	C16H30O7S	sodium 1,4-bis(1,3-dimethylbutyl) sulphonatosuccinate
2374-14-3	C12H21F9O3Si3	2,4,6-trimethyl-2,4,6-tris(3,3,3-trifluoropropyl)cyclotrisiloxane
23779-32-0	C10H24N2O4Si	[3-(triethoxysilyl)propyl]urea
23847-08-7	C12H20N2O2S2	1,1'-dithiobis[hexahydro-2H-azepin-2-one]
2385-77-5	C10H18O	(R)-3,7-dimethyloct-6-enal
23911-85-5	C29H24O7	2,2''-dihydroxy-4,4''-(2-hydroxy-propane-1,3-diyldioxy)dibenzophenone
2398-81-4	C6H10NO3	oxiniacic acid
2402-58-6	C28H52O4	didodecyl fumarate
2402-77-9	C5H3Cl2N	2,3-dichloropyridine
2404-44-6	C10H20O	octyloxirane
24085-03-8	C20H27NO3	α-[(benzyl-tert-butylamino)methyl]-m-xylene-4,α,α'-triol
24124-40-1	C23H21N3O8S2	1-amino-4-(3-amino-2,4,6-trimethyl-5-sulphoanilino)-9,10-dihydro-9,10-dioxoanthracene-2-sulphonic acid
2421-28-5	C17H6O7	benzophenone-3,3':4,4'-tetracarboxylic dianhydride
2422-91-5	C22H13N3O3	methylidynetri-p-phenylene triisocyanate
2425-85-6	C17H13N3O3	1-(4-methyl-2-nitrophenylazo)-2-naphthol
24293-43-4	C20H38O4S	bis(2-ethylhexyl) 2,2'-thiobisacetate
24338-09-8	C14H28O2Si	trimethylsilyl 10-undecenoate
2441-41-0	C18H35NO3	2-(hexadecanoylamino)acetic acid
24424-99-5	C10H18O5	di(tert-butyl) carbonate
24461-61-8	C9H11NO2	methyl (R)-aminophenylacetate

244768-32-9	C11H7ClN4	4-[(4-CHLOROPYRIMIDIN-2-YL)AMINO]BENZONITRILE
201624	C12H24O2	zinc dilaurate
24544-04-5	C12H19N	2,6-diisopropylaniline
203446	C8H16O2	barium bis(2-ethylhexanoate)
204023	C24H38O5	3α,7α-dihydroxy-12-oxo-5β-cholan-24-oic acid
2461-15-6	C11H22O2	[[(2-ethylhexyl)oxy]methyl]oxirane
24634-61-5	C6H8O2	potassium (E,E)-hexa-2,4-dienoate
24650-42-8	C16H16O3	2,2-dimethoxy-1,2-diphenylethan-1-one
211391	C7H12O3	4-hydroxybutyl acrylate
215256	C22H44O2	silver docosanoate
24916-90-3	C22H28O5	9β,11β-epoxy-17,21-dihydroxy-16α-methylpregna-1,4-diene-3,20-dione
2494-88-4	C8H11NO6S2	2-[(3-aminophenyl)sulphonyl] hydrogensulphate
2495-37-6	C11H12O2	benzyl methacrylate
2500-88-1	C36H74S2	dioctadecyl disulphide
25013-16-5	C11H16O2	tert-butyl-4-methoxyphenol
25015-63-8	C6H13BO2	4,4,5,5-Tetramethyl-1,3,2-dioxaborolane
2511-00-4	C11H20O2	ethyl 2-cyclohexylpropionate
2512-29-0	C17H16N4O4	2-[(4-methyl-2-nitrophenyl)azo]-3-oxo-N-phenylbutyramide
25134-21-8	C10H10O3	1,2,3,6-tetrahydromethyl-3,6-methanophthalic anhydride
25151-96-6	C41H76O6	2,2-bis(hydroxymethyl)-1,3-propanediyl dioleate
25157-64-6	C8H6N6O6	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5'-(1,2-diazenediyl)bis-
25168-05-2	C7H7Cl	chloromethylbenzene
2516-96-3	C7H4ClNO4	2-chloro-5-nitrobenzoic acid
2526-62-7	C6H13NO3Si	3-(trimethoxysilyl)propiononitrile
2528-61-2	C7H13ClO	heptanoyl chloride
25306-75-6	C5H10OS2	sodium O-isobutyl dithiocarbonate
25321-09-9	C12H18	diisopropylbenzene
25360-10-5	C9H20S	1,1-dimethylheptanethiol
25371-54-4	C20H43O3P	dimethyl octadecylphosphonate
25377-83-7	C8H16	octene
25448-25-3	C30H63O3P	triisodecyl phosphite
237449	C9H22O3Si	triethoxypropylsilane
2550-26-7	C10H12O	4-phenylbutan-2-one
239026	C9H20O4Si4	2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane
25550-98-5	C26H47O3P	diisodecyl phenyl phosphite
25618-55-7	C3H8O3	1,2,3-Propanetriol, homopolymer
2580-78-1	C22H18N2O11S3	2-(3-(4-amino-9,10-dihydro-3-sulpho-9,10-dioxoanthracen-4-yl)aminobenzenesulphonyl)vinyl) disodium sulphate
2594-21-0	C6H13NO2	Methyl N-butylcarbamate
25956-17-6	C18H16N2O8S2	disodium 6-hydroxy-5-[(2-methoxy-4-sulphonato-m-tolyl)azo]naphthalene-2-sulphonate

25973-55-1	C22H29N3O	2-(2H-benzotriazol-2-yl)-4,6-ditertpentylphenol
2602-34-8	C12H26O5Si	[3-(2,3-epoxypropoxy)propyl]triethoxysilane
26040-51-7	C24H34Br4O4	bis(2-ethylhexyl) tetrabromophthalate
2605-79-0	C12H27NO	N,N-dimethyldecylamine N-oxide
26090-29-9	C28H40N2O4	2-(diethylamino)ethyl 4-(2-(octyloxy)benzamido)benzoate
259636	C29H21N5O8S2	disodium 7-benzamido-4-hydroxy-3-[[4-[(4-sulphonatophenyl)azo]phenyl]azo]naphthalene-2-sulphonate
26116-12-1	C7H16N2	1-ethylpyrrolidin-2-ylmethylamine
2611-82-7	C20H14N2O10S3	trisodium 1-(1-naphthylazo)-2-hydroxynaphthalene-4',6,8-trisulphonate
26266-57-9	C22H42O6	sorbitan palmitate
26266-58-0	C60H108O8	anhydro-D-glucitol trioleate
2627-86-3	C8H11N	L-α-methylbenzylamine
2627-95-4	C8H18OSi2	1,1,3,3-tetramethyl-1,3-divinyldisiloxane
26322-14-5	C34H66O6	dihexadecyl peroxodicarbonate
26391-06-0	C7H12N2O	Acetamide, 2-cyano-N,N-diethyl-
26412-87-3	C5H5N	sulphur trioxide--pyridine (1:1)
26496-99-1	C13H6Cl4O3	bis(2,4-dichlorophenyl) carbonate
26537-19-9	C12H16O2	methyl 4-tert-butylbenzoate
26544-23-0	C22H31O3P	isodecyl diphenyl phosphite
26544-38-7	C16H26O3	dihydro-3-(tetrapropenyl)furan-2,5-dione
26566-95-0	C12H27O2PS2	zinc bis[O-(2-ethylhexyl)] bis[O-(isobutyl)] bis(dithiophosphate)
26658-19-5	C60H114O8	sorbitan tristearate
26680-54-6	C12H18O3	dihydro-3-(octenyl)furan-2,5-dione
2668-75-9	C23H28O4	17-Acetoxy-1,4,6-pregnatriene-3,20-dione
26741-53-7	C33H50O6P2	3,9-bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane
26748-41-4	C14H28O3	tert-butyl peroxyneodecanoate
26762-92-5	C10H20O2	menthane, monohydroperoxy derivative
26762-93-6	C12H18O2	diisopropylbenzene hydroperoxide
26787-78-0	C16H19N3O5S	Amoxicillin
284957	C4H9NO	N,N-dimethylacrylamide
2687-96-9	C16H31NO	N-(n-dodecyl)pyrrolidinone
2691-41-0	C4H8N8O8	octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine
26919-50-6	C13H19NO4S	6-[methyl(phenylsulphonyl)amino]hexanoic acid, compound with 2,2',2''-nitrilotriethanol (1:1)
27006-83-3	C6H6Cl2N2O	5-chloro-1,3-dimethyl-1H-pyrazole-4-carbonyl chloride
27014-42-2	C18H40N2O8	Poly(oxy-1,2-ethanediyl), a,a',a'',a'''-[1,2-ethanediylbis(nitrilodi-2,1-ethanediyl)]tetrakis[w-hydroxy-
2705-87-5	C12H20O2	allyl 3-cyclohexylpropionate
27138-01-8	C12H18O2	α,α,α',α'-tetramethylxylene-α,α-diol
27157-94-4	C14H15O2PS2	O,O-bis(methylphenyl) hydrogen dithiophosphate
2720-73-2	C6H12OS2	potassium O-pentyl dithiocarbonate
27253-29-8	C10H20O2	zinc neodecanoate

27253-31-2	C10H20O2	neodecanoic acid, cobalt salt
27298-98-2	C9H13N	(S)-1-(p-tolyl)ethanamine
27306-79-2	C16H34O2	α-hydro-ω-tetradecoxy-poly(oxyethylene)
27310-25-4	C10H9NO9S3	7-aminonaphthalene-1,3,5-trisulphonic acid
2736-23-4	C7H5Cl2NO4S	2,4-dichloro-5-sulphamoylbenzoic acid
27375-52-6	C10H13NO4S	N-[4-[(2-hydroxyethyl)sulphonyl]phenyl]acetamide
274-09-9	C7H6O2	1,3-benzodioxolane
2741-57-3	C8H5Cl5	1-(dichloromethyl)-2-(trichloromethyl)benzene
2743-38-6	C18H14O8	dibenzoyl-L-tartaric acid monohydrate
27458-93-1	C18H38O	isooctadecan-1-ol
274693-53-7	C16H21NO5	benzyl [(3aS,4R,6S,6aR)-6-hydroxy-2,2-dimethyltetrahydro-3aH-cyclopenta[d][1,3]dioxol-4-yl]carbamate
27472-21-5	C12H15NO2	(3,4-diethoxyphenyl)acetonitrile
27503-81-7	C13H10N2O3S	2-phenyl-1H-benzimidazole-5-sulphonic acid
27514-08-5	C8H13NO2	N-(4-oxocyclohexyl)acetamide
2752-17-2	C4H12N2O	2,2'-oxydi(ethylamine)
27566-05-8	C16H19NO	4-[2-[(phenylmethyl)amino]propyl]- Phenol
27619-89-2	C8H4ClF13O2S	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctanesulphonyl chloride
27676-62-6	C48H69N3O6	1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione
27710-82-3	C23H28Br2NP	[3-(Dimethylamino)propyl]triphenylphosphonium bromide hydrobromide
2781-00-2	C20H34O4	di-tert-butyl α,α,α',α'-tetramethyl-(p-phenylenedimethylene) diperoxide
27830-12-2	C15H22O3	2-(octyloxy)benzoic acid
2783-94-0	C16H12N2O7S2	disodium 6-hydroxy-5-[(4-sulphonatophenyl)azo]naphthalene-2-sulphonate
27858-32-8	C15H26O7Ti	bis(ethyl acetoacetato-O1',O3)bis(propan-2-olato)titanium
2786-76-7	C26H22N4O4	4-[[4-(aminocarbonyl)phenyl]azo]-N-(2-ethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide
27871-49-4	C4H8O3	methyl (S)-(-)-lactate
27970-79-2	C6H12O2	Reaction mass of (2S)-1-hydroxy-2-methylpentan-3-one and (2R)-1-hydroxy-2-methylpentan-3-one
280-57-9	C6H12N2	1,4-diazabicyclooctane
2814-77-9	C16H10ClN3O3	1-[(2-chloro-4-nitrophenyl)azo]-2-naphthol
28178-42-9	C13H17NO	2,6-diisopropylphenyl isocyanate
28219-61-6	C14H24O	2-ethyl-4-(2,2,3-trimethyl-3-cyclopenten-1-yl)-2-buten-1-ol
28281-49-4	C10H10O3	1-(1,3-benzodioxol-5-yl)propan-1-one
28305-25-1	C3H6O3	calcium (S)-2-hydroxypropionate
2835-68-9	C7H8N2O	p-aminobenzamide
28390-91-2	C16H19ClN2O	4-[(4-aminophenyl)methyl]aniline; 2-(chloromethyl)oxirane
284461-73-0	C21H16ClF3N4O3	4-(4-((((4-CHLORO-3-(TRIFLUOROMETHYL)PHENYL)AMINO)CARBONYL)AMINO)PHENOXY)-N-METHYL-2-PYRIDINECARBOXAMIDE
284462-37-9	C13H13N3O2	4-(4-aminophenoxy)-N-methylpyridine-2-carboxamide

28473-19-0	C30H58O4	diisodecyl sebacate
28510-23-8	C21H40O4	2,2-dimethylpropane-1,3-diyl 2-ethylhexanoate
28535-81-1	C29H44O7	methyl 3-α,7-α-diacetoxy-12-oxo-5-β-cholan-24-oate
2855-19-8	C12H24O	decyloxirane
286-20-4	C6H10O	1,2-epoxycyclohexane
28629-66-5	C16H35O2PS2	zinc bis(O,O-diisooctyl) bis(dithiophosphate)
28654-73-1	C47H49CuN11	[N,N,N',N',N'',N''-hexaethyl-29H,31H-phthalocyaninetrimethylaminato(2-)-N29,N30,N31,N32]copper
286938-65-6	C21H50O2Si3	Trisiloxane, 1,1,1,3,5,5,5-Heptamethyl-3-Tetradecyl-
28706-25-4	C31H22N4O14S4	tetrasodium 7,7'-(carbonyldiimino)bis[4-hydroxy-3-[(6-sulphonato-2-naphthyl)azo]naphthalene-2-sulphonate]
2873-97-4	C9H15NO2	N-(1,1-dimethyl-3-oxobutyl)acrylamide
28770-01-6	C8H17NO2	2-[2-(propan-2-yl)-1,3-oxazolidin-3-yl]ethanol
288-13-1	C3H4N2	pyrazole
28855-17-6	C24H42O3S	octadecylbenzenesulphonic acid
28874-51-3	C5H7NO3	sodium 5-oxo-L-prolinate
2890-61-1	C8H13ClO	1-methylcyclohexanecarbonyl chloride
2896-70-0	C9H16NO2	2,2,6,6-tetramethyl-4-oxopiperidinooxy
2901-13-5	C12H16O2	α,α-Dimethyl-ethyl ester benzeneacetic acid
2905-62-6	C7H3Cl3O	3,5-dichlorobenzoyl chloride
2915-57-3	C20H38O4	bis(2-ethylhexyl) succinate
29171-20-8	C10H16O	3,7-dimethyloct-6-en-1-yn-3-ol
2920-38-9	C13H9N	p-phenylbenzonitrile
29253-36-9	C13H14	isopropylnaphthalene
292605-05-1	C10H18O	(3Z)-hex-3-en-1-yl 2-methylprop-2-en-1-yl ether
29385-43-1	C7H7N3	methyl-1H-benzotriazole
2941-20-0	C9H13N	1-Phenylpropylamine
2941-23-3	C6H8N2	2-amino-1-cyclopentene-1-carbonitrile
2941-64-2	C3H5ClOS	ethyl chlorothiolformate
2942-59-8	C6H4ClNO2	2-chloronicotinic acid
2943-75-1	C14H32O3Si	triethoxyoctylsilane
2973-59-3	C8H7BrO3	2-bromo-5-hydroxy-4-methoxybenzaldehyde
29736-75-2	C6H12O6Sb2	2,5,7,10,11,14-hexaoxa-1,6-distibabicyclo[4.4.4]tetradecane
297730-93-9	C9H5F15O	3-Ethoxyperfluoro(2-methylhexane)
2978-58-7	C5H9N	1,1-dimethylprop-3-ynylamine
29806-73-3	C24H48O2	2-ethylhexyl palmitate
298-07-7	C16H35O4P	bis(2-ethylhexyl) hydrogen phosphate
29878-91-9	C22H14O4	1,1'-binaphthyl-8,8'-dicarboxylic acid
29920-31-8	C21H19N5O7	dimethyl 5-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azoterephthalate
29923-31-7	C17H31NO5	sodium hydrogen N-(1-oxododecyl)-L-glutamate
2996-92-1	C9H14O3Si	trimethoxyphenylsilane

2997-92-4	C8H18N6	2,2'-azobis[2-methylpropionamidine] dihydrochloride
3006-86-8	C14H28O4	cyclohexylidenebis[tert-butyl] peroxide
3010-96-6	C8H16O2	2,2,4,4-tetramethylcyclobutane-1,3-diol, mixed isomers
30125-47-4	C26H6Cl8N2O4	3,4,5,6-tetrachloro-N-[2-(4,5,6,7-tetrachloro-2,3-dihydro-1,3-dioxo-1H-inden-2-yl)-8-quinolyl]phthalimide
30246-33-4	C11H12N4O3S3	(6R-trans)-7-amino-3-[[(5-methyl-1,3,4-thiadiazol-2-yl)thio]methyl]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
302964-08-5	C16H13Cl2N5OS	2-[(6-chloro-2-methylpyrimidin-4-yl)amino]-N-(2-chloro-6-methylphenyl)-1,3-thiazole-5-carboxamide
3030-47-5	C9H23N3	bis(2-dimethylaminoethyl)(methyl)amine
3031-66-1	C6H10O2	hex-3-yne-2,5-diol
3033-62-3	C8H20N2O	N,N,N',N'-tetramethyl-2,2'-oxybis(ethylamine)
3034-38-6	C3H3N3O2	4-nitroimidazole
30414-54-1	C7H12O3	methyl 3-oxohexanoate
30433-91-1	C6H9NS	thiophene-2-ethylamine
3047-32-3	C6H12O2	3-ethyloxetane-3-methanol
3048-64-4	C9H12	5-vinylnorborn-2-ene
3049-71-6	C48H26N6O4	2,9-bis[4-(phenylazo)phenyl]anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone
3061-75-4	C22H45NO	docosanamide
30618-84-9	C5H10O4S	mercaptoacetic acid, monoester with propane-1,2,3-triol
30674-80-7	C7H9NO3	2-isocyanatoethyl methacrylate
3069-29-2	C8H22N2O2Si	N-[3-(dimethoxymethylsilyl)propyl]ethylenediamine
30693-53-9	C6H6N2O5S	sodium 2-amino-5-nitrobenzenesulphonate
3069-40-7	C11H26O3Si	trimethoxyoctylsilane
3082-64-2	C9H13N	(R)-1-PHENYLPROPYLAMINE
3088-31-1	C16H34O6S	sodium 2-(2-dodecyloxyethoxy)ethyl sulphate
3101-60-8	C13H18O2	p-tert-butylphenyl 1-(2,3-epoxy)propyl ether
31024-56-3	C10H25NO3Si	N-[3-(trimethoxysilyl)propyl]butylamine
31138-65-5	C7H14O8	sodium glucoheptonate
3115-49-9	C17H26O3	(4-nonylphenoxy)acetic acid
3120-74-9	C8H10OS	4-(methylthio)-m-cresol
3121-61-7	C6H10O3	2-methoxyethyl acrylate
31221-06-4	C4H2N4O3	5-Diazo-2,4,6(1H, 3H, 5H)-pyrimidinetrione
312-94-7	C8H4ClF3O	α,α,α-trifluoro-o-toluoyl chloride
31335-74-7	C21H40O4	2,2-dimethyl-1,3-propanediyl dioctanoate
3147-75-9	C20H25N3O	2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol
3148-73-0	C4H8N2O2	N,N'-diacetylhydrazine
31560-20-0	C13H15NO4	SQ 29,242
3159-62-4	C18H36O3	calcium(2+) 12-hydroxyoctadecanoate
3164-85-0	C8H16O2	potassium 2-ethylhexanoate

31778-10-6	C29H25N5O5	butyl 2-[[3-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-hydroxy-1-naphthyl]azo]benzoate
3179-47-3	C14H26O2	decyl methacrylate
3179-63-3	C5H13NO	3-dimethylaminopropan-1-ol
3179-76-8	C8H21NO2Si	3-(diethoxymethylsilyl)propylamine
3179-80-4	C17H36N2O	N-[3-(dimethylamino)propyl]dodecanamide
31837-42-0	C18H15N5O5	2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]benzoic acid
320-60-5	C7H3Cl2F3	2,4-dichloro-α,α,α-trifluorotoluene
32162-27-9	C10H16O	(1α,2β,4β,6α)-2,2,7-trimethyl-3-oxatricyclo[4.1.1.02,4]octane
3217-00-3	C8H14N4	3,3'-(ethylenediimino)bispropiononitrile
3218-36-8	C13H10O	p-phenylbenzaldehyde
32210-23-4	C12H22O2	4-tert-butylcyclohexyl acetate
3234-28-4	C14H28O	dodecyloxirane
3234-85-3	C28H56O2	tetradecyl myristate
3238-40-2	C6H4O5	furan-2,5-dicarboxylic acid
32388-55-9	C17H26O	[3R-(3α,3aβ,7β,8aα)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)ethan-1-one
32454-35-6	C10H11BrO2	2-(4-bromophenyl)-2-methylpropanoic acid
32492-61-8	C19H24O4	2-[4-[2-[4-(2-hydroxyethoxy)phenyl]propan-2-yl]phenoxy]ethanol
32509-66-3	C50H66O8	ethylene bis[3,3-bis(3-tert-butyl-4-hydroxyphenyl)butyrate]
32588-76-4	C18H4Br8N2O4	N,N'-ethylenebis(3,4,5,6-tetrabromophthalimide)
32687-78-8	C34H52N2O4	2',3-bis[[3-[3,5-di-tert-butyl-4-hydroxyphenyl]propionyl]]propionohydrazide
32724-62-2	C36H38N2O2	1,4-bis[(2,6-diethyl-4-methylphenyl)amino]anthraquinone
32765-81-4	C9H21Br2N	Ammonium, (6-bromohexyl)trimethyl-, bromide
32768-54-0	C7H6Cl2	2,3-dichlorotoluene
3277-26-7	C4H14OSi2	1,1,3,3-tetramethyldisiloxane
327-78-6	C8H3ClF3NO	1-chloro-4-isocyanato-2-(trifluoromethyl) benzene
328-84-7	C7H3Cl2F3	3,4-dichloro-α,α,α-trifluorotoluene
328-99-4	C8H4F4O	3-(trifluoromethyl)benzoyl fluoride
329-01-1	C8H4F3NO	α,α,α-trifluoro-3-tolyl isocyanate
3296-90-0	C5H10Br2O2	2,2-bis(bromomethyl)propane-1,3-diol
33125-90-5	C23H31ClO4	6ß-chloro-17α-hydroxypregna-4-ene-3,20-dione, 17-acetate
3332-27-2	C16H35NO	N,N-dimethyltetradecylamine N-oxide
33329-35-0	C15H36N4	N,N-bis[3-(dimethylamino)propyl]-N',N'-dimethylpropane-1,3-diamine
3338-24-7	C4H11O2PS2	sodium O,O-diethyl dithiophosphate
33422-23-0	C13H21NO2	ethyl 2-allyl-2-cyano-3-methylhexanoate
33494-80-3	C8H19O4P	Di-tert-butyl hydrogen phosphate; potassium salt
530089	C32H23N5O6S2	sodium 8-phenylamino-5-(4-(3-sulphonatophenylazo)-1-naphthylazo)naphthalenesulphonate

33704-61-9	C14H22O	1,2,3,5,6,7-hexahydro-1,1,2,3,3-pentamethyl-4H-inden-4-one
337906-36-2	C8H12N2O	1,4-Benzenediamine, 2-(methoxymethyl)-
338-83-0	C9F21N	perfluamine
34041-09-3	C8H16O2	2-ethylhexanoic acid, molybdenum salt
3407-42-9	C16H28O	3-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol
34184-82-2	C21H28O3	17-hydroxypregna-4,9(11)-diene-3,20-dione
34206-40-1	C16H32N4O4Si	butan-2-one O,O',O'',O'''-silanetetrayltetraoxime
342-25-6	C13H8F2O	2,4'-difluorobenzophenone
3423-25-4	C10H19NO	endo-8-isopropyl-8-azabicyclo[3.2.1]octan-3-ol
3423-28-7	C10H17NO	8-isopropyl-8-azabicyclo[3.2.1]octan-3-one
3425-61-4	C5H12O2	tert-pentyl hydroperoxide
34316-64-8	C18H36O2	hexyl laurate
3437-84-1	C8H14O4	bisisobutyryl peroxide
34396-03-7	C11H26O3Si	trimethoxy(2,4,4-trimethylpentyl)silane
34432-92-3	C22H31N3O2	N-ethyl-N-[2-[1-(2-methylpropoxy)ethoxy]ethyl]-4-(phenylazo)aniline
34443-12-4	C13H26O4	OO-tert-butyl O-(2-ethylhexyl) peroxycarbonate
564607	C6H11NO2	1-(2-hydroxyethyl)pyrrolidin-2-one
34455-22-6	C13H17F13N2O2S	N-[3-(dimethylamino)propyl]-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-octane-1-sulfonamide
3452-97-9	C9H20O	3,5,5-trimethylhexan-1-ol
3457-61-2	C13H20O2	tert-butyl α,α-dimethylbenzyl peroxide
3468-63-1	C16H10N4O5	1-[(2,4-dinitrophenyl)azo]-2-naphthol
34690-00-1	C17H44N3O15P5	[[(phosphonomethyl)imino]bis[hexamethylenenitrilobis(methylene)]]tetrakisphosphonic acid
34708-08-2	C10H21NO3SSi	triethoxy(3-thiocyanatopropyl)silane
34730-59-1	C4H12N2O3S	sodium 2-[(2-aminoethyl)amino]ethanesulphonate
34841-35-5	C9H9ClO	3'-chloropropiophenone
3490-06-0	C11H17NO2	3,4-dimethoxy-N-methylphenethylamine
349-76-8	C9H7F3O	3'-(trifluoromethyl)acetophenone
35037-73-1	C8H4F3NO2	p-(trifluoromethoxy)phenyl isocyanate
350-46-9	C6H4FNO2	1-fluoro-4-nitrobenzene
3508-98-3	C12H15N	2-phenylhexanenitrile
35092-89-8	C9H7NO6	methyl hydrogen 2-nitroterephthalate
35113-48-5	C13H22O6	2-ISOPROPYL-1,3-DIOXANE-5,5-DICARBOXYLIC ACID DIETHYL ESTER
35123-06-9	C5H11NO2	2-hydroxy-N,N-dimethyl-propanamide
3520-72-7	C25H17Cl2N8O2	4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[2,4-dihydro-5-methyl-2-phenyl-3H-pyrazol-3-one]
35265-04-4	C6H15NO	2-[(1-methylpropyl)amino]ethanol
352-70-5	C7H7F	3-fluorotoluene
352-93-2	C4H10S	diethyl sulphide
353497-37-7	C17H15NO3	methyl 10-methoxy-5H-dibenzo[b,f]azepine-5-carboxylate

354-15-4	C2HCl3F2	Reaction mass of (2R)-1,1,2-trichloro-1,2-difluoroethane and (2S)-1,1,2-trichloro-1,2-difluoroethane
3547-33-9	C10H22OS	2-(octylthio)ethanol
3558-60-9	C9H12O	(2-methoxyethyl)benzene
35636-63-6	C21H19N5O7	dimethyl 2-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]terephthalate
3576-88-3	C6H9N11	2,2'-iminobis[4,6-diamino-1,3,5-triazine]
3577-63-7	C7H7NO5S	5-sulphoanthranilic acid
35836-72-7	C13H20O2	(1R,5S)-2-(6,6-dimethylbicyclo[3.1.1]hept-2-en-2-yl) ethyl acetate
35836-73-8	C11H18O	(1R)-6,6-dimethylbicyclo[3.1.1]hept-2-en-2-ethanol
35869-64-8	C40H23Cl3N8O8	N,N'-(2-chloro-1,4-phenylene)bis[4-[(4-chloro-2-nitrophenyl)azo]-3-hydroxynaphthalene-2-carboxamide]
35948-25-5	C12H9O2P	6H-dibenz[c,e][1,2]oxaphosphorin 6-oxide
360-64-5	C8H6F3NO	o-(trifluoromethyl)benzamide
36078-10-1	C30H58O2	dodecyl oleate
361366-15-6	C19H26O4	ethyl 1-(2-mesitylacetoxy)cyclopentanecarboxylate
3624-77-9	C21H39NO3	sodium N-methyl-N-(1-oxo-9-octadecenyl)aminoacetate
3634-83-1	C10H8N2O2	1,3-bis(isocyanatomethyl)benzene
36443-68-2	C34H50O8	ethylenebis(oxyethylene) bis[3-(5-tert-butyl-4-hydroxy-m-tolyl)propionate]
3648-18-8	C40H80O4Sn	dioctyltin dilaurate
36483-57-5	C5H9Br3O	2,2-dimethylpropan-1-ol, tribromo derivative
365411-50-3	C16H26O2	Reaction mass of (4aR,8R,9bS)-7,7,8,9,9-pentamethyl-4,4a,5,6,7,8,9,9b-octahydroindeno[4,5-d][1,3]dioxine and (4aR,8S,9bS)-7,7,8,9,9-pentamethyl-4,4a,5,6,7,8,9,9b-octahydroindeno[4,5-d][1,3]dioxine
36631-30-8	C39H66O6	triisodecyl benzene-1,2,4-tricarboxylate
3673-79-8	C5H8Br2O2	[Name not available]
36788-39-3	C18H39O9P	7-[2-(2-hydroxymethylethoxy)methylethoxy]tetramethyl-3,6,8,11-tetraoxa-7-phosphatridecane-1,13-diol
3681-71-8	C8H14O2	(Z)-hex-3-enyl acetate
3687-45-4	C36H68O2	(Z)-octadec-9-enyl oleate
36888-99-0	C16H9N5O6	5,5'-(1H-isoindole-1,3(2H)-diylidene)dibarbituric acid
36894-69-6	C19H24N2O3	labetalol
36968-27-1	C25H20N4O4	4-[[4-(aminocarbonyl)phenyl]azo]-3-hydroxy-N-(2-methoxyphenyl)naphthalene-2-carboxamide
3698-89-3	C13H28S	dodecyl methyl sulphide
3699-54-5	C5H10N2O2	1-(2-hydroxyethyl)imidazolidin-2-one
37052-78-1	C8H8N2OS	1,3-dihydro-5-methoxy-2H-benzimidazole-2-thione
3709-43-1	C14H10N2O10S2	disodium 4,4'-dinitrostilbene-2,2'-disulphonate
3710-30-3	C8H14	octa-1,7-diene
3710-84-7	C4H11NO	N,N-diethylhydroxylamine

371-40-4	C6H6FN	4-fluoroaniline
371-41-5	C6H5FO	4-fluorophenol
3717-40-6	C12H21N	N,N-dimethyl-1-adamantanamine
37187-22-7	C10H14O6	2,4-Pentanedione, peroxide
372-31-6	C6H7F3O3	ethyl 4,4,4-trifluoroacetoacetate
37310-83-1	C18H37O4P	9-Octadecen-1-ol, (Z)-, phosphate
373-44-4	C8H20N2	octamethylenediamine
3738-00-9	C16H28O	dodecahydro-3a,6,6,9a-tetramethylnaphtho[2,1-b]furan
374067-80-8	C11H8N4O2	4-[(4,6-DIHYDROXYPYRIMIDIN-2-YL)AMINO]BENZONITRILE
37441-29-5	C8H2Cl2I3NO2	5-amino-2,4,6-triiodo-1,3-benzenedicarbonyldichloride
3749-87-9	C29H46O7	methyl 3-α,7-α-diacetoxy-12-α-hydroxy-5-β-cholan-24-oate
375-72-4	C4F10O2S	1,1,2,2,3,3,4,4,4-nonafluorobutane-1-sulphonyl fluoride
3775-90-4	C10H19NO2	2-tert-butylaminoethyl methacrylate
3779-63-3	C24H36N6O6	(2,4,6-trioxotriazine-1,3,5(2H,4H,6H)-triyl)tris(hexamethylene) isocyanate
3806-34-6	C41H82O6P2	O,O'-dioctadecylpentaerythritol bis(phosphite)
38109-77-2	C6H8N2O2	ethyl 3-amino-2-cyanoprop-2-enoate
382-26-3	C5H4F8O	2-[difluoro(methoxy)methyl]-1,1,1,3,3,3-hexafluoropropane
382-28-5	C5F11NO	2,2,3,3,5,5,6,6-octafluoro-4-(trifluoromethyl)morpholine
383-63-1	C4H5F3O2	ethyl trifluoroacetate
3851-87-4	C18H34O4	bis(3,5,5-trimethylhexanoyl) peroxide
3855-32-1	C11H27N3	N-[3-(dimethylamino)propyl]-N,N',N'-trimethylpropane-1,3-diamine
38668-48-3	C13H21NO2	1,1'-(p-tolylimino)dipropan-2-ol
3886-69-9	C8H11N	D-α-methylbenzylamine
38888-98-1	C14H14	(phenylethyl)benzene
3891-98-3	C15H32	2,6,10-trimethyldodecane
729335	C17H18ClN3O	bumetrizole
3900-45-6	C13H12O2	1-(6-methoxy-2-naphthyl)ethan-1-one
3905-19-9	C40H24Cl4N6O4	N,N'-phenylene-1,4-bis[4-[(2,5-dichlorophenyl)azo]-3-hydroxynaphthalene-2-carboxamide]
39072-70-3	C22H30N4O2	N,N''-hexane-1,6-diylbis[N'-benzylurea]
39083-38-0	C10H20	3,4,5,5-tetramethylhex-2-ene
3910-51-8	C11H14ClNO	2-chloro-N-(2,4,6-trimethylphenyl)acetamide
39118-50-8	C6H13O5P	dimethyl (2-acetoxyethyl)phosphonate
735273	C12H26O	2-butyloctan-1-ol
39236-46-9	C11H16N8O8	N,N''-methylenebis[N'-[3-(hydroxymethyl)-2,5-dioxoimidazolidin-4-yl]urea]
3923-79-3	C5H10N2O3	4,5-dihydroxy-1,3-dimethylimidazolidin-2-one
39255-32-8	C8H16O2	ethyl 2-methylvalerate
393-52-2	C7H4ClFO	2-fluorobenzoyl chloride
39489-75-3	C13H4Cl4N2O7	bis(2,4-dichloro-5-nitrophenyl) carbonate
39590-81-3	C5H10O2	1,1-BIS-(HYDROXYMETHYL)-CYCLOPROPANE

3965-55-7	C10H10O7S	sodium dimethyl 5-sulphonatoisophthalate
39670-09-2	C12H22O5	2-[2-(2-ethoxyethoxy)ethoxy]ethyl methacrylate
39811-17-1	C13H13NO	5-phenyl-o-anisidine
398489-26-4	C8H13NO3	3-Oxo-azetidine-1-carboxylic acid tert-butyl ester
39856-50-3	C5H3BrN2O2	5-bromo-2-nitropyridine
40039-93-8	C18H17Br4ClO3	2,2',6,6'-Tetrabromo-4,4'-isopropylidenediphenol, oligomeric reaction products with 1-chloro-2,3-epoxypropane
4009-98-7	C20H21OP	(methoxymethyl)triphenylphosphonium chloride
40137-22-2	C4H11NO2	3-(methylamino)propane-1,2-diol
4013-94-9	C8H20N2	N,N'-diisopropylethylenediamine
402-31-3	C8H4F6	α,α,α,β,β,β-hexafluoro-m-xylene
4023-34-1	C4H5ClO	cyclopropanecarbonyl chloride
402913-84-2	C33H54N6O10	benzyl (3,14,25-trihydroxy-2,10,13,21,24-pentaoxo-3,9,14,20,25-pentaazatriacontan-30-yl)carbamate
40306-75-0	C8H10N2O5S	3-acetamido-5-amino-4-hydroxybenzenesulphonic acid
4039-32-1	C6H19NSi2	lithiumbis(trimethylsilyl)amide
4051-63-2	C28H16N2O4	4,4'-diamino[1,1'-bianthracene]-9,9',10,10'-tetraone
40601-76-1	C42H57N3O6	1,3,5-tris[[4-tert-butyl-3-hydroxy-2,6-xylyl]methyl]-1,3,5-triazine-2,4,6(1H,3H,5H)-trione
40618-31-3	C40H24Cl4N6O3	N,N'-(2,5-dichloro-1,4-phenylene)bis[4-[(2,5-dichlorophenyl)azo]-3-hydroxynaphthalene-2-carboxamide]
4065-45-6	C14H12O6S	sulisobenzone
407-25-0	C4F6O3	trifluoroacetic anhydride
4075-81-4	C3H6O2	calcium dipropionate
4083-64-1	C8H7NO3S	p-toluenesulphonyl isocyanate
4090-51-1	C10H20O5P2S2	2,2'-oxybis[5,5-dimethyl-1,3,2-dioxaphosphorinane] 2,2'-disulphide
41026-17-9	C21H28O8	2,2-dimethylpropane-1,3-diyl cyclohex-4-ene-1,2-dicarboxylate
41078-06-2	C6H9N3O2	2-cyano-N-[(ethylamino)carbonyl]acetamide
41200-96-8	C9H11Cl2NO	2,4-dichloro-5-isopropoxyaniline
41200-97-9	C9H9Cl2NO3	1,5-dichloro-2-(1-methylethoxy)-4-nitrobenzene
811543	C12H22O4S	dibutyl 2,2'-thiobisacetate
41272-40-6	C23H26N2O	[4-[α-[4-(dimethylamino)phenyl]benzylidene]cyclohexa-2,5-dien-1-ylidene]dimethylammonium acetate
814713	C8H12O6Si	triacetoxyvinylsilane
41435-93-2	C11H18O	1-[(1R,2S)-2,6,6-trimethylcyclohex-3-en-1-yl]ethanone
41438-38-4	C11H13NO4	2,4-Pyridinedicarboxylic acid, diethyl ester
41484-35-9	C38H58O6S	thiodiethylene bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]
41506-62-1	C19H16N2O3	N-(4-acetylaminophenyl)-3-hydroxynaphthalene-2-carboxamide
4151-51-3	C21H12N3O6PS	tris(p-isocyanatophenyl) thiophosphate
4156-21-2	C9H6Cl2N4O3S	sodium p-[(4,6-dichloro-1,3,5-triazin-2-yl)amino]benzenesulphonate

41611-76-1	C32H30N2O2	1,4-bis[(2-ethyl-6-methylphenyl)amino]anthraquinone
41637-38-1	C27H32O6	Esterification products of 4,4'-isopropylidenediphenol, ethoxylated and 2-methylprop-2-enoic acid.
41687-30-3	C8H9NO5S	2-[(3-nitrophenyl)sulphonyl]ethanol
4180-23-8	C10H12O	(E)-anethole
41851-59-6	C9H13NO	(S)-1-(4-Methoxyphenyl)ethylamine
4187-38-6	C9H13N	(R)-1-(p-tolyl)ethanamine
41965-95-1	C8H11Cl2NO	(3-chloro-4-methoxyphenyl)methanaminium chloride
42019-78-3	C13H9ClO2	4-chloro-4'-hydroxybenzophenone
42142-52-9	C10H15NO	α-[2-(methylamino)ethyl]benzyl alcohol
42222-50-4	C41H76O4	2,2-dimethyl-1,3-propanediyl dioleate
848522	C11H21NO	N-(1,1,3,3-tetramethylbutyl)acrylamide
423165-13-3	C20H28N4	8-Azabicyclo[3.2.1]octane, 3-[3-methyl-5-(1-methylethyl)-4H-1,2,4-triazol-4-yl]-8-(pehnylmethyl)-, (3-exo)-
4246-51-9	C10H24N2O3	3,3'-oxybis(ethyleneoxy)bis(propylamine)
42487-72-9	C9H15N3O	2-(diethylamino)-6-methyl-1H-pyrimidin-4-one
4253-34-3	C7H12O6Si	methylsilanetriyl triacetate
4273-92-1	C19H16ClNO4	4'-chloro-3-hydroxy-2',5'-dimethoxy-2-naphthanilide
428-59-1	C3F6O	trifluoro(trifluoromethyl)oxirane
42872-29-7	C10H8ClNO	3-(1-cyanoethyl)benzoyl chloride
42872-30-0	C16H13NO	2-(m-benzoylphenyl)propionitrile
430-67-1	C2H5F2N	2,2-Difluoroethan-1-amine
43133-95-5	C6H14	methylpentane
4316-74-9	C3H9NO3S	sodium N-methyltaurinate
434-16-2	C27H44O	7,8-didehydrocholesterol
4378-61-4	C22H20Br2O2	4,10-dibromodibenzo[def,mno]chrysene-6,12-dione
4402-30-6	C7H17NO2	1,1'-(methylimino)dipropan-2-ol
4431-83-8	C7H16O4	2,5,7,10-tetraoxaundecane
443-83-4	C7H6ClF	2-chloro-6-fluorotoluene
4443-26-9	C14H15NO4	1,3-dihydro-1,3-dioxo-2H-isoindole-2-hexanoic acid
929727	C24H42	octadecylbenzene
445-03-4	C7H5ClF3N	4-chloro-α,α,α-trifluoro-o-toluidine
4457-71-0	C6H14O2	3-methylpentane-1,5-diol
447-61-0	C8H5F3O	o-(trifluoromethyl)benzaldehyde
44914-03-6	C8H14O2	2-methylbutyl acrylate
4498-67-3	C8H6N2O2	1H-indazole-3-carboxylic acid
4499-86-9	C12H29NO	tetrapropylammonium hydroxide
4500-29-2	C10H21NO2	2,2'-(cyclohexylimino)bisethanol
4501-58-0	C10H16O	(R)-2,2,3-trimethylcyclopent-3-ene-1-acetaldehyde
454-31-9	C4H6F2O2	ethyl difluoroacetate
4559-86-8	C17H36N2O	tetrabutylurea

4584-46-7	C4H10ClN	2-chloroethyldimethylammonium chloride
460-00-4	C6H4BrF	1-bromo-4-fluorobenzene
461-82-5	C7H6F3NO	4-(trifluoromethoxy)aniline
462-34-0	C4H8O	trifluoro(tetrahydrofuran)boron
462-95-3	C5H12O2	diethoxymethane
4651-67-6	C24H38O4	3-α-hydroxy-7-oxo-5-β-cholan-24-oic acid
4672-38-2	C3H9O3P	propylphosphonic acid
4684-28-0	C16H19NO4	[7(S)-(1α,.2β,4β,5α,7β)]-3-oxa-9-azatricyclo[3.3.1.02,4]non-7-yl (hydroxymethyl)phenylacetate
1022261	C15H13NO	10-methoxy-5H-dibenz[b,f]azepine
1025699	C3H7Cl2OP	propylphosphonic dichloride
471-01-2	C9H14O	3,5,5-trimethylcyclohex-3-en-1-one
4711-68-6	C19H17NO3	4'-ethoxy-3-hydroxy-2-naphthanilide
4724-48-5	C8H19O3P	octylphosphonic acid
474-25-9	C24H40O4	chenodeoxycholic acid
4747-21-1	C4H11N	N-methylisopropylamine
479-27-6	C10H10N2	1,8-naphthylenediamine
48076-38-6	C23H44O2	icosyl acrylate
4813-57-4	C21H40O2	octadecyl acrylate
48145-04-6	C11H12O3	2-phenoxyethyl acrylate
488-43-7	C6H15NO5	1-amino-1-deoxy-D-glucitol
488-98-2	C7H4Cl3F	o-fluoro-α,α,α-trichlorotoluene
4890-85-1	C15H14O2	o-phenethylbenzoic acid
4948-15-6	C32H17N2O4	2,9-bis(3,5-dimethylphenyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone
49553-76-6	C24H46O6	oleic acid, monoester with oxybis(propanediol)
49701-24-8	C9H14N2O4S	4-amino-2,5-dimethoxy-N-methylbenzenesulphonamide
4985-85-7	C7H18N2O2	N-(3-aminopropyl)iminodiethanol
499-80-9	C7H5NO4	pyridine-2,4-dicarboxylic acid
500011-92-7	C11H9BrClN3O2	Ethyl 3-bromo-1-(3-chloropyridin-2-yl)-1H-pyrazole-5-carboxylate
5026-62-0	C8H8O3	sodium 4-(methoxycarbonyl)phenolate
5026-74-4	C15H19NO4	p-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline
503614-91-3	C27H28N4O5	ethyl 1-(4-methoxyphenyl)-7-oxo-6-(4-(2-oxo-1-piperidinyl)phenyl)-4,5,6,7-tetrahydro-1H-pyrazolo[3,4-c]pyridine-3-carboxylate
5036-48-6	C6H11N3	1H-imidazole-1-propylamine
503-74-2	C5H10O2	isovaleric acid
504-29-0	C5H6N2	2-pyridylamine
505-52-2	C13H24O4	tridecanedioic acid
50594-82-6	C7H2Cl3F3	1,2,3-trichloro-5-(trifluoromethyl)benzene
506-30-9	C20H40O2	icosanoic acid
50650-75-4	C14H22O2	4-methyl-6-(2,4,4-trimethylpentyl)-2H-pyran-2-one
507-20-0	C4H9Cl	2-chloro-2-methylpropane

50-78-2	C9H8O4	Acetyl salicylic acid
5080-22-8	C3H9NO	N-isopropylhydroxylamine
50-89-5	C10H14N2O5	thymidine
50-98-6	C10H15NO	ephedrine hydrochloride
510729-01-8	C14H11BrFNO2	N-(4-bromo-3-fluorophenyl)carbamic acid phenylmethyl ester
51167-18-1	C14H20Cl2N2O2	2'-[2,4-dichloro-5-(1-methylethoxy)phenyl]-2,2-dimethylpropionohydrazide
51-21-8	C4H3FN2O2	5-Fluorouracil
51240-95-0	C18H36O3	1,1,3,3-tetramethylbutyl peroxyneodecanoate
51-28-5	C6H4N2O5	2,4-dinitrophenol
51-34-3	C17H21NO4	hyoscine
51410-72-1	C10H22N2O2	(3-methacrylamidopropyl)trimethylammonium chloride
5153-24-2	C4H6O5Zr	zirconium di(acetate) oxide
51566-62-2	C10H17N	3,7-dimethyloct-6-enenitrile
515-84-4	C4H5Cl3O2	ethyl trichloroacetate
1190723	C17H13ClN2O4S	barium bis[2-chloro-5-[(2-hydroxy-1-naphthyl)azo]toluene-4-sulphonate]
51661-19-9	C14H12N2O6	1,1'-[1,2-Ethanediylbis(oxy)]bis(2-nitrobenzene)
51772-35-1	C24H29N	N-[(1,1,3,3-tetramethylbutyl)phenyl]naphthalen-1-amine
51867-77-7	C17H10Cl2N2O3	4-[(2,5-dichlorophenyl)azo]-3-hydroxy-2-naphthoic acid
5187-23-5	C7H14O3	5-ethyl-1,3-dioxane-5-methanol
51920-12-8	C27H24N6O6S	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxy-4-[[2-methoxy-5-methyl-4-[(methylamino)sulphonyl]phenyl]azo]naphthalene-2-carboxamide
520-26-3	C22H24O12	hesperidin
52238-92-3	C35H20Cl3F3N5O4	N,N'-(2,5-dichloro-1,4-phenylene)bis[4-[[2-chloro-5-(trifluoromethyl)phenyl]azo]-3-hydroxynaphthalene-2-carboxamide]
52334-81-3	C6H3ClF3N	2-chloro-5-(trifluoromethyl)pyridine
52408-42-1	C16H26O8	1,4-butanediylbis[oxy(2-hydroxy-3,1-propanediyl)] diacrylate
52411-34-4	C14H16N2O2	1,2-Bis(2-aminophenoxy)ethane
52449-76-0	C9H6N2O4	methyl 4-cyano-2-nitrobenzoate
5246-57-1	C8H11NO3S	2-[(3-aminophenyl)sulphonyl]ethanol
52-51-7	C3H6BrNO4	bronopol
52556-42-0	C6H12O5S	sodium 3-(allyloxy)-2-hydroxypropanesulphonate
52602-39-8	C12H9NO	9H-carbazol-4-ol
52628-03-2	C6H11O6P	2-Propenoic acid, 2-methyl-, 2-hydroxyethyl ester, phosphate
52636-67-6	C4H9NO	morpholinium sulphamate
52698-46-1	C7H16O3	1,1,1-Trimethoxy-2-methylpropane
5280-68-2	C33H27ClN4O6	N-(4-chloro-2,5-dimethoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide

5280-78-4	C40H24Cl4N6O3	N,N'-(2-chloro-1,4-phenylene)bis[4-[(2,5-dichlorophenyl)azo]-3-hydroxynaphthalene-2-carboxamide]
5280-80-8	C36H32Cl3N7O5	3,3'-[(2,5-dimethyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(5-chloro-o-tolyl)benzamide]
5283-66-9	C8H17Cl3Si	octyltrichlorosilane
52846-56-7	C17H14N6O5	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(4-nitrophenyl)azo]-3-oxobutyramide
52-89-1	C3H7NO2S	cysteine hydrochloride
5292-45-5	C10H9NO6	dimethyl 2-nitroterephthalate
5292-53-5	C14H16O4	diethyl (phenylmethylene)malonate
52937-90-3	C8H15NO2	isobutyl (2Z)-3-aminobut-2-enoate
52980-28-6	C12H11NO3	ethyl 4-oxo-1,4-dihydroquinoline-3-carboxylate
530-48-3	C14H12	1,1-diphenylethylene
5308-25-8	C6H14N2	1-ethylpiperazine
53220-22-7	C30H58O6	ditetradecyl peroxydicarbonate
1250744	C7H16O3S2	1,3-bis[(2-hydroxyethyl)sulfanyl]propan-2-ol
5332-73-0	C4H11NO	3-methoxypropylamine
533-68-6	C6H11BrO2	ethyl 2-bromobutyrate
53378-51-1	C8H19O2PS2	sodium O,O-diisobutyl dithiophosphate
534-03-2	C3H9NO2	2-aminopropane-1,3-diol
53-43-0	C19H28O2	prasterone
5349-60-0	C10H14O2	α-ethyl-p-methoxybenzyl alcohol
53817-61-1	C24H44O4	diisodecyl maleate
5384-21-4	C17H20O2	4,4'-methylenedi-2,6-xylenol
53-84-9	C16H27N7O12P2	nadide
538-75-0	C13H22N2	dicyclohexylcarbodiimide
53928-30-6	C30H34O6	3,5,6-tri-O-.benzyl-1,2-O-isopropylidene-α-D-glucofuranose
53988-05-9	C9H18O2	calcium isononanoate
53988-10-6	C8H8N2S	1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione
53994-69-7	C7H7ClN2O3S	(6R-trans)-7-amino-3-chloro-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
54041-17-7	C11H14FNO2	N-(4-Fluorophenyl)-2-hydroxy-N-(1-methylethyl) acetamide
1281001	C5H12ClN	3-chloropropyldimethylammonium chloride
54112-23-1	C27H32N4O4	N,N'-(methylenedi-p-phenylene)bis[hexahydro-2-oxo-1H-azepine-1-carboxamide]
5413-60-5	C12H16O2	3a,4,5,6,7,7a-hexahydro-4,7-methanoinden-6-yl acetate
541-85-5	C8H16O	5-methylheptan-3-one
542-02-9	C4H7N5	6-methyl-1,3,5-triazine-2,4-diyldiamine
542-05-2	C5H6O5	3-oxoglutaric acid
542-08-5	C7H12O3	isopropyl acetoacetate
54-21-7	C7H6O3	sodium salicylate
542-18-7	C6H11Cl	chlorocyclohexane
542-28-9	C5H4O2	δ-valerolactone

5423-22-3	CH8N3O4P	guanidinium phosphate (1:1)
1287116	C5H5N3O2	3-aminopyrazine-2-carboxylic acid
54253-62-2	CH4O3S	copper(II) methanesulfonate
542-92-7	C5H6	cyclopentadiene
543-39-5	C10H18O	2-methyl-6-methyleneoct-7-en-2-ol
543-49-7	C7H16O	heptan-2-ol
544-01-4	C10H22O	diisopentyl ether
544-10-5	C6H13Cl	1-chlorohexane
5444-75-7	C15H22O2	2-ethylhexyl benzoate
544-76-3	C16H34	hexadecane
5459-93-8	C8H17N	cyclohexyl(ethyl)amine
54634-94-5	C17H24N2O3	2-ethylhexyl (3-isocyanatomethylphenyl)-carbamate
54914-37-3	C18H34N2	1,3,3-trimethyl-N-(2-methylpropylidene)-5-[(2-methylpropylidene)amino]cyclohexanemethylamine
5505-16-8	C7H5I3N2O2	3,5-diamino-2,4,6-triiodobenzoic acid
55066-48-3	C12H18O	3-methyl-5-phenylpentanol
55117-15-2	C7H5Cl2F	alpha,2-dichloro-6-fluorotoluene
55172-98-0	C10H20O2	barium neodecanoate
5521-31-3	C26H14N2O4	2,9-dimethylanthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone
552-37-4	C7H7NO2	sodium anthranilate
552-89-6	C7H5NO3	2-nitrobenzaldehyde
5534-13-4	C25H33FO6	9-fluoro-11β,17,21-trihydroxy-16β-methylpregna-1,4-diene-3,20-dione 17-propionate
5537-71-3	C10H9NO2	m-(1-cyanoethyl)benzoic acid
554-68-7	C6H15N	triethylammonium chloride
555-06-6	C7H7NO2	sodium 4-aminobenzoate
555-31-7	C9H21AlO3	aluminium triisopropanolate
55542-26-2	C22H30O3	17β-hydroxy-17-(3-hydroxy-1-propynyl)androst-4-ene-3-one
55542-27-3	C22H34O3	17β-hydroxy-17-(3-hydroxypropyl)androst-4-ene-4-one
555-43-1	C57H110O6	glycerol tristearate
55-56-1	C22H30Cl2N10	chlorhexidine
557-05-1	C18H36O2	zinc distearate
5578-42-7	C7H14Cl2Si	dichlorocyclohexylmethylsilane
5580-57-4	C35H29Cl4N7O5	3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(3-chloro-o-tolyl)benzamide]
5580-58-5	C34H26Cl5N7O5	3,3'-[(2,5-dichloro-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-(5-chloro-o-tolyl)benzamide]
5586-73-2	C15H17N	3-3-diphenylpropylamine
55900-27-1	C4H6ClFO2	3-Chloro-2-fluoro-propionic acid methyl ester
5593-70-4	C4H10O	titanium tetrabutanolate
55974-25-9	C12H12O4	7-Methoxy-4,4-dimethyl-1,3-isochromandione
5614-37-9	C6H12O	Cyclopentyl methyl ether

56-18-8	C6H17N3	3,3'-iminodi(propylamine)
56341-37-8	C8H6ClNO	6-chloro-1,3-dihydroindol-2-one
56358-09-9	C32H37N5	N-(2-ethylhexyl)-1-[[2-methyl-4-[(2-methylphenyl)azo]phenyl]azo]naphthalen-1-amine
5637-42-3	C8H8N4	1-(4-CYANOPHENYL)GUANIDINE
56375-79-2	C13H31NO	tributylmethylammonium chloride
56-41-7	C3H7NO2	L-alanine
56-45-1	C3H7NO3	L-serine
56539-66-3	C6H14O2	3-methoxy-3-methylbutan-1-ol
56554-53-1	C30H56O6	propane-1,2,3-triyl 3,5,5-trimethylhexanoate
565-61-7	C6H12O	3-methylpentan-2-one
5660-53-7	C9H18O3	2-isobutyl-2-methyl-1,3-dioxolane-4-methanol
5661-03-0	C7H13N	octahydrocyclopenta[c]pyrrole
56677-60-2	C15H29ClO2	tetradecyl chloroformate
56718-70-8	C12H16O3	[[p-(2-methoxyethyl)phenoxy]methyl]oxirane
56-89-3	C6H12N2O4S2	cystine
56-93-9	C10H17NO	benzyltrimethylammonium chloride
56973-87-6	C13H22O	1-(3,3-dimethylcyclohexyl)pent-4-en-1-one
57-00-1	C4H9N3O2	N-amidinosarcosine
57-09-0	C19H43NO	cetrimonium bromide
57090-45-6	C3H7ClO2	(R)-3-chloropropane-1,2-diol
571188-59-5	C14H22N4O2	tert-butyl 4-(6-aminopyridin-3-yl)piperazine-1-carboxylate
571189-16-7	C14H20N4O4	tert-Butyl 4-(6-nitropyridin-3-yl)piperazine-1-carboxylate
57260-71-6	C9H18N2O2	tert-butyl piperazine-1-carboxylate
5726-19-2	C9H16O2	2-methylcyclohexyl acetate
57499-57-7	C16H26O	1-[1,6-dimethyl-4-(4-methylpent-3-enyl)-3-cyclohexen-1-yl]ethan-1-one
575-61-1	C15H10O2	3-benzylidenephthalide
57625-74-8	C11H14O2	methyl 2-methyl-2-phenylpropanoate
5763-44-0	C7H9NO2	tetrahydrocyclopenta[c]pyrrole-1,3(2H,3aH)-dione
5766-67-6	C10H12N6	ethylenediaminetetraacetonitrile
57843-53-5	C18H36N2O6	N,N,N',N'-tetrakis(2-hydroxypropyl)adipamide
57-88-5	C27H46O	cholesterol
1427951	C8H18O2	1,1,3,3-tetramethylbutyl hydroperoxide
1428410	C6H10ClNO2	2-chloro-N,N-dimethyl-3-oxobutyramide
58210-03-0	C9H18O	2,3,6-trimethylcyclohexanol
5831-80-1	C26H51NO	N,N-dibutyloleamide
583-39-1	C7H6N2S	benzimidazole-2-thiol
58353-68-7	C22H41NO6S	disodium (Z)-4-(9-octadecenylamino)-4-oxo-2(or 3)-sulphonatobutyrate
583-59-5	C7H14O	2-methylcyclohexanol, mixed isomers
583-78-8	C6H4Cl2O	2,5-dichlorophenol
58430-94-7	C11H22O2	3,5,5-trimethylhexyl acetate
58567-11-6	C15H30O2	(ethoxymethoxy)cyclododecane
5856-77-9	C6H11ClO	2,2-dimethylbutyryl chloride

586-62-9	C10H16	p-mentha-1,4(8)-diene
586-70-9	C9H13N	1-(p-tolyl)ethanamine
58-73-1	C17H21NO	diphenhydramine
5888-33-5	C13H20O2	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acrylate
5888-87-9	C20H34N4O4	N,N'-hexane-1,6-diylbis(hexahydro-2-oxo-1H-azepine-1-carboxamide)
58909-56-1	C12H13N5O5S2	(6R-trans)-7-amino-8-oxo-3-[[(1,2,5,6-tetrahydro-2-methyl-5,6-dioxo-1,2,4-triazin-3-yl)thio]methyl]-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
5892-47-7	C18H30O	2,4,6-tri-sec-butylphenol
5894-60-0	C16H33Cl3Si	trichloro(hexadecyl)silane
5894-79-1	C10H10O3	methyl formylphenylacetate
59113-36-9	C6H14O5	oxybispropanediol
591-22-0	C7H9N	3,5-dimethylpyridine
591-27-5	C6H7NO	3-aminophenol
59130-69-7	C24H48O2	hexadecyl 2-ethylhexanoate
59231-34-4	C28H54O2	isodecyl oleate
5927-18-4	C5H11O5P	trimethyl phosphonoacetate
593-45-3	C18H38	octadecane
59-42-7	C9H13NO2	phenylephrine
59447-55-1	C10H5Br5O2	(pentabromophenyl)methyl acrylate
59487-23-9	C34H28ClN5O7	4-[[5-[[[4-(aminocarbonyl)phenyl]amino]carbonyl]-2-methoxyphenyl]azo]-N-(5-chloro-2,4-dimethoxyphenyl)-3-hydroxynaphthalene-2-carboxamide
59-50-7	C7H7ClO	chlorocresol
595-37-9	C6H12O2	2,2-dimethylbutyric acid
59-67-6	C6H5NO2	nicotinic acid
59690-88-9	C7H9N3O	(3-aminophenyl)uronium chloride
59719-67-4	C24H46N4O6	bis[2-[2-(1-methylethyl)-3-oxazolidinyl]ethyl] hexan-1,2-diylbiscarbamate
5977-14-0	C4H7NO2	acetoacetamide
59776-88-4	C7H11NO3	methyl 2-oxopyrrolidin-1-acetate
597-82-0	C18H15O3PS	O,O,O-triphenyl phosphorothioate
598-30-1	C4H9Li	sec-butyllithium
598-72-1	C3H5BrO2	2-bromopropionic acid
59875-04-6	C7H13NO3	N-butyrylalanine
59886-90-7	C7H12ClNO	4-chloro-2,3-dimethyl-1-oxidopyridin-1-ium
5989-54-8	C10H16	(S)-p-mentha-1,8-diene
598-99-2	C3H3Cl3O2	methyl trichloroacetate
599-61-1	C12H12N2O2S	3,3'-sulphonyldianiline
6001-74-7	C9H7Cl3N2O3	5-(2-chloroethyl)-4-methyl-1,3-thiazole hydrochloride (1:1)
60111-54-8	C16H36O4Si5	3,3-bis[(dimethylvinylsilyl)oxy]-1,1,5,5-tetramethyl-1,5-divinyltrisiloxane
60113-43-1	C11H18O	2,6,6-trimethylbicyclo[3.1.1]heptane-3-carbaldehyde
60-12-8	C8H10O	2-phenylethanol

60207-89-8	C13H15BrCl2O2	2-(bromomethyl)-2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolane
60209-82-7	C15H30O2	isodecyl pivalate
6041-94-7	C23H15Cl2N3O2	4-[(2,5-dichlorophenyl)azo]-3-hydroxy-N-phenylnaphthalene-2-carboxamide
608-25-3	C7H8O2	2-methylresorcinol
60857-05-8	C10H16O	tetrahydro-4-methylene-2-(2-methyl-1-propenyl)-2H-pyran
609-66-5	C7H6ClNO	2-chlorobenzamide
611-07-4	C6H4ClNO3	5-chloro-2-nitrophenol
61358-25-6	C20H26F6IP	bis(4-tert-butylphenyl)iodonium hexafluorophosphate
613-92-3	C7H8N2O	benzamide oxime
61477-40-5	C4H11NO	3-aminobutan-1-ol
61516-73-2	C8H13NO3	ethyl 2-oxopyrrolidine-1-acetate
615-20-3	C7H4ClNS	2-chlorobenzothiazole
615-50-9	C7H10N2	2-methyl-p-phenylenediamine sulfate
615-60-1	C8H9Cl	4-chloro-o-xylene
61597-98-6	C13H24O3	Propanoic acid, 2-hydroxy-, (1R,2S,5R)-5-methyl-2-(1-methylethyl)cyclohexyl ester, (2S)-
616-02-4	C5H4O3	citraconic anhydride
6161-65-5	C9H10O3	2-methoxy-6-methylbenzoic acid
616-29-5	C3H10N2O	1,3-diaminopropan-2-ol
616-47-7	C4H6N2	1-methylimidazole
617-45-8	C4H7NO4	acid D,L-aspart
617-89-0	C5H7NO	furfurylamine
61792-11-8	C11H17N	3,7-dimethylnona-2,6-dienenitrile
617-94-7	C9H12O	2-phenylpropan-2-ol
61826-76-4	C14H11NO2	SCMB
618-36-0	C8H11N	DL-α-methylbenzylamine
61847-48-1	C33H24Cl2N4O6	methyl 4-[[(2,5-dichlorophenyl)amino]carbonyl]-2-[[2-hydroxy-3-[[(2-methoxyphenyl)amino]carbonyl]-1-naphthyl]azo]benzoate
618-62-2	C6H3Cl2NO2	3,5-dichloronitrobenzene
618-83-7	C8H6O5	5-hydroxyisophthalic acid
618-88-2	C8H5NO6	5-nitroisophthalic acid
61-90-5	C6H13NO2	L-leucine
620-67-7	C27H50O6	propane-1,2,3-triyl trisheptanoate
62125-22-8	C77H148O8	2,2-bis[[(1-oxoisooctadecyl)oxy]methyl]-1,3-propanediyl bis(isooctadecanoate)
621-29-4	C8H7NO	m-tolyl isocyanate
621-76-1	C10H22O3	1,1',1''-[methylidynetris(oxy)]trispropane
62202-86-2	C6H14Mg	butylethylmagnesium
622-29-7	C8H9N	benzylidene(methyl)amine
62-23-7	C7H5NO4	4-nitrobenzoic acid
622-40-2	C6H13NO2	2-morpholinoethanol
622-58-2	C8H7NO	p-tolyl isocyanate
623-33-6	C4H9NO2	ethyl glycinate hydrochloride

62-33-9	C10H16N2O8	sodium calcium edetate
623-40-5	C5H11NO	2-Pentanone oxime
624-03-3	C34H66O4	ethane-1,2-diyl palmitate
62409-13-6	C9H13NO	1-(3-methoxyphenyl)ethanamine
62435-71-6	C7H14O2	Ethyl 2-tetrahydrofurfuryl ether
624-54-4	C8H16O2	pentyl propionate
624-89-5	C3H8S	ethyl methyl sulphide
62518-65-4	C14H20O	3-(m-tert-butylphenyl)-2-methylpropionaldehyde
62-54-4	C2H4O2	calcium di(acetate)
1591885	C14H8BrNO5S	sodium 1-amino-4-bromo-9,10-dioxoanthracene-2-sulphonate
626-67-5	C6H13N	1-methylpiperidine
6271-80-3	C12H8ClNO2	4'-Chloro-2-nitrobiphenyl
627-83-8	C38H74O4	ethylene distearate
6284-40-8	C7H17NO5	meglumine
6284-43-1	C21H42O5	2,3-dihydroxypropyl 12-hydroxyoctadecanoate
628-89-7	C4H9ClO2	2-(2-chloroethoxy)ethanol
62899-75-6	C9H16ClNO	cyclohexylethylcarbamoyl chloride
629-03-8	C6H12Br2	1,6-dibromohexane
629-15-2	C4H6O4	ethylene diformate
6291-85-6	C5H13NO	3-ethoxypropylamine
62932-92-7	C8H7BrO3	Ethanone, 2-bromo-1-(3,5-dihydroxyphenyl)-
629-40-3	C8H12N2	suberonitrile
629-62-9	C15H32	pentadecane
1606038	C36H74O	dioctadecyl ether
6298-96-0	C9H13NO	1-(4-methoxyphenyl)ethanamine
6309-51-9	C17H34O2	isopentyl laurate
63141-09-3	C5H7ClO	1-(1-chlorocyclopropyl)ethanone
1613893	C15H26N2	1,3,5-triisopropyl-2,4-diaminobenzene
6335-76-8	C11H15NO2	ethyl 3-amino-3-phenylpropanoate
63422-71-9	C15H17N3O5	(R)-[[(4-ethyl-2,3-dioxopiperazin-1-yl)carbonyl]amino]phenylacetic acid
63432-37-1	C8H7N3O2S	2-(methylsulfanyl)-3-nitropyrazolo[1,5-a]pyridine
63451-47-8	C4H6O2	hydroxy(2-methylprop-2-enoato-O)zinc
63469-23-8	C11H26N2O2	1,1'-[[3-(dimethylamino)propyl]imino]bispropan-2-ol
63562-34-5	C21H23O8P	bis(2-hydroxyethyl) (6H-dibenz[c,e][1,2]oxaphosphorin-6-ylmethyl)succinate P-oxide
1628467	C6H5ClN2O3	2-amino-4-chloro-6-nitrophenol
6358-87-8	C36H28Cl2N8O6	diethyl 4,4'-[(3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[4,5-dihydro-5-oxo-1-phenyl-1H-pyrazole-3-carboxylate]
63589-25-3	C10H5N3O6S	4-diazo-3,4-dihydro-7-nitro-3-oxonaphthalene-1-sulphonic acid
6362-79-4	C8H6O7S	sodium hydrogen-5-sulphoisophthalate
6362-80-7	C18H20	1,1'-(1,1-dimethyl-3-methylene-1,3-propanediyl)bisbenzene

63659-15-4	C19H22O2	1-(benzyloxy)-4-[2-(cyclopropylmethoxy)ethyl]benzene
63659-17-6	C11H14O3	1-[4-(2-Hydroxyethyl)phenoxy]-2,3-epoxypropane
63721-05-1	C8H14O2	methyl 3,3-dimethylpent-4-enoate
638-29-9	C5H9ClO	valeryl chloride
63843-89-0	C42H72N2O5	bis(1,2,2,6,6-pentamethyl-4-piperidyl) [[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]butylmalonate
6401-97-4	C10H11N3	2,4-dihydro-5-methyl-2-phenyl-3H-pyrazol-3-imine
64-04-0	C8H11N	phenethylamine
640-67-5	C2H2O4	manganese oxalate
6410-32-8	C25H20N4O4	3-hydroxy-4-[(2-methyl-4-nitrophenyl)azo]-N-(o-tolyl)naphthalene-2-carboxamide
6410-41-9	C30H31ClN4O7S	N-(5-chloro-2,4-dimethoxyphenyl)-4-[[5-[(diethylamino)sulphonyl]-2-methoxyphenyl]azo]-3-hydroxynaphthalene-2-carboxamide
1648615	C8H14O4	ethyl 2-methyl-1,3-dioxolane-2-acetate
64131-85-7	C18H12N3O9PS	O,O,O-tris(4-nitrophenyl) thiophosphate
6422-99-7	C10H18O4	sebacic acid, compound with hexane-1,6-diamine (1:1)
6425-39-4	C12H24N2O3	2,2'-dimorpholinyldiethyl ether
6428-31-5	C34H29N13O7S2	disodium 4-amino-3,6-bis[[4-[(2,4-diaminophenyl)azo]phenyl]azo]-5-hydroxynaphthalene-2,7-disulphonate
6440-58-0	C7H12N2O4	1,3-bis(hydroxymethyl)-5,5-dimethylimidazolidine-2,4-dione
6443-69-2	C10H14O3	3,4,5-trimethoxytoluene
6448-95-9	C24H18N4O4	3-hydroxy-4-[(2-methyl-5-nitrophenyl)azo]-N-phenylnaphthalene-2-carboxamide
644-97-3	C6H5Cl2P	dichloro(phenyl)phosphine
646-24-2	C9H22N2	nonamethylenediamine
646-25-3	C10H24N2	decamethylenediamine
64665-57-2	C7H6N3Na	sodium 4(or 5)-methyl-1H-benzotriazolide
6471-50-7	C24H17ClN4O4	4-[(4-chloro-2-nitrophenyl)azo]-3-hydroxy-N-(2-methylphenyl)naphthalene-2-carboxamide
64-73-3	C21H22N2O7	demeclocycline hydrochloride
647-42-7	C8H5F13O	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctan-1-ol
6485-40-1	C10H14O	l-p-mentha-1(6),8-dien-2-one
6485-67-2	C8H10N2O	2-Amino-2-phenylacetamide, (R)-
6486-23-3	C16H12Cl2N4O4	2-[(4-chloro-2-nitrophenyl)azo]-N-(2-chlorophenyl)-3-oxobutyramide
65113-95-3	C14H22O	3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-3-en-2-one
65140-91-2	C17H29O4P	calcium diethyl bis[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]phosphonate]
6528-34-3	C18H18N4O6	2-[(4-methoxy-2-nitrophenyl)azo]-N-(2-methoxyphenyl)-3-oxobutyramide
65405-77-8	C13H16O3	(Z)-3-hexenyl salicylate
65473-13-4	C12H14ClN	N-methyl-1-naphthalen-1-ylmethanamine hydrochloride
65520-46-9	C26H50O10	bis[2-[2-(2-butoxyethoxy)ethoxy]ethyl] adipate
6574-99-8	C7H3Cl2N	3,4-dichlorobenzonitrile

6600-31-3	C19H28O4	3,9-dicyclohex-3-enyl-2,4,8,10-tetraoxaspiro[5.5]undecane
66068-84-6	C16H28O	4-(5,5,6-trimethylbicyclo[2.2.1]hept-2-yl)cyclohexan-1-ol
6610-29-3	C2H7N3S	4-methylthiosemicarbazide
66108-89-2	C14H18I3N3O6	(R*,R*)-(±)-5-amino-N,N'-bis(2,3-dihydroxypropyl)-2,4,6-triiodoisophthaldiamide
66108-95-0	C19H26I3N3O9	Iohexol
6615-00-5	C18H24O3	11a-Hydroxy-estr-4-ene-3,17-dione
661-95-0	C3Br2F6	1,2-dibromo-1,1,2,3,3,3-hexafluoropropane
66212-25-7	C21H26O3	17-Hydroxy-1,4,6-pregnatriene-3,20-dione
66-25-1	C6H12O	hexanal
6635-20-7	C8H7NO5	5-nitrovanillin
66357-35-5	C13H22N4O3S	Ranitidine
6640-22-8	C23H16O6	disodium 4,4'-methylenebis[3-hydroxy-2-naphthoate]
6640-24-0	C10H13ClN2	1-(m-chlorophenyl)piperazine
66415-55-2	C5H11NO	3-vinyloxypropan-1-amine
66422-95-5	C8H12N2O2	2-(2,4-diaminophenoxy)ethanol dihydrochloride
66423-13-0	C18H27ClO3	octyl (R)-2-(4-chloro-2-methylphenoxy)propionate
66492-51-1	C10H16O4	(5-ethyl-1,3-dioxan-5-yl)methyl acrylate
66546-92-7	C10H17NO2	Methyl 2-cyano-2-propylpentanoate
665-66-7	C10H17N	amantadine hydrochloride
6674-22-2	C9H16N2	1,8-diazabicyclo[5.4.0]undec-7-ene
66-84-2	C6H13NO5	glucosamine hydrochloride
67014-36-2	C8H9N3O	5-amino-6-methyl-1,3-dihydrobenzimidazol-2-one
67075-37-0	C40H26N2O4	2,9-bis(2-phenylethyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone
6711-48-4	C10H25N3	N'-[3-(dimethylamino)propyl]-N,N-dimethylpropane-1,3-diamine
67124-09-8	C15H32OS	1-(tert-dodecylthio)propan-2-ol
6712-98-7	C7H17NO3	1-(N,N-bis(2-hydroxyethyl)amino)propan-2-ol
67151-63-7	C13H31N3O	1-[bis[3-(dimethylamino)propyl]amino]propan-2-ol
67442-07-3	C4H8ClNO2	2-Chloro-N-methoxy-N-methylacetamide
674773-12-7	C10H10N2O4S	methyl 5-amino-4-cyano-3-(2-methoxy-2-oxoethyl)thiophene-2-carboxylate
67-48-1	C5H15NO2	choline chloride
67-51-6	C5H8N2	3,5-dimethylpyrazole
675-62-7	C4H7Cl2F3Si	dichloromethyl(3,3,3-trifluoropropyl)silane
67584-55-8	C10H10F9NO4S	2-[methyl[(nonafluorobutyl)sulphonyl]amino]ethyl acrylate
67762-64-5	C18H34O5	Heptanoic acid, ester with 2-ethyl-2-(hydroxymethyl)-1,3-propanediol pentanoate
67801-01-8	C18H15ClN2O4S	barium bis[5-chloro-4-ethyl-2-[(2-hydroxy-1-naphthyl)azo]benzenesulphonate]
67801-15-4	C14H22O	3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-one
67801-20-1	C14H24O	3-methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-ol
67845-93-6	C31H54O3	hexadecyl 3,5-bis-tert-butyl-4-hydroxybenzoate

67859-51-2	C10H16N2O8	diammonium [[N,N'-ethylenebis[N-(carboxylatomethyl)glycinato]](4-)-N,N',O,O',ON,ON']zincate(2-)
67938-21-0	C42H82O7	di(isooctadecanoic) acid, diester with oxydi(propanediol)
67952-33-4	C4H11NO2	orthoboric acid, compound with 2,2'-iminodiethanol
67989-88-2	C10H16N2O8	diammonium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,N',O,O',ON,ON']cuprate(2-)
67990-05-0	C32H25ClN4O5	N-(5-chloro-2-methoxyphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide
68015-77-0	C10H16N2O8	dipotassium [[N,N'-ethylenebis[N-(carboxymethyl)glycinato]](4-)-N,N',O,O',ON,ON']manganate(2-)
68109-88-6	C28H48O8Sn	ethyl 9,9-dioctyl-4,7,11-trioxo-3,8,10-trioxa-9-stannatetradeca-5,12-dien-14-oate
68127-59-3	C9H10ClF3O2	reaction mass of (1R,3R)-3-[(1Z)-2-chloro-3,3,3-trifluoroprop-1-en-1-yl]-2,2-dimethylcyclopropanecarboxylic acid and (1S,3S)-3-[(1Z)-2-chloro-3,3,3-trifluoroprop-1-en-1-yl]-2,2-dimethylcyclopropanecarboxylic acid
68130-53-0	C30H56O6	Decanoic acid, mixed esters with heptanoic acid, octanoic acid and trimethylolpropane
68133-60-8	C13H13NO3	1-benzyl-3-carboxylatopyridinium sodium chloride
68134-22-5	C18H14F3N5O3	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxo-2-[[2-(trifluoromethyl)phenyl]azo]butyramide
68171-33-5	C21H42O2	isopropyl isodecanoate
681-84-5	C4H12O4Si	tetramethyl orthosilicate
682-01-9	C12H28O4Si	tetrapropyl orthosilicate
682-11-1	C9H18O4	2-allyloxymethyl-2-ethylpropanediol
68227-78-1	C32H25ClN4O4	N-(5-chloro-2-methylphenyl)-3-hydroxy-4-[[2-methoxy-5-[(phenylamino)carbonyl]phenyl]azo]naphthalene-2-carboxamide
68259-05-2	C40H33ClN5O6	bis(2-chloroethyl) 3,3'-[(2,5-dimethyl-p-phenylene)bis[iminocarbonyl(2-hydroxy-1,3-naphthylene)azo]]di-p-toluate
68400-38-4	C22H17N5O9S3	trisodium 7-[[4-[(4-aminophenyl)azo]phenyl]azo]naphthalene-1,3,5-trisulphonate
68424-85-1	C23H42ClN	Quaternary ammonium compounds, benzyl-C12-16-alkyldimethyl, chlorides
6843-66-9	C14H16O2Si	dimethoxydiphenylsilane
68443-84-5	C61H112O13	triisononanoic acid, triester with 2,2'-[oxybis(methylene)]bis[2-(hydroxymethyl)propane-1,3-diol] tris(2-ethylhexanoate)
68511-03-5	C6H15O4P	Phosphoric acid, hexyl ester
68516-73-4	C34H32N6O12	tetramethyl 2,2'-[1,4-phenylenebis[imino(1-acetyl-2-oxoethane-1,2-diyl)azo]]bisterephthalate
68516-75-6	C44H26Cl4N6O4	N,N'-naphthalene-1,5-diylbis[4-[(2,3-dichlorophenyl)azo]-3-hydroxynaphthalene-2-carboxamide]
68517-10-2	C19H38O2	methyl isostearate

68526-84-1	C9H20O	Alcohols, C8-10-iso-, C9-rich
68541-50-4	C60H116O6	2-ethyl-2-[[(1-oxoisooctadecyl)oxy]methyl]-1,3-propanediyl bis(isooctadecanoate)
68604-84-2	C38H70O4	Fatty acids, C18-unsatd., dimers, methyl esters
6860-97-5	C17H15NO9S3	4-hydroxy-5-[[(p-tolyl)sulphonyl]amino]naphthalene-2,7-disulphonic acid
686-31-7	C13H26O3	tert-pentyl 2-ethylperoxyhexanoate
68909-32-0	C19H38N2O	Propanenitrile, 3-[[3-(tridecyloxy)propyl]amino]-, branched
68912-13-0	C13H18O2	3a,4,5,6,7,7a-hexahydro-4,7-methano-1H-indenyl propionate
689293-69-4	C31H36N6O3	Carbamic acid, N-[2-[[[[1-methyl-5-[(triphenylmethyl)amino]-1H-pyrazol-4-yl]amino]carbonyl]amino]ethyl]-, 1,1-dimethylethyl ester
689294-28-8	C28H33ClN6O8S2	(6R,7R)-3-chloromethyl-7-{(Z)-2-(5-amino-1,2,4-thiadiazol-3-yl)2-[(1-carboxy-1-methylethoxy)imino]acetylamino}-8-oxo-5-thia-1-azbicyclo[4.2.0]oct-2-ene-2-carboxylic acid p-methoxybenzyl ester
68958-77-0	C28H37ClO10	2-Propenoic acid, monoester with 1,2-propanediol, polymer with 2-(chloromethyl)oxirane, dihydro-2,5-furandione and 4,4'-(1-methylethylidene)bis[phenol]
690-39-1	C3H2F6	1,1,1,3,3,3-Hexafluoropropane
691-37-2	C6H12	4-methylpent-1-ene
6920-22-5	C6H14O2	DL-hexane-1,2-diol
692-49-9	C4H2F6	(2Z)-1,1,1,4,4,4-hexafluorobut-2-ene
6925-69-5	C18H10N2O	12H-phthaloperin-12-one
693-21-0	C4H10O3	oxydiethylene dinitrate
693-57-2	C12H25NO2	12-aminododecanoic acid
6938-94-9	C12H22O4	diisopropyl adipate
694-83-7	C6H14N2	cyclohex-1,2-ylenediamine
69-53-4	C16H19N3O4S	Ampicillin
696-29-7	C9H18	isopropylcyclohexane
697235-49-7	C16H15NO4	2-((3-(4-Hydroxyphenyl)propanoylamino)benzoic acid
698-90-8	C7H14N2O	cyclohexylurea
6990-43-8	C8H19O2PS2	zinc O,O,O',O'-tetrabutyl bis(phosphorodithioate)
1860127	C24H15Cl2N5O3	4-[(2,5-dichlorophenyl)azo]-N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-hydroxynaphthalene-2-carboxamide
6994-25-8	C6H9N3O2	ethyl 3-amino-1H-pyrazole-4-carboxylate
7005-47-2	C6H15NO	2-(dimethylamino)-2-methylpropan-1-ol
70174-49-1	C9H12O2	(1R,6S)- 4,7,7-Trimethyl-3-oxabicyclo[4.1.0]hept-4-en-2-one
701-97-3	C9H16O2	3-cyclohexylpropionic acid
70223-33-5	C9H14O3	(1R,3S)-2,2-Dimethyl-3-(2-oxopropyl)cyclopropanecarboxylic acid
70321-86-7	C30H29N3O	2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol

70356-09-1	C20H22O3	1-[4-(1,1-dimethylethyl)phenyl]-3-(4-methoxyphenyl)propane-1,3-dione
70516-41-5	C34H34N2O3	2'-anilino-6'-[ethyl(3-methylbutyl)amino]-3'-methylspiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one
70-54-2	C6H14N2O2	DL-lysine
70-55-3	C7H9NO2S	toluene-4-sulphonamide
705-86-2	C10H18O2	decan-5-olide
706-14-9	C10H18O2	decan-4-olide
7065-46-5	C6H11ClO	3,3-dimethylbutyryl chloride
707-36-8	C12H19Cl	1-chloro-3,5-dimethyladamantane
707-72-2	C8H5Cl2F3	1-(dichloromethyl)-2-(trifluoromethyl)benzene
70833-40-8	C14H28O4	O-(2-ethylhexyl) O,O-tert-pentyl peroxycarbonate
7087-68-5	C8H19N	ethyldiisopropylamine
709031-43-6	C23H33N3O4	tert-butyl ((1S)-2-((1S,3S,5S)-3-cyano-2-azabicyclo[3.1.0]hex-2-yl)-1-(3-hydroxyadamantan-1-yl)-2-oxoethyl)carbamate
70969-58-3	C16H28O4	diisobutyl hexahydrophthalate
71301-98-9	C11H14O4	ethyl 2-(4-hydroxyphenoxy)propanoate
71-30-7	C4H5N3O	cytosine
713-95-1	C12H22O2	dodecan-5-olide
7148-78-9	C13H18O2	(3,3-diethoxy-1-propenyl)benzene
71566-54-6	C50H42Cl2N6O8	diisopropyl 3,3'-[(2,5-dichloro-1,4-phenylene)bis[iminocarbonyl(2-hydroxy-3,1-naphthylene)azo]]bis[4-methylbenzoate]
7159-96-8	C9H11NO3	ethyl-N-(3-hydroxyphenyl)-carbamate ethyl 3-hydroxyphenylcarbamate
71604-74-5	C15H19NO4	m-(2,3-epoxypropoxy)-N,N-bis(2,3-epoxypropyl)aniline
7173-51-5	C22H49NO	didecyldimethylammonium chloride
71735-74-5	C11H23O4PS2	ethyl 3-[[bis(1-methylethoxy)phosphinothioyl]thio]propionate
717-74-8	C15H24	1,3,5-triisopropylbenzene
71786-67-9	C16H17NO2	benzyl(3-hydroxyphenacyl)methylammonium chloride
71902-01-7	C23H48O8	Sorbitan, isooctadecanoate
71902-23-3	C15H29NO3	6-[(1-oxomethyloctyl)amino]hexanoic acid
719-80-2	C14H15OP	ethyl diphenylphosphinite
72162-46-0	C16H36N2O	N-[3-(isodecyloxy)propyl]propane-1,3-diamine
72162-47-1	C17H34N2O	3-[3-(decylalkyl-(branched)oxy)propylamino]propiononitrile
72-17-3	C3H6O3	sodium lactate
72-18-4	C5H11NO2	L-valine
7235-40-7	C40H56	β,β-carotene
72361-35-4	C48H84O6	triisotridecyl benzene-1,2,4-tricarboxylate
7237-83-4	C18H18O9	tris(oxiranylmethyl) benzene-1,2,4-tricarboxylate
72576-80-8	C34H68O2	isooctadecyl palmitate
72624-02-3	C13H20O	Phenol, heptyl derivs.
72752-52-4	C12H14N2	2-piperidin-1-yl-benzonitrile

72811-73-5	C12H13N3O2S	4-(3-METHYLPHENYL)AMINO-3-PYRIDINESULFONAMIDE
72903-27-6	C12H20O4	diethyl 1,4-cyclohexanedicarboxylate
7300-34-7	C10H24N2O2	3,3'-[butane-1,4-diylbis(oxy)]bispropanamine
7305-71-7	C4H6N2S	2-amino-5-methylthiazole
73097-51-5	C8H12N2O2S	2-Amino-4-methylsulfonyl-N-methylaniline
7320-37-8	C16H32O	tetradecyloxirane
73-22-3	C11H12N2O2	L-tryptophan
7328-22-5	C12H22O4	2-(2-butoxyethoxy)ethyl methacrylate
7360-38-5	C27H50O6	propane-1,2,3-triyl 2-ethylhexanoate
73609-36-6	C9H7Cl2F13Si	dichloromethyl(3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)silane
7379-51-3	C9H12OS	4-(methylthio)-3,5-xylenol
73936-91-1	C29H35N3O	2-(2H-Benzotriazol-2-yl)-6-(1-methyl-1-phenylethyl)-4-(1,1,3,3-tetramethylbutyl)phenol
73942-87-7	C12H13NO3	7,8-dimethoxy-1,3-dihydro-2H-3-benzazepin-2-one
7400-27-3	C4H12N2	tert-butylhydrazine monohydrochloride
74124-79-1	C9H8N2O7	di(succinimido) carbonate
74336-59-7	C17H11ClN6O3	3-[(4-chloro-2-nitrophenyl)azo]-2-methylpyrazolo[5,1-b]quinazolin-9(1H)-one
74441-05-7	C25H21N7O5	N-[4-(aminocarbonyl)phenyl]-4-[[1-[[(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)amino]carbonyl]-2-oxopropyl]azo]benzamide
74462-02-5	C20H26O2	4-[2-ethyl-1-(4-hydroxyphenyl)hexyl]phenol
7452-79-1	C7H14O2	ethyl 2-methylbutyrate
746595-79-9	C4H10N2O	1,4,5-oxadiazepane
7474-78-4	C6H8N2O3S	3,4-diaminobenzenesulphonic acid
74-79-3	C6H14N4O2	arginine
7486-38-6	C6H10O4	disodium adipate
2042106	C16H30O4	diisopropyl sebacate
7491-09-0	C20H38O7S	potassium 1,2-bis(2-ethylhexyloxycarbonyl)ethanesulphonate
75128-73-3	C12H15N5O5	2-[(2-acetamido-6,9-dihydro-6-oxo-1H-purin-9-yl]methoxy]ethyl acetate
7526-26-3	C13H13O3P	diphenyl methylphosphonate
7529-16-0	C6H9NO	5-Ethenyl-2-pyrrolidinone
7529-22-8	C5H11NO2	4-methylmorpholine 4-oxide, monohydrate
7531-52-4	C5H10N2O	(S)-pyrrolidine-2-carboxamide
75330-75-5	C24H36O5	(1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl (2S)-2-methylbutanoate
75-57-0	C4H13NO	tetramethylammonium chloride
75-59-2	C4H13NO	tetramethylammonium hydroxide
75-85-4	C5H12O	2-methylbutan-2-ol
7597-60-6	C7H10N4O3	6-amino-5-formamido-1,3-dimethyluracil
75980-60-8	C22H21O2P	diphenyl(2,4,6-trimethylbenzoyl)phosphine oxide
760-93-0	C8H10O3	methacrylic anhydride
76-16-4	C7H15AsN2S4	perfluoroethane
76-19-7	C3F8	octafluoropropane

76199-85-4	C16H11N5O4	2-cyano-2-[2,3-dihydro-3-(tetrahydro-2,4,6-trioxo-5(2H)-pyrimidinylidene)-1H-isoindol-1-ylidene]-N-methylacetamide
762-04-9	C4H11O3P	diethyl phosphonate
7620-77-1	C18H36O3	lithium 12-hydroxystearate
762-12-9	C20H38O4	bisdecanoyl peroxide
76-22-2	C10H16O	bornan-2-one
762240-92-6	C6H7F3N4	3-(trifluoromethyl)-5,6,7,8-tetrahydro[1,2,4]triazolo[4,3-a]pyrazine hydrochloride (1:1)
76272-34-9	C14H18N2O	8-Azabicyclo[3.2.1]octan-3-one, 8-(phenylmethyl)-, oxime
764667-65-4	C16H12F6N4O2	1-[3-(trifluoromethyl)-5,6-dihydro[1,2,4]triazolo[4,3-a]pyrazin-7(8H)-yl]-4-(2,4,5-trifluorophenyl)butane-1,3-dione
764-99-8	C8H14O3	1,1'-[oxybis(ethyleneoxy)]diethylene
2100549	C23H48N2O	N-[3-(dimethylamino)propyl]stearamide
76524-94-2	C10H23NO4Si	N-[3-(Triethoxysilyl)propyl]formamide
765-30-0	C3H7N	cyclopropylamine
765-43-5	C5H8O	cyclopropyl methyl ketone
765-63-9	C3H2F4O	2,2,3,3-tetrafluorooxetane
766-09-6	C7H15N	1-ethylpiperidine
766-36-9	C7H11NO	4-ethyl-3-methyl-1,2-dihydropyrrol-5-one
767340-03-4	C16H13F6N5O	(2Z)-3-amino-1-[3-(trifluoromethyl)-5,6-dihydro[1,2,4]triazolo[4,3-a]pyrazin-7(8H)-yl]-4-(2,4,5-trifluorophenyl)but-2-en-1-one
76811-98-8	C32H37NO4	Benzeneacetic acid, 4-[4-[4-(hydroxydiphenylmethyl)-1-piperidinyl]-1-oxobutyl]-α,α-dimethyl-
76-89-1	C15H14O3	methyl benzilate
768-94-5	C10H17N	amantadine
2115155	C8H19NSi2	N-(dimethylvinylsilyl)-1,1-dimethyl-1-vinylsilylamine
77017-20-0	C23H28O6	16α,17,21-trihydroxypregna-1,4,9(11)-triene-3,20-dione 21-acetate
77326-36-4	C7H5FN2	6-fluoroanhranilonitrile
77-48-5	C5H6Br2N2O2	1,3-dibromo-5,5-dimethylhydantoin
77501-63-4	C19H15ClF3NO7	(2-ethoxy-1-methyl-2-oxoethyl)-5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoate
77538-19-3	C25H50O4	Docosanoic acid, ester with 1,2,3-propanetriol
7756-94-7	C12H24	2-Methylpropene, trimers
77-76-9	C5H12O2	acetone-dimethyl acetal
77804-81-0	C36H32N10O8	2,2'-[ethylenebis(oxyphenyl-2,1-eneazo)]bis[N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-3-oxobutyramide
77820-58-7	C8H8ClNO2	Methyl 2-amino-3-chlorobenzoate
77-83-8	C13H16O3	ethyl 2,3-epoxy-3-phenylbutyrate
7785-26-4	C10H16	(-)-pin-2(3)-ene
7785-70-8	C10H16	(+)-pin-2(3)-ene
77-86-1	C4H11NO3	trometamol
7786-17-6	C33H52O2	2,2'-methylenebis(6-nonyl-p-cresol)

7787-93-1	C4H9Cl3Si	dichloro(3-chloropropyl)methylsilane
77881-13-1	C20H27NO2	(17α)-17-hydroxy-3-oxoandrost-4-ene-17-carbonitrile
77-93-0	C12H20O7	triethyl citrate
77-94-1	C18H32O7	tributyl citrate
780-69-8	C12H20O3Si	triethoxy(phenyl)silane
78-08-0	C8H18O3Si	triethoxy(vinyl)silane
78-16-0	C27H50O6	2-ethyl-2-[[(1-oxoheptyl)oxy]methyl]propane-1,3-diyl bisheptanoate
78-27-3	C8H12O	1-ethynylcyclohexanol
78491-02-8	C8H14N4O7	1-[1,3-bis(hydroxymethyl)-2,5-dioxoimidazolidin-4-yl]-1,3-bis(hydroxymethyl)urea
78521-39-8	C13H19NO4S	6-[[(4-methylphenyl)sulphonyl]amino]hexanoic acid
78683-74-6	C12H18O3	Pentapropenyl succinic anhydride
78-73-9	C5H15NO2	choline hydrogen carbonate
78-77-3	C4H9Br	1-bromo-2-methylpropane
78-86-4	C4H9Cl	2-chlorobutane
78-98-8	C3H4O2	pyruvaldehyde
79-03-8	C3H5ClO	propionyl chloride
79-30-1	C4H7ClO	isobutyryl chloride
79560-19-3	C16H12Cl2O	4-(3,4-DICHLOROPHENYL)-3,4-DIHYDRO-1-(2H)-NAPHTHALENONE
79665-24-0	C44H34Cl2N6O4	N,N'-(2,5-dimethyl-1,4-phenylene)bis[4-[(5-chloro-2-methylphenyl)azo]-3-hydroxynaphthalene-2-carboxamide
79710-86-4	C5H8O2	tetrahydrofuran-3-carbaldehyde
79723-02-7	C12H17NO4	tetramethylammonium hydrogen phthalate
79815-20-6	C9H9NO2	(S)-2,3-dihydro-1H-indol-2-carbonic acid
79953-85-8	C55H37Cl5F6N8O8	3,3'-[(2-chloro-5-methyl-p-phenylene)bis[imino(1-acetyl-2-oxoethylene)azo]]bis[4-chloro-N-[2-(4-chlorophenoxy)-5-(trifluoromethyl)phenyl]benzamide]
80-04-6	C15H28O2	4,4'-isopropylidenedicyclohexanol
8007-43-0	C42H76O7	Sorbitan, (Z)-9-octadecenoate (2:3)
80-08-0	C12H12N2O2S	dapsone
80-10-4	C12H10Cl2Si	dichloro(diphenyl)silane
8024-53-1	C10H18O	cineole
80-26-2	C12H20O2	p-menth-1-en-8-yl acetate
80-46-6	C11H16O	p-(1,1-dimethylpropyl)phenol
80-51-3	C12H14N4O5S2	4,4'-oxydi(benzenesulphonohydrazide)
80584-91-4	C21H36N6O6	6,6',6''-(1,3,5-triazine-2,4,6-triyltriimino)trihexanoic acid
80693-00-1	C35H54O6P2	3,9-bis(2,6-di-tert-butyl-4-methylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro[5.5]undecane
80-73-9	C5H10N2O	1,3-dimethylimidazolidin-2-one
80841-78-7	C5H5ClO3	4-Chloromethyl-5-methyl-1,3-dioxol-2-one
81058-27-7	C26H43BrO9	2,3,4,6-TETRAKIS-O-(2,2-DIMETHYLPROPANOYL)-ALPHA-D-GLUCOPYRANOSYL BROMIDE

81-07-2	C7H5NO3S	1,2-benzisothiazol-3(2H)-one 1,1-dioxide
81-13-0	C9H19NO4	dexpanthenol
81-25-4	C24H40O5	cholic acid
81-33-4	C24H10N2O4	perylene-3,4:9,10-tetracarboxydiimide
813-60-5	C8H18O2	2-methyl-2-(1-methylpropyl)propane-1,3-diol
813-93-4	C6H8O7	bismuth citrate
814-80-2	C3H6O3	calcium dilactate
81-64-1	C14H8O4	1,4-dihydroxyanthraquinone
81-77-6	C28H14N2O4	6,15-dihydroanthrazine-5,9,14,18-tetrone
81778-06-5	C5H10ClNO2	3-chloro-N-hydroxy-2,2-dimethylpropanamide
81778-07-6	C5H9NO2	4,4-dimethyl-1,2-oxazolidin-3-one
81782-77-6	C11H22O	4-methyl-3-decen-5-ol
81-83-4	C12H7NO2	naphthalene-1,8-dicarboximide
82104-74-3	C9H5NO2	1,3-dihydro-1-oxoisobenzofuran-5-carbonitrile
821-38-5	C14H26O4	tetradecanedioic acid
82199-12-0	C18H17N5O4	N-(2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-2-[(2-methoxyphenyl)azo]-3-oxobutyramide
822-36-6	C4H6N2	4-methylimidazole
826-55-1	C10H12O2	2-phenylisobutyric acid
82796-69-8	C9H13NO	(S)-1-(3-methoxyphenyl)ethylamine
82985-35-1	C12H31NO6Si2	bis(trimethoxysilylpropyl)amine
83016-70-0	C9H22N2O2	2-[(2-[2-(dimethylamino)ethoxy]ethyl)methylamino]ethanol
831-52-7	C6H5N3O5	sodium 2-amino-4,6-dinitrophenoxide
83161-22-2	C11H22O5	pentyl 6-deoxy-alpha-L-mannopyranoside
83196-58-1	C22H31NO3	3,3-Ethylenedioxy-17 alpha-hydroxy-5-androstene-17 beta-carbonitrile
833-86-3	C13H17NO	3-(1-pyrrolidinyl)propiophenone hydrochloride
83411-71-6	C16H35O2P	bis(2,4,4-trimethylpentyl)phosphinic acid
83-42-1	C7H6ClNO2	2-chloro-6-nitrotoluene
83447-96-5	C8H14I2	trans-1,4-bis(iodomethyl)cyclohexane
83524-75-8	C40H26N2O6	2,9-bis(p-methoxybenzyl)anthra[2,1,9-def:6,5,10-d'e'f']diisoquinoline-1,3,8,10(2H,9H)-tetrone
83-56-7	C10H8O2	naphthalene-1,5-diol
83-73-8	C9H5I2NO	diiodohydroxyquinoline
83877-91-2	C20H36O8Ti	bis(ethyl acetoacetato-O1',O3)bis(2-methylpropan-1-olato)titanium
840-65-3	C14H12O4	dimethyl naphthalene-2,6-dicarboxylate
84348-37-8	C10H15NO5	(2S)-1-(tert-butoxycarbonyl)-4-oxopyrrolidine-2-carboxylic acid
84434-11-7	C18H21O3P	ethyl phenyl(2,4,6-trimethylbenzoyl)phosphinate
84434-23-1	C13H16O	p-tert-butylcinnamaldehyde
84449-65-0	C16H14O6S3	4-(6-(methylsulfonyloxy)benzo[b]thiophen-2-yl)phenyl methanesulfonate
84-51-5	C16H12O2	2-ethylanthraquinone
84-61-7	C20H26O4	dicyclohexyl phthalate
84731-70-4	C24H44O4	bis(2-ethylhexyl) cyclohexane-1,4-dicarboxylate

848655-78-7	C10H14N2O2	N-(4-amino-2-ethoxyphenyl)acetamide
84-87-7	C10H8O4S	4-hydroxynaphthalene-1-sulphonic acid
849727-62-4	C11H12Cl2N2O2	3-(2-CHLOROETHYL)-9-HYDROXY-2-METHYL-4H-PYRIDO[1,2-A]PYRIMIDIN-4-ONE HYDROCHLORIDE (1:1)
85114-00-7	C11H22O3	2-ethylhexanoic acid, monoester with propane-1,2-diol
85-18-7	C7H7ClN4O2	8-chlorotheophylline
85187-23-1	C15H22N2O4	1,3,5-triisopropyl-2,4-dinitrobenzene
85-60-9	C26H38O2	6,6'-di-tert-butyl-4,4'-butylidenedi-m-cresol
85-73-4	C17H13N3O5S2	phthalylsulfathiazole
85-98-3	C17H20N2O	1,3-diethyldiphenylurea
862574-88-7	C11H8F2O4	1-(2,2-Difluorobenzo[d][1,3]dioxol-5-yl)cyclopropanecarboxylic acid
86261-90-7	C9H14N2O3	2-(2-oxoimidazolidin-1-yl)ethyl methacrylate
86-28-2	C14H13N	9-ethylcarbazole
86404-04-8	C8H12O6	(5R)-5-[(1S)-1,2-Dihydroxyethyl]-4-ethoxy-3-hydroxy-5H-furan-2-one
865-47-4	C4H10O	potassium tert-butanolate
865-48-5	C4H10O	sodium 2-methylpropan-2-olate
86552-32-1	C10H15O2P	SQ 28,303
86604-78-6	C9H13NO2	4-methoxy-3,5-dimethylpyridine-2-methanol
867-13-0	C8H17O5P	triethyl phosphonoacetate
867-56-1	C3H6O3	sodium (S)-lactate
868-14-4	C4H6O6	potassium hydrogen tartrate
86-84-0	C11H7NO	1-naphthyl isocyanate
868-84-8	C3H6OS2	S,S-dimethyl carbonodithioate
86-92-0	C11H12N2O	3-methyl-1-p-tolyl-5-pyrazolone
869-24-9	C6H14ClN	2-chloroethyldiethylammonium chloride
870-08-6	C16H34OSn	dioctyltin oxide
87-02-5	C10H9NO4S	7-amino-4-hydroxynaphthalene-2-sulphonic acid
87061-04-9	C13H26O3	3-[[5-methyl-2-(1-methylethyl)cyclohexyl]oxy]propane-1,2-diol
87-13-8	C10H16O5	diethyl ethoxymethylenemalonate
871-70-5	C18H34O4	1,18-octadecanedioic acid
87199-17-5	C7H7BO3	4 FPBA
873055-55-1	C16H23NO5	2,4-Di-tert-butyl-5-nitrophenyl methyl carbonate
87428-99-7	C19H19NO3	Glycine, N-[1-oxo-2-(phenylmethyl)-2-propen-1-yl]-, phenylmethyl ester
87460-09-1	C19H23O4P	benzyl [hydroxy-(4-phenylbutyl)phosphinyl] acetate
87-56-9	C4H2Cl2O3	mucochloric acid
87787-67-5	C8H19NO2	7,7-dimethyl-3-oxa-6-azaoctan-1-ol
87-99-0	C5H12O5	xylitol
88-17-5	C7H6F3N	α,α,α-trifluoro-o-toluidine
88-18-6	C10H14O	2-tert-butylphenol
88196-70-7	C9H13NO	(R)-1-(3-methoxyphenyl)ethylamine
88-19-7	C7H9NO2S	toluene-2-sulphonamide

88-21-1	C6H7NO3S	2-aminobenzenesulphonic acid
88-23-3	C6H6ClNO4S	3-amino-5-chloro-2-hydroxybenzenesulphonic acid
88-27-7	C17H29NO	2,6-di-tert-butyl-α-dimethylamino-p-cresol
88374-05-4	C14H10F2O	2-(2-Fluorophenyl)-2-(4-fluorophenyl)oxirane
88-45-9	C6H8N2O3S	2,5-diaminobenzenesulphonic acid
88-50-6	C6H5Cl2NO3S	4-amino-2,5-dichlorobenzenesulphonic acid
88-51-7	C7H8ClNO3S	4-amino-6-chlorotoluene-3-sulphonic acid
885-82-5	C12H9NO3	3-nitro[1,1'-biphenyl]-4-ol
88-75-5	C6H5NO3	2-nitrophenol
887-76-3	C10H8N2O5S	4,4'-azo-3-hydroxynaphthalene-1-sulphonate
88-95-9	C8H4Cl2O2	phthaloyl dichloride
89-00-9	C7H5NO4	pyridine-2,3-dicarboxylic acid
89-04-3	C33H54O6	trioctyl benzene-1,2,4-tricarboxylate
89-25-8	C10H10N2O	3-methyl-1-phenyl-5-pyrazolone
89-33-8	C12H12N2O3	ethyl 5-oxo-1-phenyl-2-pyrazoline-3-carboxylate
89-36-1	C10H10N2O4S	4-(3-methyl-5-oxo-2-pyrazolin-1-yl)benzenesulphonic acid
89402-42-6	C6H2F5N	2,3-Difluoro-5-trifluoromethyl-pyridine
89-48-5	C12H22O2	menthyl acetate
89-57-6	C7H7NO3	Sulfasalazine metabolite: Mesalazine
89-58-7	C8H9NO2	2-nitro-p-xylene
89-62-3	C6H6N2O3	2-nitro-p-toluidine
89-63-4	C6H5ClN2O2	4-chloro-2-nitroaniline
89-65-6	C6H8O6	2,3-didehydro-D-erythro-hexono-1,4-lactone
897-06-3	C19H24O2	androsta-1,4-diene-3,17-dione
90-02-8	C7H6O2	salicylaldehyde
9005-00-9	C18H38O	2-octadecoxyethanol
9005-64-5	C32H60O10	Sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated)
9005-67-8	C22H42O8	Sorbitan monostearate, ethoxylated
9016-45-9	C17H28O2	Poly(oxy-1,2-ethanediyl), .alpha.-(nonylphenyl)-.omega.-hydroxy-
90-17-5	C10H9Cl3O2	2,2,2-trichloro-1-phenylethyl acetate
90-20-0	C10H9NO7S2	4-amino-5-hydroxynaphthalene-2,7-disulphonic acid
902146-43-4	C11H16N2O2S	(2S)-2-benzyl-N,N-dimethylaziridine-1-sulfonamide
90-31-3	C10H9ClN2O	2-(3-chlorophenyl)-2,4-dihydro-5-methyl-3H-pyrazol-3-one
90474-13-8	C11H18O4	diethyl 1,2-cyclopentanedicarboxylate
90-51-7	C10H9NO4S	6-amino-4-hydroxynaphthalene-2-sulphonic acid
90-82-4	C10H15NO	pseudoephedrine
91-16-7	C8H10O2	veratrole
91-21-4	C9H11N	1,2,3,4-tetrahydroisoquinoline
91-35-0	C13H12N2O5S	2-[[(3-amino-4-hydroxyphenyl)sulphonyl]amino]benzoic acid
91-64-5	C9H6O2	coumarin
91-66-7	C10H15N	N,N-diethylaniline

920-66-1	C3H2F6O	1,1,1,3,3,3-hexafluoropropan-2-ol
92077-08-2	C13H20O3	dihydro-3-(tripropenyl)furan-2,5-dione
923-02-4	C5H9NO2	N-(hydroxymethyl)methacrylamide
92-36-4	C14H12N2S	4-(6-methylbenzothiazol-2-yl)aniline
924-50-5	C6H10O2	methyl 3-methyl-2-butenoate
924663-38-7	C18H21N3O4S	2-[[4-(3-methoxypropoxy)-3-methyl-1-oxypyridin-2-yl]methylsulfinyl]-1H-benzimidazole
925-21-3	C8H12O4	butyl hydrogen maleate
92-55-7	C9H9NO7	5-nitrofurfurylidene di(acetate)
926-63-6	C5H13N	dimethyl(propyl)amine
92-69-3	C12H10O	biphenyl-4-ol
927-07-1	C9H18O3	tert-butyl peroxypivalate
92-72-8	C19H16ClNO4	5'-chloro-3-hydroxy-2',4'-dimethoxy-2-naphthanilide
927395-20-8	C12H30O2SSi2	3-Methoxy-3,8,8,9,9-pentamethyl-2-oxa-7-thia-3,8-disiladecane
927-62-8	C6H15N	N,N-dimethylbutylamine
92-77-3	C17H13NO2	3-hydroxy-2-naphthanilide
92-79-5	C18H15NO3	3-hydroxy-4'-methoxy-2-naphthanilide
928-70-1	C6H12OS2	potassium isopentyl dithiocarbonate
92-88-6	C12H10O2	biphenyl-4,4'-diol
928-96-1	C6H12O	cis-hex-3-en-1-ol
930-02-9	C20H40O	1-(vinyloxy)octadecane
93-01-6	C10H8O4S	6-hydroxynaphthalene-2-sulphonic acid
93-04-9	C11H10O	methyl 2-naphthyl ether
93-08-3	C12H10O	2'-acetonaphthone
931-36-2	C6H10N2	2-ethyl-4-methylimidazole
93-17-4	C10H11NO2	3,4-dimethoxyphenylacetonitrile
93-20-9	C12H12O2	2-(2-naphthyloxy)ethanol
93-55-0	C9H10O	propiophenone
93-58-3	C8H8O2	methyl benzoate
93-69-6	C9H13N5	1-o-tolylbiguanide
93803-87-3	C38H76O2	2-octyldodecyl isooctadecanoate
93803-89-5	C41H76O8	2,2-bis[[(1-oxoisononyl)oxy]methyl]-1,3-propanediyl diisononanoate
938-18-1	C10H11ClO	2,4,6-trimethylbenzoyl chloride
93820-33-8	C17H35NO	N-(2-ethylhexyl)isononan-1-amide
93-83-4	C22H43NO3	N,N-bis(2-hydroxyethyl)oleamide
93-92-5	C10H12O	1-phenylethyl acetate
94-05-3	C8H11NO3	ethyl 2-cyano-3-ethoxyacrylate
94108-97-1	C24H34O9	2-[[2,2-bis[[(1-oxoallyl)oxy]methyl]butoxy]methyl]-2-ethyl-1,3-propanediyl diacrylate
94-13-3	C10H12O3	propyl 4-hydroxybenzoate
94239-04-0	C6H3F4N	2-Fluoro-6-trifluoromethylpyridine
94-58-6	C10H12O2	5-propyl-1,3-benzodioxole
94-60-0	C10H16O4	dimethyl cyclohexane-1,4-dicarboxylate
94-70-2	C8H11NO	o-phenetidine

94744-50-0	C19H19NO4	N-a-Fmoc-a-aminoisobutyric acid, N-Fmoc-C-a-methylalanine
947701-81-7	C27H31NO2	10-undecenyl 2-cyano-3,3-diphenylpropenoate
94-91-7	C15H18N2O2	α,α'-propylenedinitrilodi-o-cresol
94-96-2	C8H18O2	2-ethylhexane-1,3-diol
95-14-7	C6H5N3	benzotriazole
95-52-3	C7H7F	2-fluorotoluene
95-64-7	C8H11N	3,4-xylidine
95-73-8	C7H6Cl2	2,4-dichlorotoluene
95748-46-2	C24H38N4O7	Benzyl (5-{[4-({5-[acetyl(hydroxy)amino]pentyl}amino)-4-oxobutanoyl](hydroxy)amino}pentyl)carbamate
95-75-0	C7H6Cl2	3,4-dichlorotoluene
957-68-6	C10H12N2O5S	3-acetoxymethylen-7-amino-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid
95-78-3	C8H11N	2,5-xylidine
95-79-4	C7H8ClN	5-chloro-o-toluidine
95-87-4	C8H10O	2,5-xylenol
959-14-8	C14H19N3O	oxolamine
959-52-4	C12H15N3O3	hexahydro-1,3,5-tris(1-oxoallyl)-1,3,5-triazine
96-05-9	C7H10O2	allyl methacrylate
96-10-6	C4H10AlCl	diethylaluminium chloride
96-32-2	C3H5BrO2	methyl bromoacetate
96-47-9	C5H10O	tetrahydro-2-methylfuran
96562-58-2	C10H12O4	methyl (R)-2-(4-hydroxyphenoxy)propionate
96-67-3	C6H6N2O6S	3-amino-2-hydroxy-5-nitrobenzenesulphonic acid
96-93-5	C6H6N2O6S	3-amino-4-hydroxy-5-nitrobenzenesulphonic acid
96-96-8	C7H8N2O3	2-nitro-p-anisidine
96-97-9	C7H5NO5	5-nitrosalicylic acid
96-99-1	C7H4ClNO4	4-chloro-3-nitrobenzoic acid
971-15-3	C12H20N2S8	bis(piperidinothiocarbonyl) hexasulphide
97-39-2	C15H17N3	1,3-di-o-tolylguanidine
97-53-0	C10H12O2	eugenol
97-59-6	C4H6N4O3	allantoin
97-61-0	C6H12O2	2-methylvaleric acid
976-71-6	C22H28O3	canrenone
97-74-5	C6H12N2S3	tetramethylthiuram monosulphide
97-78-9	C15H29NO3	N-lauroylsarcosine
97-90-5	C10H14O4	ethylene dimethacrylate
97-97-2	C4H9ClO2	2-chloro-1,1-dimethoxyethane
97-99-4	C5H10O2	tetrahydrofurfuryl alcohol
98231-71-1	C6H15Cl2NO3S	2(2-Amino-ethoxy)-2'chloro-diethylsulfone Hydrochloride
98298-66-9	C6H11ClO3	chloro-1-ethyl isopropyl carbonate
98-32-8	C6H8N2O3S	3-amino-4-hydroxybenzenesulphonamide
98-37-3	C6H7NO4S	3-amino-4-hydroxybenzenesulphonic acid
98-42-0	C7H9NO4S	3-amino-4-methoxybenzenesulphonic acid

98-43-1	C7H7NO5S	4-sulphoanthranilic acid
98-52-2	C10H20O	4-tert-butylcyclohexanol
98-55-5	C10H18O	p-menth-1-en-8-ol
98-59-9	C7H7ClO2S	tosyl chloride
98-60-2	C6H4Cl2O2S	4-chlorobenzenesulphonyl chloride
98-89-5	C7H12O2	cyclohexanecarboxylic acid
98-92-0	C6H6N2O	nicotinamide
991-84-4	C33H56N4OS2	2,6-di-tert-butyl-4-(4,6-bis(octylthio)-1,3,5-triazin-2-ylamino)phenol
99-34-3	C7H4N2O6	3,5-dinitrobenzoic acid
99-51-4	C8H9NO2	4-nitro-o-xylene
99-59-2	C7H8N2O3	5-nitro-o-anisidine
99-62-7	C12H18	1,3-diisopropylbenzene
996-35-0	C5H13N	N,N-dimethylisopropylamine
99-75-2	C9H10O2	methyl p-toluate
99-82-1	C10H20	1-isopropyl-4-methylcyclohexane
998-30-1	C6H16O3Si	triethoxysilane
99-93-4	C8H8O2	4'-hydroxyacetophenone
99-97-8	C9H13N	N,N-dimethyl-p-toluidine
no CAS	C7H7NO3	Sulfasalazine metabolite: Mesalazine

REACH SVHC

101-14-4	C13H12Cl2N2	4,4'-methylenebis[2-chloroaniline]
101-61-1	C17H22N2	N,N,N',N'-tetramethyl-4,4'-methylenedianiline (Michlerâ€™s base)
101-77-9	C13H14N2	4,4'-methylenedianiline
101-80-4	C12H12N2O	4,4'-oxydianiline
106-94-5	C3H7Br	1-bromopropane
109-86-4	C3H8O2	2-methoxyethanol
110-00-9	C4H4O	furan
110-71-4	C4H10O2	1,2-dimethoxyethane
110-80-5	C4H10O2	2-ethoxyethanol
111-15-9	C6H12O3	2-Ethoxyethyl acetate
111-96-6	C6H14O3	bis(2-methoxyethyl) ether
112-49-2	C8H18O4	1,2-bis(2-methoxyethoxy)ethane
115-96-8	C6H12Cl3O4P	tris(2-chloroethyl) phosphate
1163-19-5	C12Br10O	bis(pentabromophenyl) ether
117-81-7	C24H38O4	bis(2-ethylhexyl) phthalate
117-82-8	C14H18O6	Bis(2-methoxyethyl) phthalate
120-12-7	C14H10	anthracene
120-71-8	C8H11NO	6-methoxy-m-toluidine
121-14-2	C7H6N2O4	2,4-Dinitrotoluene
12578-12-0	C36H70O6Pb3	dioxobis(stearato)trilead
127-19-5	C4H9NO	N,N-dimethylacetamide
131-18-0	C18H26O4	di-n-pentyl phthalate

140-66-9	C14H22O	4-(1,1,3,3-tetramethylbutyl)phenol
143860-04-2	C11H23NO	3-ethyl-2-methyl-2-(3-methylbutyl)-1,3-oxazolidine
19438-60-9	C9H12O3	hexahydro-4-methylphthalic anhydride
2058-94-8	C11HF21O2	Perfluoro-n-undecanoic acid (PFUnA)
2451-62-9	C12H15N3O6	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione
25155-23-1	C24H27O4P	trixylyl phosphate
25550-51-0	C9H12O3	hexahydromethylphthalic anhydride
25637-99-4	C12H18Br6	hexabromocyclododecane
307-55-1	C12HF23O2	Perfluorododecanoic acid (PFDoA)
3194-55-6	C12H18Br6	Hexabromocyclododecane
335-67-1	C8HF15O2	PFOA, C8
376-06-7	C14HF27O2	Perfluorotetradecanoic acid (PFTDA)
561-41-1	C24H29N3O	4,4'-bis(dimethylamino)-4''-(methylamino)trityl alcohol [with â‰¥ 0.1% of Michler's ketone (EC No. 202-027-5) or Michler's base (EC No. 202-959-2)]
56-35-9	C24H54OSn2	bis(tributyltin) oxide
59653-74-6	C12H15N3O6	1,3,5-tris[(2S and 2R)-2,3-epoxypropyl]-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione (Î²-TGIC)
60-09-3	C12H11N3	4-aminoazobenzene
605-50-5	C18H26O4	diisopentyl phthalate
625-45-6	C3H6O3	methoxyacetic acid
629-14-1	C6H14O2	1,2-Diethoxyethan
64-67-5	C4H10O4S	diethyl sulphate
6786-83-0	C33H33N3O	Î±,Î±-Bis[4-(dimethylamino)phenyl]-4 (phenylamino)naphthalene-1-methanol (C.I. Solvent Blue 4) [with â‰¥ 0.1% of Michler's ketone (EC No. 202-027-5) or Michler's base (EC No. 202-959-2)]
68-12-2	C3H7NO	N,N-dimethylformamide
683-18-1	C8H18Cl2Sn	dibutyltin dichloride
69011-06-9	C8H4O6Pb3	[phthalato(2-)]dioxotrilead
75-56-9	C3H6O	methyloxirane
77-09-8	C20H14O4	phenolphthalein
78-00-2	C8H20Pb	tetraethyllead
79-06-1	C3H5NO	acrylamide
79-16-3	C3H7NO	N-methylacetamide
81-15-2	C12H15N3O6	5-tert-butyl-2,4,6-trinitro-m-xylene (musk xylene)
838-88-0	C15H18N2	4,4'-methylenedi-o-toluidine
84-69-5	C16H22O4	diisobutyl phthalate
84-74-2	C16H22O4	dibutyl phthalate
84777-06-0	C18H24O4	1,2-benzenedicarboxylic acid, dipentylester, branched and linear
85-42-7	C8H10O3	cyclohexane-1,2-dicarboxylic anhydride
85-68-7	C19H20O4	benzyl butyl phthalate
872-50-4	C5H9NO	1-methyl-2-pyrrolidone
88-85-7	C10H12N2O5	dinoseb

90-04-0	C7H9NO	o-anisidine
90-94-8	C17H20N2O	4,4'-bis(dimethylamino)benzophenone (Michlerâ€™s ketone)
92-67-1	C12H11N	biphenyl-4-ylamine; xenylamine; 4-aminobiphenyl
95-53-4	C7H9N	o-toluidine
95-80-7	C7H10N2	4-methyl-m-phenylenediamine
96-18-4	C3H5Cl3	1,2,3-trichloropropane
96-45-7	C3H6N2S	imidazolidine-2-thione
97-56-3	C14H15N3	4-o-tolylazo-o-toluidine; 4-amino-2',3-dimethylazobenzene; fast garnet GBC base; AAT; o-aminoazotoluene

CMR

100-44-7	C7H7Cl	α-chlorotoluene
100-63-0	C6H8N2	phenylhydrazine
101-14-4	C13H12Cl2N2	4,4'-methylenebis[2-chloroaniline]
101-61-1	C17H22N2	N,N,N',N'-tetramethyl-4,4'-methylenedianiline (Michlerâ€™s base)
101-80-4	C12H12N2O	4,4'-oxydianiline
103112-35-2	C12H8Cl5N3O2	ethyl 1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazole-3-carboxylate
103122-66-3	C8H15NO3S	O-isobutyl-N-ethoxy carbonylthiocarbamate
103-33-3	C12H10N2	azobenzene
103361-09-7	C19H15FN2O4	flumioxazin (ISO); N-(7-fluoro-3,4-dihydro-3-oxo-4-prop-2-ynyl-2H-1,4-benzoxazin-6-yl)cyclohex-1-ene-1,2-dicarboxamide
105024-66-6	C25H29FO2Si	(4-ethoxyphenyl)(3-(4-fluoro-3-phenoxyphenyl)propyl)dimethylsilane
10605-21-7	C9H9N3O2	carbendazim (ISO); methyl benzimidazol-2-ylcarbamate
106-47-8	C6H6ClN	4-chloroaniline
106-89-8	C3H5ClO	1-chloro-2,3-epoxypropane
106-94-5	C3H7Br	1-bromopropane
106-97-8	C4H10	butane
106-99-0	C4H6	buta-1,3-diene
107-13-1	C3H3N	acrylonitrile
109-86-4	C3H8O2	2-methoxyethanol
110-00-9	C4H4O	furan
110-49-6	C5H10O3	2-methoxyethyl acetate; methylglycol acetate
110-71-4	C4H10O2	1,2-dimethoxyethane
110-80-5	C4H10O2	2-ethoxyethanol
111-15-9	C6H12O3	2-Ethoxyethyl acetate
111-41-1	C4H12N2O	2-(2-aminoethylamino)ethanol
1116-54-7	C4H10N2O3	2,2'-(nitrosoimino)bisethanol
111-96-6	C6H14O3	bis(2-methoxyethyl) ether
1120-71-4	C3H6O3S	1,3-propanesultone
112-49-2	C8H18O4	1,2-bis(2-methoxyethoxy)ethane
115-29-7	C9H6Cl6O3S	Endosulfan

115-32-2	C14H9Cl5O	Dicofol
115-96-8	C6H12Cl3O4P	tris(2-chloroethyl) phosphate
117-82-8	C14H18O6	Bis(2-methoxyethyl) phthalate
118-74-1	C6Cl6	hexachlorobenzene
119738-06-6	C21H19ClN2O5	(±) tetrahydrofurfuryl (R)-2-[4-(6-chloroquinoxalin-2-yloxy)phenyloxy]propionate
119-90-4	C14H16N2O2	3,3'-dimethoxybenzidine; o-dianisidine
119-93-7	C14H16N2	4,4'-bi-o-toluidine
120-71-8	C8H11NO	6-methoxy-m-toluidine
120-82-1	C6H3Cl3	1,2,4-trichlorobenzene
121-14-2	C7H6N2O4	2,4-Dinitrotoluene
122-60-1	C9H10O2	2,3-epoxypropyl phenyl ether
122-66-7	C12H12N2	hydrazobenzene; 1,2-diphenylhydrazine
126-99-8	C4H5Cl	2-chlorobuta-1,3-diene
127-19-5	C4H9NO	N,N-dimethylacetamide
131-18-0	C18H26O4	di-n-pentyl phthalate
132-32-1	C14H14N2	3-amino-9-ethyl carbazole; 9-ethylcarbazol-3-ylamine
133-49-3	C6HCl5S	Pentachlorobenzenethiol
1335-32-6	C4H10O8Pb3	lead acetate, basic; lead acetate
13463-39-3	C4NiO4	tetracarbonylnickel; nickel tetracarbonyl
137-17-7	C9H13N	2,4,5-trimethylaniline
139-65-1	C12H12N2S	4,4'-thiodianiline and its salts
1420-07-1	C10H12N2O5	dinoterb (ISO); 2-tert-butyl-4,6-dinitrophenol
143860-04-2	C11H23NO	3-ethyl-2-methyl-2-(3-methylbutyl)-1,3-oxazolidine
1464-53-5	C4H6O2	2,2'-bioxirane; 1,2:3,4-diepoxybutane
1589-47-5	C4H10O2	2-methoxypropanol
16039-61-5	C6H10NiO6	nickel dilactate
1763-23-1	C8HF17O3S	perfluorooctane sulfonic acid; heptadecafluorooctane-1-sulfonic acid
17804-35-2	C14H18N4O3	benomyl (ISO); methyl 1-(butylcarbamoyl)benzimidazol-2-ylcarbamate
1836-75-5	C12H7Cl2NO3	nitrofen (ISO); 2,4-dichlorophenyl 4-nitrophenyl ether
192-97-2	C20H12	benzo[e]pyrene
199327-61-2	C16H21N3O4	Morfon, 7-methoxy-6-(3-morfolin-4-yl-propoxy)-3H-quinazolin-4-on
205-82-3	C20H12	benzo[j]fluoranthene
205-99-2	C20H12	benz[e]acephenanthrylene
207-08-9	C20H12	benzo[k]fluoranthene
21436-97-5	C9H13N	2,4,5-trimethylaniline hydrochloride
218-01-9	C18H12	chrysene
2451-62-9	C12H15N3O6	1,3,5-tris(oxiranylmethyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione
24602-86-6	C19H39NO	tridemorph (ISO); 2,6-dimethyl-4-tridecylmorpholine
2475-45-8	C14H12N4O2	1,4,5,8-tetraaminoanthraquinone; C.I. Disperse Blue 1

25321-14-6	C7H6N2O4	dinitrotoluene
294-62-2	C12H24	cyclododecane
32536-52-0	C12H2Br8O	diphenylether; octabromo derivate
330-55-2	C9H10Cl2N2O2	linuron (ISO); 3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea
3724-43-4	C3H7Cl2N	Chloromethylene dimethylammonium chloride
37894-46-5	C11H25ClO6Si	6-(2-chloroethyl)-6-(2-methoxyethoxy)-2,5,7,10-tetraoxa-6-silaundecane; etacelasil
39300-45-3	C18H24N2O6	dinocap (ISO)
399-95-1	C6H6FNO	4-amino-3-fluorophenol
485-31-4	C15H18N2O6	binapacryl (ISO); 2-sec-butyl-4,6-dinitrophenyl-3-methylcrotonate
50-29-3	C14H9Cl5	Clofenotane (= p,pDDT)
50-32-8	C20H12	benzo[a]pyrene; benzo[def]chrysene
50471-44-8	C12H9Cl2NO3	vinclozolin (ISO); N-3,5-dichlorophenyl-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione
51594-55-9	C3H5ClO	(R)-1-chloro-2,3-epoxypropane
51-79-6	C3H7NO2	urethane (INN); ethyl carbamate
5216-25-1	C7H4Cl4	α,α,α,4-tetrachlorotoluene
53-70-3	C22H14	dibenz[a,h]anthracene
540-73-8	C2H8N2	1,2-dimethylhydrazine
542-56-3	C4H9NO2	isobutyl nitrite
5543-57-7	C19H16O4	(S)-4-Hydroxy-3-(3-oxo-1-phenylbutyl)-2-benzopyron
5543-58-8	C19H16O4	(R)-4-Hydroxy-3-(3-oxo-1-phenylbu- tyl)-2-benzopyron
556-52-5	C3H6O2	2,3-epoxypropan-1-ol
5571-36-8	C20H26O3	cyclic 3-(1,2-ethanediylacetale)-estra-5(10),9(11)-diene-3,17-dione
56-55-3	C18H12	benz[a]anthracene
57044-25-4	C3H6O2	R-2,3-epoxy-1-propanol
57-57-8	C3H4O2	propiolactone
581-89-5	C10H7NO2	2-nitronaphthalene
58-89-9	C6H6Cl6	Lindane
592-62-1	C4H8N2O3	methyl-ONN-azoxymethyl acetate; methyl azoxy methyl acetate
59653-74-6	C12H15N3O6	1,3,5-tris[(2S and 2R)-2,3-epoxypropyl]-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione (Î²-TGIC)
60-09-3	C12H11N3	4-aminoazobenzene
602-01-7	C7H6N2O4	2,3-dinitrotoluene
602-87-9	C12H9NO2	5-nitroacenaphthene
605-50-5	C18H26O4	diisopentyl phthalate
606-20-2	C7H6N2O4	2,6-dinitrotoluene
610-39-9	C7H6N2O4	3,4-dinitrotoluene
613-35-4	C16H16N2O2	N,N'-diacetylbenzidine
615-05-4	C7H10N2O	2,4-diaminoanisole, 4-methoxy-m-phenylenediamine
61571-06-0	C6H10OS	tetrahydrothiopyran-3-carboxaldehyde

618-85-9	C7H6N2O4	3,5-dinitrotoluene
619-15-8	C7H6N2O4	2,5-dinitrotoluene
621-64-7	C6H14N2O	nitrosodipropylamine
625-45-6	C3H6O3	methoxyacetic acid
629-14-1	C6H14O2	1,2-Diethoxyethan
64-67-5	C4H10O4S	diethyl sulphate
64-86-8	C22H25NO6	colchicine
65277-42-1	C26H28Cl2N4O4	ketoconazole; 1-[4-[4-[[(2SR,4RS)-2-(2,4-dichlorophenyl)-2-(imidazol-1-ylmethyl)-1,3-dioxolan-4-yl]methoxy]phenyl]piperazin-1-yl]ethanone
66-81-9	C15H23NO4	cycloheximide
680-31-9	C6H18N3OP	hexamethylphosphoric triamide; hexamethylphosphoramide
1791337	C11H12N4O4	carbadox (INN); methyl 3-(quinoxalin-2-ylmethylene)carbazate 1,4-dioxide; 2-(methoxycarbonylhydrazonomethyl)quinoxaline 1,4-dioxide
68049-83-2	C15H15Cl2N3O2	azafenidin
6807-17-6	C18H22O2	4,4-isobutylethylidenediphenol
68-12-2	C3H7NO	N,N-dimethylformamide
683-18-1	C8H18Cl2Sn	dibutyltin dichloride
69806-50-4	C19H20F3NO4	fluazifop-butyl (ISO); butyl (RS)-2-[4-(5-trifluoromethyl-2-pyridyloxy)phenoxy]propionate
70657-70-4	C6H12O3	2-methoxypropyl acetate
71-43-2	C6H6	benzene
71957-07-8	C12H22NiO14	bis(D-gluconato-O1,O2)nickel
75-26-3	C3H7Br	2-bromopropane
75-28-5	C4H10	isobutane
75-55-8	C3H7N	2-methylaziridine
75-56-9	C3H6O	methyloxirane
75-74-1	C4H12Pb	Tetramethyllead
764-41-0	C4H6Cl2	1,4-dichlorobut-2-ene
77-09-8	C20H14O4	phenolphthalein
77402-03-0	C7H11NO4	methyl acrylamidomethoxyacetate (containing ≥ 0,1 % acrylamid)
77402-05-2	C6H9NO4	methyl acrylamidoglycolate (containing ≥ 0,1 % acrylamide)
78-79-5	C5H8	isoprene
79-06-1	C3H5NO	acrylamide
79-16-3	C3H7NO	N-methylacetamide
79-44-7	C3H6ClNO	dimethylcarbamoyl chloride
79-46-9	C3H7NO2	2-nitropropane
80387-97-9	C25H42O3S	2-ethylhexyl[[[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]methyl]thio]acetate
81-81-2	C19H16O4	warfarin
82413-20-5	C26H29NO2	(E)-3-[1-[4-[2-(Dimethylamino)ethoxy]phenyl]-2-phenylbut-1-enyl]phenol
838-88-0	C15H18N2	4,4'-methylenedi-o-toluidine

84245-12-5	C11H15N5O5	N-[6,9-dihydro-9-[[2-hydroxy-1-(hydroxymethyl)ethoxy]methyl]-6-oxo-1H-purin-2-yl]acetamide
84-69-5	C16H22O4	diisobutyl phthalate
84777-06-0	C18H24O4	1,2-benzenedicarboxylic acid, dipentylester, branched and linear
84852-35-7	C18H34NiO4	(isooctanoato-O)(neodecanoato-O)nickel
84852-36-8	C19H36NiO4	(isodecanoato-O)(isononanoato-O)nickel
85166-19-4	C18H34NiO4	(isodecanoato-O)(isooctanoato-O)nickel
85508-46-9	C17H32NiO4	(isononanoato-O)(isooctanoato-O)nickel
85509-19-9	C16H15F2N3Si	flusilazole (ISO); bis(4-fluorophenyl)(methyl)(1H-1,2,4-triazol-1-ylmethyl)silane
85551-28-6	C19H36NiO4	(isononanoato-O)(neodecanoato-O)nickel
872-50-4	C5H9NO	1-methyl-2-pyrrolidone
87-61-6	C6H3Cl3	1,2,3-trichlorobenzene
87-68-3	C4Cl6	Hexachlorobuta1,3-diene
88-72-2	C7H7NO2	2-nitrotoluene
88-85-7	C10H12N2O5	dinoseb
90-04-0	C7H9NO	o-anisidine
90-94-8	C17H20N2O	4,4'-bis(dimethylamino)benzophenone (Michlerâ€™s ketone)
91-22-5	C9H7N	quinoline
91-23-6	C7H7NO3	2-nitroanisole
91-59-8	C10H9N	2-naphthylamine
91-94-1	C12H10Cl2N2	3,3'-dichlorobenzidine; 3,3'-dichlorobiphenyl-4,4'-ylenediamine
91-95-2	C12H14N4	biphenyl-3,3',4,4'-tetrayltetraamine; diaminobenzidine
92-67-1	C12H11N	biphenyl-4-ylamine; xenylamine; 4-aminobiphenyl
92-87-5	C12H12N2	benzidine; 1,1'-biphenyl-4,4'-diamine; 4,4'-diaminobiphenyl; biphenyl-4,4'-ylenediamine
92-93-3	C12H9NO2	4-nitrobiphenyl
94-59-7	C10H10O2	safrole; 5-allyl-1,3-benzodioxole
95-06-7	C8H14ClNS2	sulfallate (ISO); 2-chloroallyl N,N-dimethyldithiocarbamate
95-53-4	C7H9N	o-toluidine
95-69-2	C7H8ClN	4-chloro-o-toluidine
95-80-7	C7H10N2	4-methyl-m-phenylenediamine
96-09-3	C8H8O	(epoxyethyl)benzene
96-12-8	C3H5Br2Cl	1,2-dibromo-3-chloropropane
96-13-9	C3H6Br2O	2,3-dibromopropan-1-ol; 2,3-dibromo-1-propanol
96-18-4	C3H5Cl3	1,2,3-trichloropropane
96-23-1	C3H6Cl2O	1,3-dichloropropan-2-ol
96-45-7	C3H6N2S	imidazolidine-2-thione
97-56-3	C14H15N3	4-o-tolylazo-o-toluidine; 4-amino-2',3-dimethylazobenzene; fast garnet GBC base; AAT; o-aminoazotoluene
98-07-7	C7H5Cl3	α,α,α-trichlorotoluene

no CAS		2-[2-hydroxy-3-(2-chlorophenyl)carbamoyl-1-naphthylazo]-7-[2-hydroxy-3-(3-methylphenyl)carbamoyl-1-naphthylazo]fluoren-9-one

Pesticides / Biocides

002634-33-5	C7H5NOS	1,2-benzisothiazol-3(2H)-on
079538-32-2	C17H14ClF7O2	tefluthrin
10004-44-1	C4H5NO2	HYMEXAZOLE
100646-51-3	C18H15ClN2O4	QUIZALOFOP_P_ETHYL
101200-48-0	C15H17N5O6S	tribenuron-methyl
101205-02-1	C17H27NO3S	CYCLOXYDIM
101-21-3	C10H12ClNO2	CHLORPROFAM
101463-69-8	C21H11ClF6N2O3	flufenoxuron
1014-69-3	C8H15N5S	DESMETRYN
10265-92-6	C2H8NO2PS	METHAMIDOFOS
103055-07-8	C17H8Cl2F8N2O3	lufenuron
10326-41-7	C3H6O3	(R)-lactic acid
103361-09-7	C19H15FN2O4	flumioxazin (ISO); N-(7-fluoro-3,4-dihydro-3-oxo-4-prop-2-ynyl-2H-1,4-benzoxazin-6-yl)cyclohex-1-ene-1,2-dicarboxamide
104206-82-8	C14H13NO7S	MESOTRIONE
104653-34-1	C31H23BrO2S	difethialon
10543-57-4	C10H16N2O4	N,N'-ethylenebis[N-acetylacetamide]
105512-06-9	C17H13ClFNO4	CLODINAFOP_PROPARGYL
10552-74-6	C14H17NO6	NITROTHAL_ISOPROPYL
10605-21-7	C9H9N3O2	carbendazim (ISO); methyl benzimidazol-2-ylcarbamate
1071-83-6	C3H8NO5P	GLYPHOSATE
107534-96-3	C16H22ClN3O	1-(4-chlorofenyl)-4,4-dimethyl-3-(1,2,4-tria- zole-1-ylmethyl)-3-pentanol / tebuconazole
108173-90-6	C18H41N7	GUAZATINE
1085-98-9	C9H11Cl2FN2O2S2	Dichlofluanide
108-62-3	C8H16O4	METALDEHYDE
110235-47-7	C14H13N3	MEPANIPYRIM
110488-70-5	C21H22ClNO4	DIMETHOMORF
1113-02-6	C5H12NO4PS	OMETHOAAT
111-30-8	C5H8O2	glutaral
11141-17-6	C35H44O16	AZADIRACHTINE_A
111479-05-1	C22H22ClN3O5	PROPAQUIZAFOP
111988-49-9	C10H9ClN4S	THIACLOPRID
111991-09-4	C15H18N6O6S	NICOSULFURON
112143-82-5	C13H22N4O3S	TRIAZAMAAT
112-65-2	C13H29N3	DODINE
113036-88-7	C25H20ClF2N3O3	FLUCYCLOXURON
114-26-1	C11H15NO3	PROPOXUR
116-06-3	C7H14N2O2S	ALDICARB

116255-48-2	C13H12BrCl2N3O	BROMUCONAZOLE
117428-22-5	C18H16F3NO4	PICOXYSTROBIN
118-52-5	C5H6Cl2N2O2	1,3-dichloro-5,5-dimethylhydantoine
118712-89-3	C15H12Cl2F4O2	transfluthrin
119168-77-3	C18H24ClN3O	TEBUFENPYRAD
119446-68-3	C19H17Cl2N3O3	DIFENOCONAZOLE
1194-65-6	C7H3Cl2N	DICHLOBENIL
120068-37-3	C12H4Cl2F6N4OS	FIPRONIL
120116-88-3	C13H13ClN4O2S	CYAZOFAMID
120923-37-7	C9H15N5O7S2	AMIDOSULFURON
12122-67-7	C4H6N2S4Zn	ZINEB
1214-39-7	C12H11N5	BENZYLADENINE
121552-61-2	C14H15N3	CYPRODINIL
121-75-5	C10H19O6PS2	MALATHION
122-14-5	C9H12NO5PS	FENITROTHION
122-34-9	C7H12ClN5	SIMAZIN
122-42-9	C10H13NO2	PROFAM
122931-48-0	C14H17N5O7S2	RIMSULFURON
122-99-6	C8H10O2	2-phenoxyethanol
123312-89-0	C10H11N5O	PYMETROZINE
123-33-1	C4H4N2O2	MALEINE_HYDRAZIDE
124495-18-7	C15H8Cl2FNO	QUINOXYFEN
125116-23-6	C17H22ClN3O	metconazole (ISO); (1RS,5RS;1RS,5SR)-5-(4-chlorobenzyl)-2,2-dimethyl-1-(1H-1,2,4-triazol-1-ylmethyl)cyclopentanol
125794-71-0	C4H5NOS	2-methyl-2H-isothiazol-3-on
126535-15-7	C17H19F3N6O6S	TRIFLUSULFURON_METHYL
126833-17-8	C14H17Cl2NO2	FENHEXAMIDE
12750-92-4	C19H30O5	piperonylbutoxide
12795-76-5	C30H28N6O4S4	Verticilliun
128639-02-1	C15H14Cl2F3N3O3	CARFENTRAZONE_ETHYL
129630-19-9	C15H13Cl2F3N2O4	pyraflufen-ethyl
13121-70-5	C18H34OSn	CYHEXATIN
131341-86-1	C12H6F2N2O2	FLUDIOXONIL
13171-21-6	C10H19ClNO5P	FOSFAMIDON
131807-57-3	C22H18N2O4	FAMOXADONE
131860-33-8	C22H17N3O5	AZOXYSTROBINE
13194-48-4	C8H19O2PS2	ETHOPROFOS
133-06-2	C9H8Cl3NO2S	CAPTAN
133-07-3	C9H4Cl3NO2S	FOLPET
133-32-4	C12H13NO2	3_INDOLYLBOTERZUUR
13356-08-6	C60H78OSn2	FENBUTATINOXIDE
13360-45-7	C9H10BrClN2O2	CHLORBROMURON
13457-18-6	C14H20N3O5PS	PYRAZOFOS
134-62-3	C12H17NO	N,N-Diethyltoluamide (DEET)

135319-73-2	C17H13ClFN3O	EPOXICONAZOLE
135410-20-7	C10H11ClN4	acetamiprid
135590-91-9	C16H18Cl2N2O4	MEFENPYRDIETHYL, diethyl 1-(2,4-dichlorophenyl)-5-methyl-4,5-dihydro-1H-pyrazole-3,5-dicarboxylate
13684-56-5	C16H16N2O4	DESMEDIFAM
13684-63-4	C16H16N2O4	FENMEDIFAM
137-26-8	C6H12N2S4	thiram
137-30-4	C6H12N2S4Zn	ziram
137662-59-0	C4H4ClNOS	5-chloro-2-methyl-2H-isothiazol-3-on
138261-41-3	C9H10ClN5O2	IMIDACLOPRID
141112-29-0	C15H12F3NO4S	isoxaflutol/5-cyclopropyl-1,2-oxazyl-α,α,α-trifluor-2-mesyl-p-tolylketon
141517-21-7	C20H19F3N2O4	TRIFLOXYSTROBINE
1420-07-1	C10H12N2O5	dinoterb (ISO); 2-tert-butyl-4,6-dinitrophenol
142459-58-3	C14H13F4N3O2S	flufenacet
142469-14-5	C13H9F6N5O4S	tritosulfuron
142891-20-1	C19H17Cl2NO4	CINIDON_ETHYL
143390-89-0	C18H19NO4	KRESOXIM_METHYL
144550-36-7	C14H13IN5NaO6S	IODOSULFURON_METHYL_NATRIUM
145701-23-1	C12H8F3N5O3S	FLORASULAM
14816-18-3	C12H15N2O3PS	phoxim (ISO); α-(diethoxyfosfinothioylimino) fenylacetonitril
148477-71-8	C21H24Cl2O4	SPIRODICLOFEN
148-79-8	C10H7N3S	THIABENDAZOLE
149877-41-8	C17H20N2O3	BIFENAZAAT
149979-41-9	C17H24ClNO4	tepraloxydim (ISO); (RS)-(EZ)-2-{1-[(2E)-3-chloroallyloxyimino]propyl}-3-hydroxy-5-perhydropyran-4-ylcyclohex-2-een-1-on
150114-71-9	C6H4Cl2N2O2	aminopyralid
15299-99-7	C12H17NO	napropamide
153233-91-1	C21H23F2NO2	etoxazole
153719-23-4	C19H25NO4	thiamethoxam
154592-20-8	C10H8CuN2O2S2	koperpyrithion
15545-48-9	C10H13ClN2O	chlortoluron/3-(3-chloro-p-tolyl)-1,1- dimethylurea
156052-68-5	C14H16Cl3NO2	ZOXAMIDE
1563-66-2	C12H15NO3	CARBOFURAN
158062-67-0	C9H6F3N3O	FLONICAMID
15845-66-6	C2H7O3P	fosetyl
1593-77-7	C18H35NO	DODEMORF
1596-84-5	C6H12N2O3	DAMINOZIDE
16079-88-2	C5H6BrClN2O2	bromochloro-5,5-dimethylimidazolidine-2,4-dione
161050-58-4	C22H28N2O3	methoxyfenozide
16118-45-9	C12H16N2O3	carbetamide
16118-49-3	C12H16N2O3	CARBEETAMIDE
161326-34-7	C17H17N3OS	FENAMIDONE
163515-14-8	C12H18ClNO2S	DIMETHENAMIDE_P
16752-77-5	C5H10N2O2S	METHOMYL

168316-95-8	C83H132N2O20	SPINOSAD
1689-83-4	C7H3I2NO	ioxynil/4-hydroxy-3,5-dijodiumbenzonitril en zouten
1689-84-5	C7H3Br2NO	bromoxynil/bromoxynilphenol/3,5-dibroom-4- hydroxybenzonitril en zouten
1698-60-8	C10H8ClN3O	CHLORIDAZON
1702-17-6	C6H3Cl2NO2	CLOPYRALID
173159-57-4	C17H20N6O7S	FORAMSULFURON
173584-44-6	C22H17ClF3N3O7	INDOXACARB
1746-81-2	C9H11ClN2O2	MONOLINURON
175013-18-0	C19H18ClN3O4	PYRACLOSTROBINE
175217-20-6	C13H21NOSSi	silthiofam
177406-68-7	C18H24FN3O3S	benthiavalicarb-isopropyl
17804-35-2	C14H18N4O3	benomyl (ISO); methyl 1-(butylcarbamoyl)benzimidazol-2-ylcarbamate
178928-70-6	C14H15Cl2N3OS	PROTHIOCONAZOLE
179101-81-6	C18H14Cl4F3NO3	pyridalyl
180409-60-3	C20H17F5N2O2	cyflufenamide
18181-80-1	C17H16Br2O3	BROOMPROPYLAAT
18691-97-9	C10H11N3OS	METHABENZTHIAZURON
188425-85-6	C18H12Cl2N2O	BOSCALID
1897-45-6	C8Cl4N2	CHLORTHALONIL
1912-24-9	C8H14ClN5	atrazine
1918-00-9	C8H6Cl2O3	DICAMBA
1918-16-7	C11H14ClNO	PROPACHLOR
19408-46-9	C14H25N3O9	KASUGAMYCINE
19937-59-8	C10H13ClN2O2	METOXURON
2032-65-7	C11H15NO2S	METHIOCARB
20711-10-8	C16H30O2	(Z)-11-tetradecenylacetaat
208465-21-8	C17H21N5O9S2	mesosulfuron-methyl
210631-68-8	C16H17N3O5S	TOPRAMEZONE
21087-64-9	C8H14N4OS	METRIBUZIN
210880-92-5	C6H8ClN5O2S	clothianidine
96639	C13H18N2O2	LENACIL
220899-03-6	C19H21BrO5	METRAFENONE
22144-76-9	C30H37NO6	Metarhizium
22224-92-6	C13H22NO3PS	FENAMIFOS
2227-17-0	C10Cl10	DIENOCHLOR
2275-23-2	C8H18NO4PS2	VAMIDOTHION
22781-23-3	C11H13NO4	bendiocarb
2303-17-5	C10H16Cl3NOS	TRI_ALLAAT
2310-17-0	C12H15ClNO4PS2	FOSALONE
23103-98-2	C11H18N4O2	PIRIMICARB
23135-22-0	C7H13N3O3S	OXAMYL
23560-59-0	C9H12ClO4P	HEPTENOFOS
23564-05-8	C12H14N4O4S2	THIOFANAAT_METHYL

2372-82-9	C18H41N3	N-(3-aminopropyl)-N-dodecylpropaan-1,3-diamine
239110-15-7	C14H8Cl3F3N2O	FLUOPICOLIDE
23950-58-5	C12H11Cl2NO	PROPYZAMIDE
24017-47-8	C12H16N3O3PS	TRIAZOFOS
243973-20-8	C23H32N2O4	pinoxaden
25057-89-0	C10H12N2O3S	BENTAZONE
25254-50-6	C12H27N3O3	alfa,alfa',alfa''-trimethyl-1,3,5-triazine-1,3,5(2H,4H,6H)-triethanol
2593-15-9	C5H5Cl3N2OS	ETRIDIAZOLE
26002-80-2	C23H26O3	d-fenothrin
26225-79-6	C13H18O5S	ETHOFUMESAAT
2637-34-5	C5H5NS	pyridine-2-thiol
26644-46-2	C10H14Cl6N4O2	TRIFORINE
272451-65-7	C23H22F7IN2O4S	flubendiamide
2797-51-5	C10H6ClNO2	QUINOCLAMIN
28159-98-0	C11H19N5S	Irgarol
283594-90-1	C23H30O4	SPIROMESIFEN
28772-56-7	C30H23BrO4	bromadiolon
2921-88-2	C9H11Cl3NO3PS	CHLORPYRIFOS
29232-93-7	C11H20N3O3PS	PIRIMIFOS_METHYL
301-03-1	C4H6MnN2S4	MANEB
30560-19-1	C4H10NO3PS	ACEFAAT
3060-89-7	C9H11BrN2O2	METOBROMURON
438389	C4H6	1-methylcyclopropeen
32809-16-8	C13H11Cl2NO2	PROCYMIDON
330-54-1	C9H10Cl2N2O	diuron
330-55-2	C9H10Cl2N2O2	linuron (ISO); 3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea
33089-61-1	C19H23N3	AMITRAZ
333-41-5	C12H21N2O3PS	DIAZINON
3337-71-1	C8H10N2O4S	ASULAM
334-48-5	C10H20O2	Decanoic acid
3347-22-6	C14H4N2O2S2	DITHIANON
335104-84-2	C17H16ClF3O6S	tembotrione
33956-49-9	C12H22O	CODLEMON
34123-59-6	C12H18N2O	ISOPROTURON
34681-10-2	C7H14N2O2S	BUTOCARBOXIM
348635-87-0	C13H13BrFN5O4S2	amisulbrom
35367-38-5	C14H9ClF2N2O2	DIFLUBENZURON
3586-55-8	C4H10O4	(ethyleendioxy)dimethanol
361377-29-9	C21H16ClFN4O5	FLUOXASTROBIN
36734-19-7	C13H13Cl2N3O3	IPRODION
3691-35-8	C23H15ClO3	chlorfacinon
374726-62-2	C23H22ClNO4	MANDIPROPAMID
698836	C9H6ClNO3S	BENAZOLIN

38260-54-7	C10H17N2O4PS	ETRIMFOS
3861-47-0	C15H17I2NO2	ioxyniloctanoaat/4-cyano-2,6-dijodium-fenyloctanoaat
39148-24-8	C6H18AlO9P3	fosetyl-aluminium
39515-41-8	C22H23NO3	FENPROPATHRIN
400882-07-7	C24H24F3NO4	cyflumetofen
40487-42-1	C13H19N3O4	PENDIMETHALIN
41083-11-8	C20H35N3Sn	AZOCYCLOTIN
41394-05-2	C10H10N4O	METAMITRON
41483-43-6	C13H24N4O3S	BUPIRIMAAT
422556-08-9	C14H13F3N6O5S	pyroxsulam
42576-02-3	C14H9Cl2NO5	BIFENOX
42822-86-6	C10H20O2	p-menthaan-3,8-diol
470-90-6	C12H14Cl3O4P	CHLORFENVINFOS
500008-45-7	C18H14BrCl2N5O2	chlorantraniliprole
50471-44-8	C12H9Cl2NO3	vinclozolin (ISO); N-3,5-dichlorophenyl-5-methyl-5-vinyl-1,3-oxazolidine-2,4-dione
51218-45-2	C15H22ClNO2	METOLACHLOR
51249-05-9	C18H38NO3P	BUMINAFOS
52315-07-8	C22H19Cl2NO3	cypermethrin
52645-53-1	C21H20Cl2O3	PERMETHRIN
52-68-6	C4H8Cl3O4P	TRICHLORFON
52888-80-9	C14H21NOS	PROSULFOCARB
52918-63-5	C22H19Br2NO3	DELTAMETHRIN
53112-28-0	C12H13N3	PYRIMETHANIL
533-74-4	C5H10N2S2	DAZOMET
534-52-1	C7H6N2O5	2-methyl-4,6-dinitro-phenol, DNOC
5395-50-6	C8H14N4O6	tetrahydro-1,3,4,6-tetrakis(hydroxymethyl)imidazo[4,5-d]imidazole-2,5(1H,3H)-dion
55179-31-2	C20H23N3O2	BITERTANOL
55219-65-3	C14H18ClN3O2	TRIADIMENOL
55335-06-3	C7H4Cl3NO3	TRICLOPYR
55406-53-6	C8H12INO2	3-jood-2-propynylbutylcarbamaat
55512-33-9	C19H23ClN2O2S	PYRIDAAT
55-56-1	C22H30Cl2N10	chlorhexidine
56073-07-5	C31H24O3	difenacoum
56-38-2	C10H14NO5PS	PARATHION
57018-04-9	C9H11Cl2O3PS	TOLCLOFOS_METHYL
57646-30-7	C17H19NO4	FURALAXYL
57837-19-1	C15H21NO4	METALAXYL
57960-19-7	C24H32O4	ACEQUINOCYL
57966-95-7	C7H10N4O3	CYMOXANIL
581809-46-3	C18H12Cl2F3N3O	bixafen
58-89-9	C6H6Cl6	Lindane
5915-41-3	C9H16ClN5	terbuthylazine

59-50-7	C7H7ClO	chlorocresol
59669-26-0	C10H18N4O4S3	THIODICARB
60168-88-9	C17H12Cl2N2O	fenarimol/2,4'-dichloro-α(pyrimidyl)-benzhydrylalcohol
60207-31-0	C12H11Cl2N3O2	AZACONAZOLE
60207-90-1	C15H17Cl2N3O2	PROPICONAZOLE
60-51-5	C5H12NO3PS2	DIMETHOAAT
62-73-7	C4H7Cl2O4P	DICHLORVOS
6317-18-6	C3H2N2S2	methyleenbisthiocyanaat
63-25-2	C12H11NO2	CARBARYL
640-15-3	C6H15O2PS3	THIOMETON
64359-81-5	C11H17Cl2NOS	4,5-dichloro-2-octyl-2H-isothiazol-3-on
65195-55-3	C95H142O28	abamectin
658066-35-4	C16H11ClF6N2O	fluopyram
65-85-0	C7H6O2	benzoic acid
66052-95-7	C31H23BrO3	brodifacoum
66063-05-6	C19H21ClN2O	PENCYCURON
66204-44-2	C9H18N2O2	3,3'-methyleenbis[5-methyloxazolidine]
66215-27-8	C6H10N6	CYROMAZINE
66230-04-4	C25H22ClNO3	ESFENVALERAAT
66246-88-6	C13H15Cl2N3	PENCONAZOLE
66332-96-5	C17H16F3NO2	FLUTOLANIL
67129-08-2	C14H16ClN3O	METAZACHLOR
67306-00-7	C19H31N	FENPROPIDIN
67375-30-8	C22H19Cl2NO3	alfa-cypermethrin
67485-29-4	C25H24F6N4	HYDRAMETHYLNON
67564-91-4	C20H33NO	fenpropimorf
67-63-0	C3H8O	propan-2-ol
67747-09-5	C15H16Cl3N3O2	PROCHLORAZ
67762-36-1	C9H18O2	nonaanzuur
67-99-2	C13H14N2O4S2	gliocladium
68085-85-8	C23H19ClF3NO3	lambda-cyhalothrin
68359-37-5	C22H18Cl2FNO3	CYFLUTHRIN
69327-76-0	C16H23N3OS	BUPROFEZIN
69377-81-7	C7H5Cl2FN2O3	FLUROXYPYR
69-72-7	C7H6O3	Acetyl salycilic acid metabolite: Salicylic acid
69806-40-2	C16H13ClF3NO4	HALOXYFOP_P_METHYLESTER
70630-17-0	C15H21NO4	METALAXYL_M
7085-19-0	C10H11ClO3	mecoprop (MCPP)
71-23-8	C3H8O	propan-1-ol
71283-80-2	C18H16ClNO5	FENOXAPROP_P_ETHYL
71751-41-2	C48H72O14	ABAMECTINE
7287-19-6	C10H19N5S	PROMETRYN
731-27-1	C10H13Cl2FN2O2S2	TOLYLFLUANIDE
7319-86-0	C8H16O2	Octanoic acid

73790-28-0	C14H14Cl2N2O	IMAZALIL
74051-80-2	C17H29NO3S	SETHOXYDIM
74070-46-5	C12H9ClN2O3	ACLONIFEN
74115-24-5	C14H8Cl2N4	CLOFENTEZIN
74223-64-6	C14H15N5O6S	METSULFURON_METHYL
74738-17-3	C11H6Cl2N2	FENPICLONIL
74-85-1	C2H4	ethyleen
75-21-8	C2H4O	ethyleenoxide
759-94-4	C9H19NOS	EPTC
76578-14-8	C19H17ClN2O4	QUIZALOFOP_ETHYL
76738-62-0	C15H20ClN3O	PACLOBUTRAZOL
76-87-9	C18H16OSn	fentinhydroxide/trifenyltinhydroxide
7696-12-0	C19H25NO4	tetramethrin
77-06-5	C19H22O6	GIBBERELLA_ZUUR_A3
7786-34-7	C7H13O6P	MEVINFOS
78587-05-0	C17H21ClN2O2S	HEXYTHIAZOX
79-08-3	C2H3BrO2	bromoacetic acid
79127-80-3	C17H19NO4	FENOXYCARB
79241-46-6	C19H20F3NO4	fluazifop-P-butyl/(R)-2-[4-(5-trifluormethyl)-2-pyridyloxy)fenoxy]propionaat
79622-59-6	C13H4Cl2F6N4O4	FLUAZINAM
2234562	C4H8N2S4	MANCOZEB
81405-85-8	C16H20N2O3	IMAZAMETHABENZ_METHYL
81406-37-3	C15H21Cl2FN2O3	fluroxypyr-meptyl
81591-81-3	C6H16NO5PS	GLYPHOSATE_TRIMESIUM
81777-89-1	C12H14ClNO2	CLOMAZONE
82558-50-7	C18H24N2O4	ISOXABEN
82560-54-1	C20H30N2O5S	benfuracarb (ISO); ethyl N-[2,3-dihydro- 2,2-dimethylbenzofuran-7-yloxy- carbonyl(methyl)aminothio]-N-isopropyl- β-alaninaat
83121-18-0	C14H6Cl2F4N2O2	TEFLUBENZURON
83164-33-4	C19H11F5N2O2	DIFLUFENICAN
86-50-0	C10H12N3O3PS2	AZINFOS_METHYL
865318-97-4	C15H25N5	ametoctradin
86-86-2	C12H11NO	1_NAFTYLACEETAMIDE
86-87-3	C12H10O2	1_NAFTYLAZIJNZUUR
87130-20-9	C14H21NO4	DIETHOFENCARB
87237-48-7	C19H19ClF3NO5	HALOXYFOP_ETHOXYETHYL
87392-12-9	C15H22ClNO2	S_METOLACHLOR
87-51-4	C10H9NO2	3_INDOLYLAZIJNZUUR
87674-68-8	C12H18ClNO2S	DIMETHENAMIDE
88283-41-4	C14H12Cl2N2O	PYRIFENOX
886-50-0	C10H19N5S	TERBUTRYN
89415-87-2	C6H8Cl2N2O2	1,3-dichloro-5-ethyl-5-methylimidazolidine-2,4-dion

9006-42-2	C4H6N2S4Zn	METIRAM
9008-22-4	C18H32O16	laminarin
900-95-8	C20H18O2Sn	fentinacetaat/trifenyltinacetaat
90-43-7	C12H10O	biphenyl-2-ol
90717-03-6	C11H8ClNO2	QUINMERAC
907204-31-3	C18H12F5N3O	fluxapyroxad
91465-08-6	C23H19ClF3NO3	LAMBDA_CYHALOTHRIN
94125-34-5	C15H16F3N5O4S	prosulfuron
94361-06-5	C15H18ClN3O	cyproconazole
94-74-6	C9H9ClO3	MCPA
94-75-7	C8H6Cl2O3	2_4_D
94-82-6	C10H10Cl2O3	2,4-DB
950-37-8	C6H11N2O4PS3	METHIDATION
95266-40-3	C13H16O5	TRINEXAPAC_ETHYL
95737-68-1	C20H19NO3	PYRIPROXYFEN
96489-71-3	C19H29ClN2OS	PYRIDABEN
97-17-6	C10H13Cl2O3PS	DICHLOFENTHION
98243-83-5	C20H23NO3	benalaxyl-M
98886-44-3	C9H18NO3PS2	FOSTHIAZAAT
99105-77-8	C14H13ClO5S	SULCOTRION
99-30-9	C6H4Cl2N2O2	DICHLORAN
99387-89-0	C15H15ClF3N3O	TRIFLUMIZOLE
99-49-0	C10H14O	KARVON_D
99607-70-2	C18H22ClNO3	CLOQUINTOCEET_MEXYL, heptan-2-yl [(5-chloroquinolin-8-yl)oxy]acetate
no CAS	C12H12N2Br2	diquatdibromide
no CAS	C20H23F2N3O	isopyrazam
no CAS	C23H46	cis-tricos-9-een
no CAS	C2H4NNaS2	metam-natrium
no CAS	C49H75NO13	emamectin

Pharmaceuticals

10066-90-7	C8H9NO5S	Paracetamol metabolite: 4-Acetaminophen Sulfate
1021933-98-1	C22H33NO8	Venlafaxine metabolite: O-desmethyl-(rac-venlafaxine)Glucuronide
102767-28-2	C8H14N2O2	Levetiracetam
103-90-2	C8H9NO2	Paracetamol (Acetaminophen)
114-07-8	C37H67NO13	Erythromycin A / Erythromycin h2o
114798-26-4	C22H20ClN6O	Losartan
119141-88-7	C17H19N3O3S	Omeprazole metabolite: Esomeprazole
125-33-7	C12H14N2O2	Primidone
134523-00-5	C33H35FN2O5	Atorvastatin
13523-86-9	C14H20N2O2	Pindolol
137-58-6	C14H22N2O	Lidocaine
137862-53-4	C24H29N5O3	Valsartan

138402-11-6	C25H28N6O	Irbesartan
139755-82-1	C21H28N6O4S	Sildenafil metabolite: (n-desmethyl sildenafil)
139755-83-2	C22H30N6O4S	Sildenafil = viagra
144-83-2	C11H11N3O2S	Sulfapyridine
149289-30-5	C16H25NO2	Venlafaxine metabolite: D,L N-desmethyl venlafaxine
15307-86-5	C14H11Cl2NO2	Diclofenac
15687-27-1	C13H18O2	ibuprofen
16051-77-7	C6H9NO6	Isosorbide mononitrate
18323-44-9	C18H33ClN2O5S	Clindamycin
21312-10-7	C12H13N3O4S	Sulfamethoxazole metabolite: N4-acetyl Sulfamethoxazole
22071-15-4	C16H14O3	Ketoprofen
22204-53-1	C14H14O3	Naproxen
23031-25-6	C12H19NO3	Terbutaline
23593-75-1	C22H17ClN2	Clotrimazole
2447-57-6	C12H14N4O4S	Sulfadoxin
2465-59-0	C5H4N4O2	Oxypurinol = Alloxanthine
25812-30-0	C15H22O3	Gemfibrozil
26787-78-0	C16H19N3O5S	Amoxicillin
27203-92-5	C16H25NO2	Tramadol
29122-68-7	C14H22N2O3	Atenolol
298-46-4	C15H12N2O	Carbamazepine
315-30-0	C5H4N4O	Allopurinol
31879-05-7	C15H14O3	Fenoprofen
35763-26-9	C13H21NO3	Salbutamol
36507-30-9	C15H12N2O2	Carbamazepine matebolite: Carbamazepine 10,11-epoxide
37148-27-9	C12H18Cl2N2O	Clenbuterol
37350-58-6	C15H25NO3	Metoprolol
37519-14-5	C8H9NO3	Paracetamol metabolite: 3-hydroxy paracetamol
3778-73-2	C7H15Cl2N2O2P	ifosfamide
3930-20-9	C12H20N2O3S	Sotalol
41859-67-0	C19H20ClNO4	Bezafibrate
42399-41-7	C22H26N2O4S	Diltiazem
42835-25-6	C14H12FNO3	Flumequine
439-14-5	C16H13ClN2O	Diazepam
443-48-1	C6H9N3O3	Metronidazole
479-92-5	C14H18N2O	Propyphenazone
50-02-2	C22H29FO5	Dexamethasone
50-18-0	C7H15Cl2N2O2P	Cyclophosphamide
50-24-8	C21H28O5	prednisolone
50-36-2	C21H30O5	Cocaine
50-78-2	C9H8O4	Acetyl salicylic acid
51481-61-9	C10H16N6S	Cimetidine
52-53-9	C27H38N2O4	Verapamil

525-66-6	C16H21NO2	Propranolol
54-31-9	C12H11ClN2O5S	Furosemide
54910-89-3	C17H18F3NO	Fluoxetine
564-25-0	C22H24N2O8	Doxycycline
57-27-2	C17H19NO3	Morphine
57-41-0	C15H12N2O2	Phenytoin (dilantin)
57-63-6	C20H24O2	17-alpha-ethinylestradiol
58-08-2	C8H10N4O2	caffeine
58-15-1	C13H17N3O	Aminophenazone metabolite: Dimethylaminophenazone
58-55-9	C7H8N4O2	theophylline
58-93-5	C7H8ClN3O4S2	Hydrochlorothiazide
599-79-1	C18H14N4O5S	Sulfasalazine
60166-93-0	C17H22I3N3O8	Iopamidol
604-75-1	C15H11ClN2O2	Oxazepam
60-54-8	C22H24N2O8	Tetracycline
60756-73-2	C13H12O3	Naproxen metabolite: (R)-O-Desmethyl Naproxen
60-80-0	C11H12N2O	phenazone
61869-08-7	C19H20FNO3	Paroxetine
62572-94-5	C14H23NO3	Metoprolol metabolite: O-desmethyl metoprolol
64118-84-9	C14H11Cl2NO3	Diclofenac matebolite: 4'-hydroxy diclofenac
1677687	C13H18N4O3	Pentoxifylline
657-24-9	C4H11N5	Metformin
66108-95-0	C19H26I3N3O9	Iohexol
66357-35-5	C13H22N4O3S	Ranitidine
66722-44-9	C18H31NO4	Bisoprolol
68-35-9	C10H10N4O2S	Sulfadiazine
69-53-4	C16H19N3O4S	Ampicillin
69-72-7	C7H6O3	Acetyl salycilic acid metabolite: Salicylic acid
70288-86-7	C48H74O14	Ivermectin (dihydroavermectin)
7081-44-9	C19H18ClN3O5S	Cloxacillin
723-46-6	C10H11N3O3S	Sulfamethoxazole
73334-07-3	C18H24I3N3O8	Iopromide
73590-58-6	C17H19N3O3S	Omeprazole
738-70-5	C14H18N4O3	Trimethoprim
73986-53-5	C15H23NO2	Tramadol metabolite: O-Desmethyltramadol
75377-45-6	C15H23NO2	Tramadol metabolite: N-Desmethyltramadol
75847-73-3	C20H28N2O5	Enalapril
76-57-3	C18H21NO3	Codeine
78649-41-9	C17H22I3N3O8	Iomeprol
79-57-2	C22H24N2O9	Oxytetracycline
79902-63-9	C25H38O5	Simvastatin
80214-83-1	C41H76N2O15	Roxithromycin
81103-11-9	C38H69NO13	Clarithromycin
82419-36-1	C18H20FN3O4	Ofloxacin

83891-03-6	C16H16F3NO	Fluoxetine metabolite: Norfluoxetine
846-50-4	C16H13ClN2O2	Temazepam
85721-33-1	C17H18FN3O3	Ciprofloxacin
859-18-7	C18H34N2O6S	Lincomycin
87-08-01	C16H18N2O5S	Penicillin V = Phenoxymethylpenicillin
88150-42-9	C20H25ClN2O5	Amlodipine
882-09-7	C10H11ClO3	Clofibrate metabolite: Clofibric acid
88546-55-8	C17H19N3O4S	Omeprazole metabolite: omeprazole sulfone
89-57-6	C7H7NO3	Sulfasalazine metabolite: Mesalazine
91683-38-4	C21H30O9	Gemfibrozil metabolite: Gemfibrozil 1-O-glucuronide
92340-57-3	C17H19N3O4S	Omeprazole metabolite: 5-hydroxyomeprazole
93106-60-6	C19H22FN3O3	Enrofloxacin
93413-57-1	C17H25NO	Venlafaxine metabolite: Dehydro venlafaxine
93413-62-8	C16H25NO2	4-[2-(Dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenol
93413-69-5	C17H28ClNO2	Venlafaxine, 1-[2-(dimethylamino)-1-(4-methoxyphenyl)ethyl]cyclohexanol
93413-77-5	C15H23NO2	Venlafaxine metabolite: D,L-N,N-didesmethyl venlafaxine
992-62-1	C36H65NO13	Erythromycine metabolite :N-demethyl erythromycin A
99-66-1	C8H16O2	Valproic acid
no CAS		Sulfachloropyridazine metabolite: N4-acetyl Sulfachloropyridazine
no CAS		MDA
no CAS		Lidocaine metabolite: Glycinexylidide
no CAS		metamphetamine
no CAS		Sulfachloropyridazine = Sulfaclozine
no CAS		Chloroamphenicol
no CAS		Primidone metabolite: Phenylethylmalonamide
no CAS		MDMA
no CAS		Iotalamic acid
no CAS		Ioxitalamic acid
no CAS		Primidone metabolite: Phenobarbital
no CAS		Sulfadiazine metabolite: Acetyl sulfadiazine
no CAS		Florfenicol
no CAS		MDEA
no CAS		Lidocaine metabolite: mono-ethylglycinexylidide
no CAS		Naproxen metabolite: desmethyl Naproxen sulfate
no CAS		Ketamine
no CAS		Aminophenazone (aminopyrine)
no CAS		Ibuprofen metabolite: Ibuprofen sulfate
no CAS		Ibuprofen metaboliet: hydroxy ibuprofen
no CAS		Diclofenac metabolite: 3-hydroxy diclofenac
no CAS		Diclofenac metabolite: 5'-hydroxy diclofenac
no CAS		Diclofenac metabolite: 4'-5-dihydroxy diclofenac

no CAS	Sulfaquinoxalin
no CAS	Sulfaquinoxalin metabolite: N4-acetyl Sulfaquinoxalin
no CAS	Paracetamol metabolite: 4-Acetamidophenyl-ß-D-Glucuronide
no CAS	Trimethoprim metabolite: Pyrimidine iminoquinone methide
no CAS	Trimethoprim metabolite: hydroxy trimethoprim
no CAS	Trimethoprim metabolite: dihydroxy trimethoprim
no CAS	Methylfenidaat (=ritalin)
no CAS	Atenolol metabolite: Hydroxy atenolol
no CAS	Flurazepam metabolite: Desalkyl flurazepam
no CAS	Nordazepam(desmethyldiazepam)
no CAS	Carbamazepine matebolite: 10,11-trans diol Carbamazepine (20%)
no CAS	Diclofenac metabolite: 3'-hydroxy 4'-methoxy diclofenac
no CAS	Carbamazepine matebolite: 10,11-Dihydro-10-hydroxy carbamazepine
no CAS	Mitomycin
no CAS	Gemfibrozil metabolite: Carboxy gemfibrozil
no CAS	Metoprolol metabolite: Alpha-hydroxy metoprolol (10%)
no CAS	Pantoprazol
no CAS	Clopidogrel
no CAS	Clopidogrel metabolite 92-{1-[1-(2-chlorophenyl)-2-methoxy-2-oxoethyl]-4-sulfanyl-3-piperidinylidene}acetic acid.)
no CAS	Penicillin G = Benzylpenicillin
no CAS	Colistin
no CAS	benzoylecgonine
no CAS	Penicilloic acid (amoxicilloic acid?)
no CAS	Oseltamivir (Tamiflu)
no CAS	Fenofibric acid
no CAS	Perindopril metabolite: Perindoprilate
no CAS	Enalaprilat
no CAS	Naproxen metabolite: Demethyl Naproxen Acyl-ß-D-glucuronide
no CAS	Morphine metabolite: 6-monoacetylmorphine
no CAS	Ibuprofen metabolite: Ibuprofen Acyl-ß-D-glucuronide
no CAS	Perindopril
no CAS	Citaprolam
no CAS	Methotrexate
no CAS	Desacetyl diltiazem
no CAS	Oxazepam metabolite: Oxazepam glucuronide
no CAS	Carbamazepine metabolite: 10,11-Dihydro-10-hydroxy Carbamazepine O-ß-D-Glucuronide
no CAS	Flurazepam
no CAS	17-alpha-Ethinylestradiol-3-methylether = mestranol

no CAS	Gestodene
no CAS	Prednisone
no CAS	Triamcinolone
no CAS	Methadone
no CAS	THC metabolite: 9-COOH-delta-9-THC
no CAS	Cortisone
no CAS	THC (delta-9-Tetrahydrocannabinol)
no CAS	Cortisol
no CAS	Cortisol sulfate
no CAS	Metoprolol metabolite: Metoprolol-glucuronide
no CAS	Oxytetracycline metabolite: Beta-apo oxytetracycline
no CAS	Loratidine
no CAS	Metamizole metabolite: N-acetyl-4-aminoantypyrine
no CAS	Oxytetracycline metabolite: 4-epi-oxytetracycline
no CAS	Flumethasone
no CAS	Prednisolone metabolite: 6-alpha methyl prednisolone
no CAS	Neomycin
no CAS	Valsartan metabolite: 4-hydroxy valsartan
no CAS	Triamcinolone acetonide
no CAS	Simvastatin metabolite: Simvastatin beta hydroxy acid
no CAS	Acarbose
no CAS	Verapamil metabolite: Norverapamil
no CAS	Cortisol glucuronide
no CAS	Telmisartan
no CAS	Clarythromycin metabolite: 14-hydroxy clarithromycin
no CAS	Digoxin
no CAS	Tylosin / Tilmicosin
no CAS	Timilcosin
no CAS	Isosorbide mononitrate metabolite: Isosorbide
no CAS	Niacin (vitamine B3, nicotinezuur)
no CAS	Sulfasalazine metabolite: Mesalazine
no CAS	Amfetamine
no CAS	N Acetyl mesalazine

Chemicals in EU water quality regulation

Drinking water Directive		
1024-57-3	C10H5Cl7O	heptachloroepoxide
106-89-8	C3H5ClO	1-chloro-2,3-epoxypropane
111-96-6	C6H14O3	bis(2-methoxyethyl) ether
1634-04-4	C5H12O	tert-butyl methyl ether
191-24-2	C22H12	benzo[g,h,i]peryleen

193-39-5	C22H12	indeno[1,2,3-cd]pyreen
205-99-2	C20H12	benz[e]acephenanthrylene
207-08-9	C20H12	benzo[k]fluoranthene
309-00-2	C12H8Cl6	aldrin
50-32-8	C20H12	benzo[a]pyrene; benzo[def]chrysene
60-57-1	C12H8Cl6O	dieldrin
637-92-3	C6H14O	2-ethoxy-2-methylpropane
71-43-2	C6H6	benzene
76-44-8	C10H5Cl7	heptachlor
79-06-1	C3H5NO	acrylamide

Priority substances directive

104-40-5	C15H24O	p-nonylphenol
115-29-7	C9H6Cl6O3S	Endosulfan
117-81-7	C24H38O4	bis(2-ethylhexyl) phthalate
118-74-1	C6Cl6	hexachlorobenzene
12002-48-1	C6H3Cl3	trichlorbenzenen
120-12-7	C14H10	anthracene
122-34-9	C7H12ClN5	SIMAZIN
140-66-9	C14H22O	4-(1,1,3,3-tetramethylbutyl)phenol
1582-09-8	C13H16F3N3O4	trifluralin
15972-60-8	C14H20ClNO2	alachlor
1806-26-4	C14H22O	octylphenolen
1912-24-9	C8H14ClN5	atrazine
191-24-2	C22H12	benzo[g,h,i]peryleen
193-39-5	C22H12	indeno[1,2,3-cd]pyreen
205-99-2	C20H12	benz[e]acephenanthrylene
206-44-0	C16H10	fluorantheen
207-08-9	C20H12	benzo[k]fluoranthene
25154-52-3	C15H24O	nonylphenol
2921-88-2	C9H11Cl3NO3PS	CHLORPYRIFOS
309-00-2	C12H8Cl6	aldrin
32534-81-9	C12H5Br5O	pentabroomdifenylether (congeneren 28, 47, 99, 100, 153 en 154)
330-54-1	C9H10Cl2N2O	diuron
34123-59-6	C12H18N2O	ISOPROTURON
36643-28-4	C12H27Sn	tributyltin-kation
465-73-6	C12H8Cl6	isodrin
470-90-6	C12H14Cl3O4P	CHLORFENVINFOS
50-29-3	C14H9Cl5	Clofenotane (= p,pDDT)
50-32-8	C20H12	benzo[a]pyrene; benzo[def]chrysene
60-57-1	C12H8Cl6O	dieldrin
608-73-1	C6H6Cl6	hexachloorcyclohexaan
608-93-5	C6HCl5	pentachloorbenzeen
688-73-3	C12H28Sn	tributyltinverbindingen

71-43-2	C6H6	benzene
72-20-8	C12H8Cl6O	endrin
87-68-3	C4Cl6	Hexachlorobuta1,3-diene
87-86-5	C6HCl5O	pentachlorophenol
91-20-3	C10H8	naphthalene

Attention lists

Drinking water relevant substances IAWR/RIWA

100-41-4	C8H10	ethylbenzene
100-44-7	C7H7Cl	α-chlorotoluene
100-97-0	C6H12N4	methenamine
104-40-5	C15H24O	p-nonylphenol
10605-21-7	C9H9N3O2	carbendazim (ISO); methyl benzimidazol-2-ylcarbamate
106-42-3	C8H10	p-xylene
1066-51-9	CH6NO3P	Amino Methyl Phosphoric Acid (AMPA)
1071-83-6	C3H8NO5P	GLYPHOSATE
108-20-3	C6H14O	diisopropyl ether
108-38-3	C8H10	m-xylene
108-88-3	C7H8	toluene
110488-70-5	C21H22ClNO4	DIMETHOMORF
111-96-6	C6H14O3	bis(2-methoxyethyl) ether
111991-09-4	C15H18N6O6S	NICOSULFURON
112-49-2	C8H18O4	1,2-bis(2-methoxyethoxy)ethane
115-96-8	C6H12Cl3O4P	tris(2-chloroethyl) phosphate
117-81-7	C24H38O4	bis(2-ethylhexyl) phthalate
117-96-4	C11H9I3N2O4	3,5-diacetamido-2,4,6-triiodobenzoic acid
126-73-8	C12H27O4P	tributyl phosphate
134523-00-5	C33H35FN2O5	Atorvastatin
13674-84-5	C9H18Cl3O4P	tris(2-chloro-1-methylethyl) phosphate
137-58-6	C14H22N2O	Lidocaine
139-13-9	C6H9NO6	nitrilotriacetic acid
143-24-8	C10H22O5	bis(2-(2-methoxyethoxy)ethyl) ether
150-68-5	C9H11ClN2O	Monuron
15307-86-5	C14H11Cl2NO2	Diclofenac
15545-48-9	C10H13ClN2O	chloortoluron/3-(3-chloor-p-tolyl)-1,1- dimethylurea
161326-34-7	C17H17N3OS	FENAMIDONE
1634-04-4	C5H12O	tert-butyl methyl ether
1698-60-8	C10H8ClN3O	CHLORIDAZON
2008-58-4	C7H5Cl2NO	2,6-dichloorbenzamide
205-99-2	C20H12	benz[e]acephenanthrylene
206-44-0	C16H10	fluorantheen
2276-90-6	C11H9I3N2O4	Jotalaminezuur
23135-22-0	C7H13N3O3S	OXAMYL

24579-73-5	C9H20N2O2	Propamocarb
25057-89-0	C10H12N2O3S	BENTAZONE
25812-30-0	C15H22O3	Gemfibrozil
2593-15-9	C5H5Cl3N2OS	ETRIDIAZOLE
28179-44-4	C12H11I3N2O5	Ioxitalamic acid
298-46-4	C15H12N2O	Carbamazepine
304-55-2	C4H6O4S2	2,3-bis-sulfanylbutanedioic acid (DMSA)
330-54-1	C9H10Cl2N2O	diuron
34123-59-6	C12H18N2O	ISOPROTURON
34681-24-8	C7H14N2O3S	butocarboxinsulfoxide
37350-58-6	C15H25NO3	Metoprolol
39184-27-5	C9H18N2O3S	thiofanoxsulfoxide
3930-20-9	C12H20N2O3S	Sotalol
50-32-8	C20H12	benzo[a]pyrene; benzo[def]chrysene
50-78-2	C9H8O4	Acetyl salicylic acid
51218-45-2	C15H22ClNO2	METOLACHLOOR
51-28-5	C6H4N2O5	2,4-dinitrophenol
525-66-6	C16H21NO2	Propranolol
53-16-7	C18H22O2	estrone
55297-95-5	C28H47NO4S	Tiamulin
57018-04-9	C9H11Cl2O3PS	TOLCLOFOS_METHYL
576-24-9	C6H4Cl2O	2,3-dichlorophenol
57837-19-1	C15H21NO4	METALAXYL
58-08-2	C8H10N4O2	caffeine
58-55-9	C7H8N4O2	theophylline
58-93-5	C7H8ClN3O4S2	Hydrochlorothiazide
59017-64-0	C24H21I6N5O8	joxaglinezuur
5915-41-3	C9H16ClN5	terbuthylazine
60-00-4	C10H16N2O8	edetic acid
60166-93-0	C17H22I3N3O8	Iopamidol
60-80-0	C11H12N2O	phenazone
615-22-5	C8H7NS2	2-(Methylthio)benzothiazol
634-91-3	C6H4Cl3N	3,4,5-trichlooraniline
657-24-9	C4H11N5	Metformin
66108-95-0	C19H26I3N3O9	Iohexol
69-72-7	C7H6O3	Acetyl salycilic acid metabolite: Salicylic acid
7085-19-0	C10H11ClO3	mecoprop (MCPP)
723-46-6	C10H11N3O3S	Sulfamethoxazole
73334-07-3	C18H24I3N3O8	Iopromide
78649-41-9	C17H22I3N3O8	Iomeprol
80-05-7	C15H16O2	4,4'-isopropylidenediphenol
84-69-5	C16H22O4	diisobutyl phthalate
84-74-2	C16H22O4	dibutyl phthalate
91-20-3	C10H8	naphthalene

94-74-6	C9H9ClO3	MCPA
94-75-7	C8H6Cl2O3	2_4_D

Ecosystem relevant substances NORMAN

100-42-5	C8H8	styrene
100-61-8	C7H9N	N-methylaniline
1007-28-9	C5H8ClN5	6-Deisopropylatrazine / 1,3,5-Triazine-2,4-diamine, 6-chloro-N-ethyl-
100-75-4	C5H10N2O	N-nitrosonornicotine
100-86-7	C10H14O	2-Methyl-1-phenylpropan-2-ol
101043-37-2	C49H74N10O12	Microcystin-LR
101064-48-6	C52H72N10O13	Microcystin-YR
101-20-2	C13H9Cl3N2O	triclocarban
101-21-3	C10H12ClNO2	CHLOORPROFAM
101312-92-9	C31H52N2O5S	Valnemulin
1014-60-4	C14H22	1,3-Bis(1,1-dimethylethyl)-benzene
1014-69-3	C8H15N5S	DESMETRYN
101-48-4	C10H14O2	Viridine
101-83-7	C12H23N	dicyclohexylamine
101-86-0	C15H20O	Hexylcinnamaldehyde
10206-21-0	C13H13N3O6S	Cefacetrile
102280-35-3	C17H20N6	Baquiloprim
10238-21-8	C23H28ClN3O5S	Glibenclamide (Glyburide)
102-76-1	C9H14O6	triacetin
102767-28-2	C8H14N2O2	Levetiracetam
1031-07-8	C9H6Cl6O4S	Endosulfan-sulfate
103577-45-3	C16H14F3N3O2S	Lansoprazole
103-69-5	C8H11N	N-ethylaniline
103-71-9	C7H5NO	phenyl isocyanate
103-90-2	C8H9NO2	Paracetamol (Acetaminophen)
10396-80-2	C15H24O2	2,6-Di-tert-butyl-4-hydroxy-4-methyl-2,5-cyclohexadien-1-one
104-35-8	C17H28O2	4-Nonylphenol mono-ethoxylate (NPE1O group)
104-92-7	C7H7BrO	4-bromoanisole
10543-57-4	C10H16N2O4	N,N'-ethylenebis[N-acetylacetamide]
105-95-3	C15H26O4	1,4-dioxacycloheptadecane-5,17-dione
10595-95-6	C3H8N2O	N-nitrosomethylethylamine (NMEA)
106-02-5	C15H28O2	pentadecan-15-olide
10605-21-7	C9H9N3O2	carbendazim (ISO); methyl benzimidazol-2-ylcarbamate
106-41-2	C6H5BrO	4-Bromophenol
106-44-5	C7H8O	p-cresol
106-46-7	C6H4Cl2	1,4-dichlorobenzene
106-47-8	C6H6ClN	4-chloroaniline
106-48-9	C6H5ClO	4-chlorophenol
1066-51-9	CH6NO3P	Amino Methyl Phosphoric Acid (AMPA)

106807-78-7	C19H30O4	2-(2-(4-Nonylphenoxy)ethoxy)acetic acid (NPE2C)
1071-83-6	C3H8NO5P	GLYPHOSATE
107-46-0	C6H18OSi2	hexamethyldisiloxane
107-51-7	C8H24O2Si3	octamethyltrisiloxane
108050-54-0	C46H80N2O13	Tilmicosin
108-18-9	C6H15N	diisopropylamine
108427-53-8	C6F13O3S	Perfluorohexane sulfonate (PFHxS) (anion)
108-42-9	C6H6ClN	3-chloroaniline
1085-98-9	C9H11Cl2FN2O2S2	Dichlofluanide
108-62-3	C8H16O4	METALDEHYDE
1087-02-1	C18H26	p-Dicyclohexylbenzene
1088-11-5	C15H11ClN2O	Nordiazepam
108-88-3	C7H8	toluene
1113-02-6	C5H12NO4PS	OMETHOAAT
111755-37-4	C49H75N13O12	Microcystin-RR
111-87-5	C8H18O	octan-1-ol
112-30-1	C10H22O	decan-1-ol
112398-08-0	C19H22FN3O3	Danofloxacin
1125-21-9	C9H12O2	2,6,6-trimethylcyclohex-2-ene-1,4-dione
1134-47-0	C10H12ClNO2	Baclofen
1135-99-5	C12H10Cl2Sn	Diphenyltin compounds - Diphenyltin ion
114-07-8	C37H67NO13	Erythromycin A / Erythromycin h2o
115-38-8	C13H14N2O3	Methylphenobarbital
115550-35-1	C17H21FN4O4	Marbofloxacin
115-86-6	C18H15O4P	triphenyl phosphate
115-96-8	C6H12Cl3O4P	tris(2-chloroethyl) phosphate
116-06-3	C7H14N2O2S	ALDICARB
116-16-5	C3Cl6O	hexachloroacetone
1163-19-5	C12Br10O	bis(pentabromophenyl) ether
117-84-0	C24H38O4	Di-n-octylphthalate (DOP)
117-96-4	C11H9I3N2O4	3,5-diacetamido-2,4,6-triiodobenzoic acid
118-12-7	C12H15N	1,3,3-Trimethyl-2-oxoindol
1184-89-0	CBr2ClNO2	Dibromochloronitromethane
118-56-9	C16H22O3	homosalate
118-58-1	C14H12O3	benzyl salicylate
118-79-6	C6H3Br3O	2,4,6-tribromophenol
119141-88-7	C17H19N3O3S	Omeprazole metabolite: Esomeprazole
119-36-8	C8H8O3	methyl salicylate
1194-65-6	C7H3Cl2N	DICHLOBENIL
119-61-9	C13H10O	benzophenone
119-65-3	C9H7N	isoquinoline
120-18-3	C10H8O3S	Naphthalene sulphonic acid
120-32-1	C13H11ClO	o-Benzyl-p-chlorophenol (Chlorophene)
120-47-8	C9H10O3	ethyl 4-hydroxybenzoate

120-83-2	C6H4Cl2O	2,4-dichlorophenol
121-75-5	C10H19O6PS2	MALATHION
122-11-2	C12H14N4O4S	Sulfadimethoxin
1222-05-5	C18H26O	1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyran
122-39-4	C12H11N	diphenylamine
124495-18-7	C15H8Cl2FNO	QUINOXYFEN
124-76-5	C10H18O	Isoborneol
125-12-2	C12H20O2	exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl acetate
125-28-0	C18H23NO3	Dihydrocodeine
125-29-1	C18H21NO3	Hydrocodone
125-33-7	C12H14N2O2	Primidone
126-71-6	C12H27O4P	triisobutyl phosphate
126-73-8	C12H27O4P	tributyl phosphate
126-86-3	C14H26O2	2,4,7,9-tetramethyldec-5-yne-4,7-diol
127-51-5	C14H22O	g-Methylionone
127-79-7	C11H12N4O2S	Sulfamerazine
128196-01-0	C20H21FN2O	Escitalopram
128-37-0	C15H24O	2,6-di-tert-butyl-p-cresol, BHT
128-39-2	C14H22O	2,6-di-tert-butylphenol
131-11-3	C10H10O4	dimethyl phthalate
131-56-6	C13H10O3	2,4-Dihydroxybenzophenone
131-57-7	C14H12O3	oxybenzone
13171-00-1	C17H24O	celestolide (ABDI)
13194-48-4	C8H19O2PS2	ETHOPROFOS
1330-20-7	C8H10	xylene
133-53-9	C8H8Cl2O	Dichlorodimethylphenol (2,4-Dichloro-meta-xylenol)
13392-18-2	C17H21NO4	Fenoterol
134-62-3	C12H17NO	N,N-Diethyltoluamide (DEET)
13463-41-7	C10H8N2O2S2Zn	pyrithione zinc
13523-86-9	C14H20N2O2	Pindolol
135531-25-8	CHBrClNO2	Bromochloronitromethane
13674-84-5	C9H18Cl3O4P	tris(2-chloro-1-methylethyl) phosphate
13674-87-8	C9H15Cl6O4P	tris[2-chloro-1-(chloromethyl)ethyl] phosphate
13684-56-5	C16H16N2O4	DESMEDIFAM
13684-63-4	C16H16N2O4	FENMEDIFAM
136-85-6	C7H7N3	5-Methyl-1H-benzotriazole (5-Tolyltriazole)
13710-19-5	C14H12ClNO2	Tolfenamic acid
137-58-6	C14H22N2O	Lidocaine
138261-41-3	C9H10ClN5O2	IMIDACLOPRID
139-13-9	C6H9NO6	nitrilotriacetic acid
139-40-2	C9H16ClN5	propazine
140-11-4	C9H10O2	benzyl acetate
1401-69-0	C46H77NO17	Tylosin

14035-33-7	C16H24O2	3,5-Di-tert-butyl-4-hydroxyacetophenone
1403-66-3	C19H38N4O6	Gentamicin
1404-04-2	C23H46N6O13	Neomycin B
141-62-8	C10H30O3Si4	decamethyltetrasiloxane
141-63-9	C12H36O4Si5	dodecamethylpentasiloxane
1420-07-1	C10H12N2O5	dinoterb (ISO); 2-tert-butyl-4,6-dinitrophenol
142459-58-3	C14H13F4N3O2S	flufenacet
144-83-2	C11H11N3O2S	Sulfapyridine
1461-25-2	C16H36Sn	tetrabutyltin
14698-29-4	C13H11NO5	Oxolinic acid
14816-18-3	C12H15N2O3PS	phoxim (ISO); α-(diethoxyfosfinothioylimino) fenylacetonitril
148-79-8	C10H7N3S	THIABENDAZOLE
149-30-4	C7H5NS2	benzothiazole-2-thiol
151-05-3	C12H16O2	1,1-Dimethyl-2-phenethylacetate
15234-85-2	C16H24O3	4-Octylphenoxy acetic acid (OPE1C)
15307-86-5	C14H11Cl2NO2	Diclofenac
15323-35-0	C17H24O	AHDI (Phantolide) 6-Acetyl-1,1,2,3,3,5-hexamethyldihydroindene
15545-48-9	C10H13ClN2O	chloortoluron/3-(3-chloor-p-tolyl)-1,1- dimethylurea
15686-71-2	C16H17N3O4S	Cefalexin
15687-27-1	C13H18O2	ibuprofen
1610-18-0	C10H19N5O	Prometon
1634-04-4	C5H12O	tert-butyl methyl ether
1634-36-2	C11H14O2	(1-Hydroxy-iso-propyl)acetophenone
1646-88-4	C7H14N2O4S	Aldicarb sulfone
16484-77-8	C10H11ClO3	(R)-2-(4-chloro-2-methylphenoxy)propionic acid
1668-19-5	C19H21NO	Doxepine
16752-77-5	C5H10N2O2S	METHOMYL
1678-25-7	C12H11NO2S	N-phenylbenzenesulphonamide
16846-24-5	C42H69NO15	Josamycin
1689-99-2	C15H17Br2NO2	bromoxyniloctanoaat/2,6-dibroom-4-cyano- fenyloctanoaat
1691-99-2	C12H10F17NO3S	2-(N-ethylperfluorooctanesulfonamido)-ethyl alcohol (N-Et-FOSE)
1695-77-8	C14H24N2O7	Spectinomycin
1696-20-4	C6H11NO2	4-acetylmorpholine
1698-60-8	C10H8ClN3O	CHLORIDAZON
16995-35-0	C3H2Cl4O	1,1,1,3-Tetrachloropropanone
1702-17-6	C6H3Cl2NO2	CLOPYRALID
17117-34-9	C17H9NO3	3-Nitrobenzanthrone
17164-77-1	C18H12S	2-(2-Naphthalenyl)benzothiophene
1763-23-1	C8HF17O3S	perfluorooctane sulfonic acid; heptadecafluorooctane-1-sulfonic acid
1768-31-6	C3HCl5O	1,1,1,3,3-Pentachloropropanone
1812-30-2	C14H10BrN3O	Bromazepam

18181-70-9	C8H8Cl2IO3PS	Iodofenphos
18339-16-7	C19H28O	Androstenone
18559-94-9	C13H21NO3	salbutamol
1861-32-1	C10H6Cl4O4	Chlorthal-dimethyl
1893-33-0	C21H30FN3O2	Pipamperon
1897-45-6	C8Cl4N2	CHLOORTHALONIL
1918-00-9	C8H6Cl2O3	DICAMBA
1918-16-7	C11H14ClNO	PROPACHLOOR
1929-29-9	C10H12O3	3-(Bromo-4-methoxyphenyl)propionic acid
1948-33-0	C10H14O2	2-tert-butylhydroquinone
19666-30-9	C15H18Cl2N2O3	Oxadiazon
1982-47-4	C15H15ClN2O2	Chloroxuron
1984-65-2	C7H6Cl2O	2,6-Dichloroanisole
19937-59-8	C10H13ClN2O2	METOXURON
2032-65-7	C11H15NO2S	METHIOCARB
20427-84-3	C19H32O3	4-Nonylphenol di-ethoxylate / 2-(2-(4-Nonylphenoxy)ethoxy)ethanol (NPE2O group)
2043-47-2	C6H5F9O	4:2 FTOH
2058-94-8	C11HF21O2	Perfluoro-n-undecanoic acid (PFUnA)
207122-16-5	C12H3Br7O	2,2',3,4,4',5',6-Heptabromodiphenyl ether (BDE-183)
2078-54-8	C12H18O	Di-iso-propylphenol
2082-79-3	C35H62O3	octadecyl 3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate
20830-81-3	C27H29NO10	Daunorubicine
21593-23-7	C17H17N3O6S2	Cefapirin
21702-84-1	C7H6Br2O	2,4-Dibromoanisole
21725-46-2	C9H13ClN6	Cyanazine
21850-44-2	C21H20Br8O2	1,1'-(isopropylidene)bis[3,5-dibromo-4-(2,3-dibromopropoxy)benzene]
22071-15-4	C16H14O3	Ketoprofen
2212-67-1	C9H17NOS	molinaat
22131-79-9	C11H11ClO3	Alclofenac
22204-53-1	C14H14O3	Naproxen
23031-25-6	C12H19NO3	Terbutaline
2303-17-5	C10H16Cl3NOS	TRI_ALLAAT
2315-61-9	C18H30O3	2-[2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethoxy]ethanol / 4-Octylphenol di-ethoxylate (OPE2O)
2315-67-5	C16H26O2	2-[4-(1,1,3,3-tetramethylbutyl)phenoxy]ethanol / 4-Octylphenol mono-ethoxylate (OPE1O)
23560-59-0	C9H12ClO4P	HEPTENOFOS
23593-75-1	C22H17ClN2	Clotrimazole
23726-91-2	C13H20O	Damascone
23950-58-5	C12H11Cl2NO	PROPYZAMIDE
2440-22-4	C13H11N3O	2-(2H-benzotriazol-2-yl)-p-cresol
2444-37-3	C3H6O2S	2-Methylthioacetic acid

24448-09-7	C11H8F17NO3S	2-(N-methylperfluorooctanesulfonamido)-ethyl alcohol (N-Me-FOSE)
2447-57-6	C12H14N4O4S	Sulfadoxin
24851-98-7	C13H22O3	methyl 3-oxo-2-pentylcyclopentaneacetate
25013-16-5	C11H16O2	tert-butyl-4-methoxyphenol
25057-89-0	C10H12N2O3S	BENTAZONE
25167-93-5	C6H4ClNO2	Chloronitrobenzene (2 isomers)
25268-77-3	C14H10F17NO4S	N-methylperfluorooctanesulfonamidoethyl acrylate (N-MeFOSEA)
25451-15-4	C11H14N2O4	Taloxa
256-96-2	C14H11N	5H-dibenz[b,f]azepine
25812-30-0	C15H22O3	Gemfibrozil
2591-86-8	C6H11NO	Formylpiperidine
25953-19-9	C14H14N8O4S3	Cefazoline
26225-79-6	C13H18O5S	ETHOFUMESAAT
26259-45-0	C10H19N5O	Secbumeton
268728	C11H15NO3S	Methiocarb sulfoxide
2642-71-9	C12H16N3O3PS2	Azinphos-ethyl
2642-80-0	C14H11Cl3	4,4'-DDMS
26761-40-0	C28H46O4	Diisodecyl phthalate (DIDP)
26787-78-0	C16H19N3O5S	Amoxicillin
26839-75-8	C13H24N4O3S	Timolol
26914-52-3	C18H26N2O4S2	N-Ethyltoluenesulfonamide
2719-62-2	C18H30	6-Phenyldodecane
27203-92-5	C16H25NO2	Tramadol
28159-98-0	C11H19N5S	Irgarol
28179-44-4	C12H11I3N2O5	Ioxitalamic acid
28553-12-0	C26H42O4	di-''isononyl'' phthalate
364854	C16H15ClN2	Medazepam
28981-97-7	C17H13ClN4	Alprazolam
29122-68-7	C14H22N2O3	Atenolol
29232-93-7	C11H20N3O3PS	PIRIMIFOS_METHYL
29385-43-1	C7H7N3	methyl-1H-benzotriazole
298-00-0	C8H10NO5PS	Parathion methyl
298-46-4	C15H12N2O	Carbamazepine
29878-31-7	C7H7N3	4-Methyl-1H-benzotriazole
30125-63-4	C7H12ClN5	Desethylterbutylazin
307-24-4	C6HF11O2	Perfluorohexanoic acid (PFHxA)
307-35-7	C8F18O2S	heptadecafluorooctanesulphonyl fluoride
307-55-1	C12HF23O2	Perfluorododecanoic acid (PFDoA)
3112-85-4	C7H8O2S	Methylphenylsulfone
3115-49-9	C17H26O3	(4-nonylphenoxy)acetic acid
3116-76-5	C19H17Cl2N3O5S	Dicloxacillin
314-40-9	C9H13BrN2O2	Bromacil
3149-12-0	C9H18O3	2,6-Diethoxytetrahydropyran

31506-32-8	C9H4F17NO2S	N-methylperfluorooctanesulfonamide (N-MeFOSA)
3173-53-3	C7H11NO	Cyclohexylisocyanate
31879-05-7	C15H14O3	Fenoprofen
32388-55-9	C17H26O	[3R-(3α,3aβ,7β,8aα)]-1-(2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl)ethan-1-one
330-55-2	C9H10Cl2N2O2	linuron (ISO); 3-(3,4-dichlorophenyl)-1-methoxy-1-methylurea
333-41-5	C12H21N2O3PS	DIAZINON
335-67-1	C8HF15O2	PFOA, C8
335-76-2	C10HF19O2	Perfluorodecanoic acid (PFDA)
3380-34-5	C12H7Cl3O2	triclosan
34622-58-7	C12H16ClNOS	Orbencarb
34970-00-8	CHBrClI	Bromochloroiodomethane
35507-37-0	CH2N2O3S	Sulfonyl urea
35763-26-9	C13H21NO3	Salbutamol
3622-84-2	C10H15NO2S	N-butylbenzenesulphonamide
630203	C25H35NO5	Mebeverine
36576-43-9	C9H14ClN5O2	Cyanazine acid
36861-47-9	C18H22O	4-Methylbenzylidene camphor
37148-27-9	C12H18Cl2N2O	Clenbuterol
37172-53-5	C13H22O3	Dihydromethyljasmonate
37321-09-8	C21H41N5O11	Apramycin
37350-58-6	C15H25NO3	Metoprolol
37517-30-9	C18H28N2O4	Acebutolol
375-85-9	C7HF13O2	Perfluoroheptanoic acid (PFHpA)
375-95-1	C9HF17O2	Perfluorononanoic acid (PFNA)
376-06-7	C14HF27O2	Perfluorotetradecanoic acid (PFTDA)
3778-73-2	C7H15Cl2N2O2P	ifosfamide
378-44-9	C22H29FO5	betamethasone
38640-62-9	C16H20	bis(isopropyl)naphthalene
3910-35-8	C18H20	1-Phenyl-1,3,3-trimethylindane
3922-90-5	C35H61NO12	Oleandomycin
39239-77-5	C14H5F25O	12:2 FTOH
3930-20-9	C12H20N2O3S	Sotalol
3964-56-5	C6H4BrClO	4-Bromo-2-chlorophenol
40487-42-1	C13H19N3O4	PENDIMETHALIN
4128-37-4	C7H16N2O	N,N'-Di-iso-propylurea
41318-75-6	C12H7Br3O	2,4,4'-tribromodiphenylether (BDE-28)
41394-05-2	C10H10N4O	METAMITRON
4151-50-2	C10H6F17NO2S	N-ethylperfluorooctanesulfonamide (N-EtFOSA)
4184-79-6	C8H9N3	5,6-Dimethyl-1H-benzotriazole
41859-67-0	C19H20ClNO4	Bezafibrate
42017-89-0	C17H15ClO4	Fenofibric acid (metabolite of FENOFIBRATE)
42200-33-9	C17H27NO4	Nadolol
42397-64-8	C16H8N2O4	1,6-dinitropyreen

42397-65-9	C16H8N2O4	1,8-dinitropyreen
857259	C11H14O3	Isobutyl-paraben
4253-89-8	C6H14S2	Di-iso-propyldisulfide
42576-02-3	C14H9Cl2NO5	BIFENOX
4273-98-7	C12H11NO2S	Aminodiphenylsulfone
42835-25-6	C14H12FNO3	Flumequine
43121-43-3	C14H16ClN3O2	Triadimefon
434-22-0	C18H26O2	nandrolone
439-14-5	C16H13ClN2O	Diazepam
4394-85-8	C5H9NO2	N-Formylmorpholine
445-03-4	C7H5ClF3N	4-chloro-α,α,α-trifluoro-o-toluidine
4455-13-4	C5H10O2S	2-Ethylthioacetic acid ethylester
4471-47-0	C2HNO	Cyanoformaldehyde
458-24-2	C12H16F3N	Fenfluramine
1000766	C13H9Cl3O2	Methyl triclosan
4773-83-5	C12H14	1,2,3-Trimethyl-1H-indene
479-92-5	C14H18N2O	Propyphenazone
481-97-0	C18H22O5S	Estrone sulphate
4824-78-6	C10H12BrCl2O3PS	Bromofos-ethyl
483-63-6	C13H17NO	Crotamiton
486-56-6	C10H12N2O	Cotinine
49562-28-9	C20H21ClO4	fenofibrate
50-02-2	C22H29FO5	Dexamethasone
50-06-6	C12H12N2O3	Phenobarbital
50-18-0	C7H15Cl2N2O2P	Cyclophosphamide
5022-29-7	C10H9NO2	N-Ethylphthalimide
50-24-8	C21H28O5	prednisolone
50-27-1	C18H24O3	Estriol
50-28-2	C18H24O2	estradiol
50-33-9	C19H20N2O2	Phenylbutazone
50-36-2	C21H30O5	Cocaine
50-48-6	C20H23N	Amitryptiline
50-49-7	C19H24N2	Imapramine
50-78-2	C9H8O4	Acetyl salicylic acid
51146-55-5	C13H18O3	2-Hydroxy Ibuprofen
51-21-8	C4H3FN2O2	5-Fluorouracil
51218-45-2	C15H22ClNO2	METOLACHLOOR
51235-04-2	C12H20N4O2	Hexazinone
51-28-5	C6H4N2O5	2,4-dinitrophenol
51805-45-9	C9H15O6P	TCEP
52315-07-8	C22H19Cl2NO3	cypermethrin
5234-68-4	C12H13NO2S	Carboxin
52-43-7	C10H12N2O3	Allobarbital
5250-39-5	C19H17ClFN3O5S	Flucloxacillin

52-53-9	C27H38N2O4	Verapamil
525-66-6	C16H21NO2	Propranolol
52645-53-1	C21H20Cl2O3	PERMETHRIN
52-68-6	C4H8Cl3O4P	TRICHLOORFON
5278-95-5	C2HBr2ClO2	Dibromochloroacetic acid
52918-63-5	C22H19Br2NO3	DELTAMETHRIN
529-19-1	C8H7N	Methylbenzonitrile
529-34-0	C10H10O	Tetralinone
530-48-3	C14H12	1,1-diphenylethylene
53164-05-9	C21H18ClNO6	Acemetacin
53-16-7	C18H22O2	estrone
53-19-0	C14H10Cl4	Dichlorodiphenyldichloroethane - o,p' (o,p'-DDD / Mitotane)
534-07-6	C3H4Cl2O	1,3-Dichloroketone
1263471	C11H12O	4-iso-Propenylacetophenone
53-86-1	C19H16ClNO4	indometacin
53949-53-4	C13H18O3	1-Hydroxy Ibuprofen
540-97-6	C12H36O6Si6	dodecamethylcyclohexasiloxane
541-02-6	C10H30O5Si5	decamethylcyclopentasiloxane
542-75-6	C3H4Cl2	1,3-Dichloropropene
54-31-9	C12H11ClN2O5S	Furosemide
54460-96-7	C6H12Cl2O	Bis(chloropropyl)ethers
54464-57-2	C16H26O	OTNE
5466-77-3	C18H26O3	2-ethylhexyl 4-methoxycinnamate
54739-18-3	C15H21F3N2O2	Fluvoxamine
54910-89-3	C17H18F3NO	Fluoxetine
55-18-5	C4H10N2O	4-nitropyreen
55297-95-5	C28H47NO4S	Tiamulin
553-82-2	C7H6Cl2O	2,4-Dichloroanisole
55-38-9	C10H15O3PS2	Fenthion
556-67-2	C8H24O4Si4	octamethylcyclotetrasiloxane
5575-21-3	C20H18N4O5S2	Cefalonium
5589-96-8	C2H2BrClO2	Bromochloroacetic acid
5598-13-0	C7H7Cl3NO3PS	Chlorpyriphos methyl
56038-13-2	C12H19Cl3O8	sucralose
561-27-3	C21H23NO5	Heroin
56-29-1	C12H16N2O3	Hexobarbital
563-12-2	C9H22O4P2S4	Echio (Ethion)
56-38-2	C10H14NO5PS	PARATHION
56420-45-2	C27H29NO11	Epirubicin
564-25-0	C22H24N2O8	Doxycycline
56-53-1	C18H20O2	diethylstilboestrol
56-55-3	C18H12	benz[a]anthracene
56-75-7	C11H12Cl2N2O5	Chloramphenicol
57018-04-9	C9H11Cl2O3PS	TOLCLOFOS_METHYL

57-15-8	C4H7Cl3O	Chlorobutanol
57-27-2	C17H19NO3	Morphine
57-41-0	C15H12N2O2	Phenytoin (dilantin)
57-43-2	C11H18N2O3	Amobarbital
57-53-4	C9H18N2O4	Meprobamate
57-62-5	C22H23ClN2O8	Chlortetracycline
57-63-6	C20H24O2	17-alpha-ethinylestradiol
57-68-1	C12H14N4O2S	Sulfamethazine
57775-29-8	C18H22N2O2	Carazolol
57808-66-9	C22H24ClN5O2	Domperidon
57837-19-1	C15H21NO4	METALAXYL
578-57-4	C7H7BrO	2-Bromoanisole
57-88-5	C27H46O	cholesterol
57-91-0	C18H24O2	17-alpha-Estradiol
57-92-1	C21H39N7O12	Streptomycin
58-08-2	C8H10N4O2	caffeine
58-73-1	C17H21NO	diphenhydramine
5875-23-0	C2H3I2NO	Diiodoacetamide
588-68-1	C14H12N2	Eusolex
58-90-2	C6H2Cl4O	2,3,4,6-Tetrachlorophenol
58-93-5	C7H8ClN3O4S2	Hydrochlorothiazide
5915-41-3	C9H16ClN5	terbuthylazine
59277-89-3	C8H11N5O3	Acyclovir
594-47-8	C2H2Br3NO	Tribromoacetamide
59-66-5	C4H6N4O3S2	Acetazolamide
59669-26-0	C10H18N4O4S3	THIODICARB
598-70-9	C2H3Br2NO	Dibromoacetamide
59-89-2	C4H8N2O2	N-nitrosomethylvinylamine
5989-27-5	C10H16	(R)-p-mentha-1,8-diene
60-00-4	C10H16N2O8	edetic acid
60166-93-0	C17H22I3N3O8	Iopamidol
60168-88-9	C17H12Cl2N2O	fenarimol/2,4'-dichloor-α(pyrimidyl)-benzhydrylalcohol
60207-90-1	C15H17Cl2N3O2	PROPICONAZOLE
6028-61-1	C6H14S3	Dipropyltrisulfide
604-75-1	C15H11ClN2O2	Oxazepam
60-51-5	C5H12NO3PS2	DIMETHOAAT
60-54-8	C22H24N2O8	Tetracycline
60756-73-2	C13H12O3	Naproxen metabolite: (R)-O-Desmethyl Naproxen
607-99-8	C7H5Br3O	2,4,6-Tribromoanisole
60-80-0	C11H12N2O	phenazone
608-27-5	C6H5Cl2N	2,3-dichloroaniline
61-32-5	C17H20N2O6S	Methicillin
61-33-6	C16H18N2O4S	Penicillin G
614-68-6	C8H7NO	Methylphenylisocyanate

615-22-5	C8H7NS2	2-(Methylthio)benzothiazol
615-58-7	C6H4Br2O	2,4-Dibromophenol
61-68-7	C15H15NO2	Mefenamic acid
61-70-1	C9H9NO	2,3-Dihydro-1-methyl-1H-indol
61869-08-7	C19H20FNO3	Paroxetine
6190-65-4	C6H10ClN5	Desethylatrazine
619-33-0	C6H12Cl2O2	1,1-Dichloro-2,2-diethoxyethane
62-53-3	C6H7N	aniline
62-73-7	C4H7Cl2O4P	DICHLOORVOS
62893-19-0	C25H27N9O8S2	Cefoperazone
632-21-3	C3H2Cl4O	1,1,3,3-Tetrachloropropanone
63-25-2	C12H11NO2	CARBARYL
63387-28-0	C12HBr9O	2,2',3,3',4,4',5,5',6-Nonabromodiphenylether (BDE-206)
634-67-3	C6H4Cl3N	2,3,4-Trichloroaniline
635-12-1	C14H8O2	Anthracen-1,4-dione
63659-18-7	C18H29NO3	Betaxolol
644-62-2	C14H11Cl2NO2	Meclofenamic acid
645-13-6	C11H14O	4-iso-Propylacetophenone
6452-71-7	C15H23NO3	Oxprenolol
646-01-5	C4H8O2S	3-Methylthiopropionic acid
647-42-7	C8H5F13O	3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctan-1-ol
6485-40-1	C10H14O	l-p-mentha-1(6),8-dien-2-one
1677687	C13H18N4O3	Pentoxifylline
657-24-9	C4H11N5	Metformin
658051-75-3	C12H23NO3	Bayrepel
65907-30-4	C18H26N2O5S	Furathiocarb
66108-95-0	C19H26I3N3O9	Iohexol
66357-35-5	C13H22N4O3S	Ranitidine
66722-44-9	C18H31NO4	Bisoprolol
66-79-5	C19H19N3O5S	Oxacillin
67129-08-2	C14H16ClN3O	METAZACHLOOR
67-43-6	C14H23N3O10	N-carboxymethyliminobis(ethylenenitrilo)tetra(acetic acid)
67747-09-5	C15H16Cl3N3O2	PROCHLORAZ
678-39-7	C10H5F17O	8:2 FTOH
68002-20-0	C15H30N6O6	Hexa(methoxymethyl)melamine
68140-48-7	C18H26O	ATII (Traseolide)
68-35-9	C10H10N4O2S	Sulfadiazine
6846-50-0	C16H30O4	1-isopropyl-2,2-dimethyltrimethylene diisobutyrate
686-07-7	C6H13NS2	N,N-Diethyldithiocarbamic acid methyl ester
69377-81-7	C7H5Cl2FN2O3	FLUROXYPYR
69-53-4	C16H19N3O4S	Ampicillin
70288-86-7	C48H74O14	Ivermectin (dihydroavermectin)

704-00-7	C10H10O2	2-Acetylacetophenone
70458-96-7	C16H18FN3O3	Norfloxacin
7081-44-9	C19H18ClN3O5S	Cloxacillin
7085-19-0	C10H11ClO3	mecoprop (MCPP)
709-98-8	C9H9Cl2NO	Propanil
71133-14-7	C2HBrCl2O2	Bromodichloroacetic acid
71758-44-6	C13H10ClNO	2-[(2-Chlorophenyl)amino]benzaldehyde
719-22-2	C14H20O2	2,6-Di-tert-butylquinone
7205-98-3	C7H7ClO2S	Chloromethylphenylsulfone
72-33-3	C21H26O2	Mestranol
723-46-6	C10H11N3O3S	Sulfamethoxazole
72-43-5	C16H15Cl3O2	Methoxychlor
7261-97-4	C14H10N4O5	Dantrolene
7287-19-6	C10H19N5S	PROMETRYN
7298-73-9	C11H15NO2	N-Methylphenacetine
731-27-1	C10H13Cl2FN2O2S2	TOLYLFLUANIDE
73334-07-3	C18H24I3N3O8	Iopromide
73573-88-3	C23H34O5	(1S,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxotetrahydro-2H-pyran-2-yl]ethyl}-7-methyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl(2S)-2-methylbutanoate
73590-58-6	C17H19N3O3S	Omeprazole
738-70-5	C14H18N4O3	Trimethoprim
74011-58-8	C15H19FN4O3	Enoxacin
74039-30-8	C5H2Br3NO2	2,3,5-Tribromopyrrole
74070-46-5	C12H9ClN2O3	ACLONIFEN
7425-14-1	C16H32O2	2-ethylhexyl-2-ethylhexanoaat
75321-20-9	C16H8N2O4	1,3-Dinitropyrene
75330-75-5	C24H36O5	(1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl (2S)-2-methylbutanoate
754-91-6	C8H2F17NO2S	Perfluorooctane sulfonamide (PFOSA)
75-74-1	C4H12Pb	Tetramethyllead
761-65-9	C9H19NO	N,N-dibutylformamide
76-22-2	C10H16O	bornan-2-one
76-42-6	C18H21NO4	Oxycodone
76-57-3	C18H21NO3	Codeine
76674-21-0	C16H13F2N3O	Flutriafol
76-73-3	C12H18N2O3	Secobarbital
76738-62-0	C15H20ClN3O	PACLOBUTRAZOL
76-74-4	C11H18N2O3	pentobarbital
76824-35-6	C8H15N7O2S3	Famotidine
7695-91-2	C31H52O3	3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-benzopyran-6-yl acetate
77-02-1	C10H14N2O3	Aprobarbital
77-26-9	C11H16N2O3	Butalbital
77439-76-0	C5H3Cl3O3	Mutagen X (MX)

77-66-7	C9H15BrN2O3	Acecarbromal
77-67-8	C7H11NO2	Ethosuximide
77732-09-3	C14H18N2O4	Oxadixyl
7786-34-7	C7H13O6P	MEVINFOS
77-90-7	C20H34O8	tributyl O-acetylcitrate
77-93-0	C12H20O7	triethyl citrate
78-00-2	C8H20Pb	tetraethyllead
78-40-0	C6H15O4P	triethyl phosphate
78-42-2	C24H51O4P	tris(2-ethylhexyl) phosphate
78-43-3	C9H15Cl6O4P	Tris(dichloropropyl)phosphate
78-51-3	C18H39O7P	tris(2-butoxyethyl) phosphate
78649-41-9	C17H22I3N3O8	Iomeprol
791-28-6	C18H15OP	triphenylphosphine oxide
793-23-7	C20H18	1,4-Bis(phenylmethyl) benzene
79-57-2	C22H24N2O9	Oxytetracycline
79617-96-2	C17H17Cl2N	Sertraline
79794-75-5	C22H23ClN2O2	Loratadine
79902-63-9	C25H38O5	Simvastatin
79-94-7	C15H12Br4O2	2,2',6,6'-tetrabromo-4,4'-isopropylidenediphenol
80-05-7	C15H16O2	4,4'-isopropylidenediphenol
80-08-0	C12H12N2O2S	dapsone
80135-31-5	C24H27NO2	Octocrylene
80214-83-1	C41H76N2O15	Roxithromycin
8024-53-1	C10H18O	cineole
80-54-6	C14H20O	2-(4-tert-butylbenzyl)propionaldehyde
2251180	C18H36N4O11	Kanamycin
81093-37-0	C23H36O7	Pravastatin
81103-11-9	C38H69NO13	Clarithromycin
81-14-1	C14H18N2O5	Musk ketone
81-15-2	C12H15N3O6	5-tert-butyl-2,4,6-trinitro-m-xylene (musk xylene)
82-05-3	C17H10O	7H-Benzo(de)anthracen-7-one (Benzanthrone)
82304-66-3	C17H24O3	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione
82419-36-1	C18H20FN3O4	Ofloxacin
825629-31-0	C9H13NO2S	N-Ethyl-2-tolylsulfonamide
82626-48-0	C19H21N3O	Zolpidem
83-05-6	C14H10Cl2O2	4,4’-DDA
83164-33-4	C19H11F5N2O2	DIFLUFENICAN
832-64-4	C15H12	4-Methyl-phenanthrene
834-12-8	C9H17N5S	ametryn
83463-62-1	C2HBrClN	Bromochloroacetonitrile
83-46-5	C29H50O	Beta-sitosterol
83-66-9	C12H16N2O5	Musk ambrette
83905-01-5	C38H72N2O12	Azithromycin
84057-84-1	C9H7Cl2N5	lamotrigine

84-15-1	C18H14	o-Terphenyl
84-54-8	C15H10O2	2-Methylanthraquinone
846-49-1	C15H10Cl2N2O2	Lorazepam
846-50-4	C16H13ClN2O2	Temazepam
84-65-1	C14H8O2	anthraquinone
84-66-2	C12H14O4	diethyl phthalate
84-74-2	C16H22O4	dibutyl phthalate
84852-53-9	C14H4Br10	1,1'-(ethane-1,2-diyl)bis[pentabromobenzene]
85-01-8	C14H10	Phenanthrene
85509-19-9	C16H15F2N3Si	flusilazole (ISO); bis(4-fluorophenyl)(methyl)(1H-1,2,4-triazol-1-ylmethyl)silane
85-68-7	C19H20O4	benzyl butyl phthalate
85688-81-9	C10H16N2	2,3-Diethyl-2,3-dimethylsuccinonitrile
85721-33-1	C17H18FN3O3	Ciprofloxacin
859-18-7	C18H34N2O6S	Lincomycin
85-98-3	C17H20N2O	1,3-diethyldiphenylurea
86-30-6	C12H10N2O	N-Nitrosodiphenylamine (NDPA)
865-86-1	C12H5F21O	10:2 FTOH
86-74-8	C12H9N	carbazole
867-54-9	C3H4Br2O	1,1-Dibromopropanone
87075-14-7	C20H22O3	Butyl methoxydibenzoylmethane
87-08-1	C16H18N2O5S	Penicillin V
872-50-4	C5H9NO	1-methyl-2-pyrrolidone
87-40-1	C7H5Cl3O	2,4,6-Trichloroanisole
87-56-9	C4H2Cl2O3	mucochloric acid
87674-68-8	C12H18ClNO2S	DIMETHENAMIDE
88-04-0	C8H9ClO	Chlorodimethylphenol (Chloroxylenol)
88-06-2	C6H3Cl3O	2,4,6-Trichlorophenol
882-09-7	C10H11ClO3	Clofibrate metabolite: Clofibric acid
886-50-0	C10H19N5S	TERBUTRYN
88-75-5	C6H5NO3	2-nitrophenol
89796-99-6	C16H13Cl2NO4	Aceclofenac
90-30-2	C16H13N	N-1-naphthylaniline
90717-03-6	C11H8ClNO2	QUINMERAC
90-98-2	C13H8Cl2O	DBP
91-17-8	C10H18	decahydronaphthalene
91-19-0	C8H6N2	Chinoxaline
91-22-5	C9H7N	quinoline
918-02-5	C6H15N	Bromodichloronitromethane
921-03-9	C3H3Cl3O	1,1,3-trichloroacetone
924-16-3	C8H18N2O	N-nitrosodiisopropylamine
92-52-4	C12H10	biphenyl
92-94-4	C18H14	p-Terphenyl
930-55-2	C4H8N2O	N-nitrosopiperidine
93106-60-6	C19H22FN3O3	Enrofloxacin

934-32-7	C7H7N3	2-Aminobenzimidazole
94-13-3	C10H12O3	propyl 4-hydroxybenzoate
941-57-1	C7H5NO3S2	Benzothiazol-2-sulfonic acid
947-19-3	C13H16O2	hydroxycyclohexyl phenyl ketone
94-74-6	C9H9ClO3	MCPA
94-75-7	C8H6Cl2O3	2_4_D
94-81-5	C11H13ClO3	4-(4-chloro-o-tolyloxy) butyric acid (2,4-mcpb)
95-14-7	C6H5N3	benzotriazole
95-16-9	C7H5NS	benzothiazole
95-56-7	C6H5BrO	2-Bromophenol
95-57-8	C6H5ClO	2-Chlorophenol
95-95-4	C6H3Cl3O	2,4,5-Trichlorophenol
95975-55-6	C21H28O2	4,4'-DDOH
96180-79-9	C46H67N7O12	Microcystin-LA / Cyanoginosin-LA
96-19-5	C3H3Cl3	1,2,3-Trichloropropene (TRCP)
98-10-2	C6H7NO2S	Benzenesulfonamide
98105-99-8	C20H19F2N3O3	Sarafloxacin
98106-17-3	C21H21F2N3O3	Difloxacin
98136-99-3	C2H2BrClO	Bromochloroacetaldehyde
98-52-2	C10H20O	4-tert-butylcyclohexanol
98-53-3	C10H18O	4-tert-butylcyclohexanone
98-54-4	C10H14O	4-tert-butylphenol
98-55-5	C10H18O	p-menth-1-en-8-ol
98-95-3	C6H5NO2	nitrobenzene
99-66-1	C8H16O2	Valproic acid
99-76-3	C8H8O3	methyl 4-hydroxybenzoate
no CAS	C19H16ClNO4	Indometacin

Attachment II

21 identified compounds

Of the 158 prioritized accurate masses, 21 compounds had a confirmed structure (see table below).

Plant protection products	Pharmaceuticals	Industrial compounds
chloridazon	caffeine	1,2-benzisothiazol-3(2H)-on
dimethenamide P	carbamazepine 10,11-epoxide	4-Methyl-1H-benzotriazole
metolachloor	metoprolol	benzotriazole
N,N-Diethyltoluamide (DEET)	N-acetylaminoantipyrine	tributyl phosphate
simazine	oxazepam	triethyl phosphate
terbuthylazine	phenazone	triphenylphosphine oxide
	propyphenazone	tris(2-chloro-1-methylethyl) phosphate
	tramadol	

Attachment III

1220 Chemical Descriptors

1	mode	Ionisation mode
2	peak	Peak number
3	mass_p	Mass of peak
4	mass_s	Mass of suspect
5	dev	Mass deviation
6	tR	Retention time
7	nAcid	Number of acidic groups. The list of acidic groups is defined by these SMARTS "$([O;H1]-[C,S,P]=O)", "$([*;-;!$(*~[*;+])])", "$([NH](S(=O)=O)C(F)(F)F)", and "$(n1nnnc1)" originally presented in JOELib
8	ALogP	Ghose-Crippen LogKow
9	ALogp2	Square of ALogP
10	AMR	Molar refractivity
11	apol	Sum of the atomic polarizabilities (including implicit hydrogens)
12	naAromAtom	Number of aromatic atoms
13	nAromBond	Number of aromatic bonds
14	nAtom	Number of atoms
15	nHeavyAtom	Number of heavy atoms (i.e. not hydrogen)
16	nH	Number of hydrogen atoms
17	nC	Number of carbon atoms
18	nN	Number of nitrogen atoms
19	nO	Number of oxygen atoms
20	nS	Number of sulphur atoms
21	nP	Number of phosphorus atoms
22	nF	Number of fluorine atoms
23	nCl	Number of chlorine atoms
24	nX	Number of halogen atoms (F, Cl, Br, I, At, Uus)
25	ATS0m	Broto-Moreau autocorrelation - lag 0 / weighted by mass
26	ATS1m	Broto-Moreau autocorrelation - lag 1 / weighted by mass
27	ATS2m	Broto-Moreau autocorrelation - lag 2 / weighted by mass
28	ATS3m	Broto-Moreau autocorrelation - lag 3 / weighted by mass
29	ATS4m	Broto-Moreau autocorrelation - lag 4 / weighted by mass
30	ATS5m	Broto-Moreau autocorrelation - lag 5 / weighted by mass
31	ATS6m	Broto-Moreau autocorrelation - lag 6 / weighted by mass
32	ATS7m	Broto-Moreau autocorrelation - lag 7 / weighted by mass
33	ATS8m	Broto-Moreau autocorrelation - lag 8 / weighted by mass

34	ATS0v	Broto-Moreau autocorrelation - lag 0 / weighted by van der Waals volumes
35	ATS1v	Broto-Moreau autocorrelation - lag 1 / weighted by van der Waals volumes
36	ATS2v	Broto-Moreau autocorrelation - lag 2 / weighted by van der Waals volumes
37	ATS3v	Broto-Moreau autocorrelation - lag 3 / weighted by van der Waals volumes
38	ATS4v	Broto-Moreau autocorrelation - lag 4 / weighted by van der Waals volumes
39	ATS5v	Broto-Moreau autocorrelation - lag 5 / weighted by van der Waals volumes
40	ATS6v	Broto-Moreau autocorrelation - lag 6 / weighted by van der Waals volumes
41	ATS7v	Broto-Moreau autocorrelation - lag 7 / weighted by van der Waals volumes
42	ATS8v	Broto-Moreau autocorrelation - lag 8 / weighted by van der Waals volumes
43	ATS0e	Broto-Moreau autocorrelation - lag 0 / weighted by Sanderson electronegativities
44	ATS1e	Broto-Moreau autocorrelation - lag 1 / weighted by Sanderson electronegativities
45	ATS2e	Broto-Moreau autocorrelation - lag 2 / weighted by Sanderson electronegativities
46	ATS3e	Broto-Moreau autocorrelation - lag 3 / weighted by Sanderson electronegativities
47	ATS4e	Broto-Moreau autocorrelation - lag 4 / weighted by Sanderson electronegativities
48	ATS5e	Broto-Moreau autocorrelation - lag 5 / weighted by Sanderson electronegativities
49	ATS6e	Broto-Moreau autocorrelation - lag 6 / weighted by Sanderson electronegativities
50	ATS7e	Broto-Moreau autocorrelation - lag 7 / weighted by Sanderson electronegativities
51	ATS8e	Broto-Moreau autocorrelation - lag 8 / weighted by Sanderson electronegativities
52	ATS0p	Broto-Moreau autocorrelation - lag 0 / weighted by polarizabilities
53	ATS1p	Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities
54	ATS2p	Broto-Moreau autocorrelation - lag 2 / weighted by polarizabilities
55	ATS3p	Broto-Moreau autocorrelation - lag 3 / weighted by polarizabilities
56	ATS4p	Broto-Moreau autocorrelation - lag 4 / weighted by polarizabilities
57	ATS5p	Broto-Moreau autocorrelation - lag 5 / weighted by polarizabilities
58	ATS6p	Broto-Moreau autocorrelation - lag 6 / weighted by polarizabilities
59	ATS7p	Broto-Moreau autocorrelation - lag 7 / weighted by polarizabilities
60	ATS8p	Broto-Moreau autocorrelation - lag 8 / weighted by polarizabilities
61	ATS0i	Broto-Moreau autocorrelation - lag 0 / weighted by first ionization potential
62	ATS1i	Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential
63	ATS2i	Broto-Moreau autocorrelation - lag 2 / weighted by first ionization potential
64	ATS3i	Broto-Moreau autocorrelation - lag 3 / weighted by first ionization potential
65	ATS4i	Broto-Moreau autocorrelation - lag 4 / weighted by first ionization potential
66	ATS5i	Broto-Moreau autocorrelation - lag 5 / weighted by first ionization potential
67	ATS6i	Broto-Moreau autocorrelation - lag 6 / weighted by first ionization potential
68	ATS7i	Broto-Moreau autocorrelation - lag 7 / weighted by first ionization potential
69	ATS8i	Broto-Moreau autocorrelation - lag 8 / weighted by first ionization potential
70	ATS0s	Broto-Moreau autocorrelation - lag 0 / weighted by I-state
71	ATS1s	Broto-Moreau autocorrelation - lag 1 / weighted by I-state
72	ATS2s	Broto-Moreau autocorrelation - lag 2 / weighted by I-state
73	ATS3s	Broto-Moreau autocorrelation - lag 3 / weighted by I-state
74	ATS4s	Broto-Moreau autocorrelation - lag 4 / weighted by I-state
75	ATS5s	Broto-Moreau autocorrelation - lag 5 / weighted by I-state
76	ATS6s	Broto-Moreau autocorrelation - lag 6 / weighted by I-state
77	ATS7s	Broto-Moreau autocorrelation - lag 7 / weighted by I-state

78	ATS8s	Broto-Moreau autocorrelation - lag 8 / weighted by I-state
79	AATS0m	Average Broto-Moreau autocorrelation - lag 0 / weighted by mass
80	AATS1m	Average Broto-Moreau autocorrelation - lag 1 / weighted by mass
81	AATS2m	Average Broto-Moreau autocorrelation - lag 2 / weighted by mass
82	AATS3m	Average Broto-Moreau autocorrelation - lag 3 / weighted by mass
83	AATS4m	Average Broto-Moreau autocorrelation - lag 4 / weighted by mass
84	AATS5m	Average Broto-Moreau autocorrelation - lag 5 / weighted by mass
85	AATS6m	Average Broto-Moreau autocorrelation - lag 6 / weighted by mass
86	AATS7m	Average Broto-Moreau autocorrelation - lag 7 / weighted by mass
87	AATS8m	Average Broto-Moreau autocorrelation - lag 8 / weighted by mass
88	AATS0v	Average Broto-Moreau autocorrelation - lag 0 / weighted by van der Waals volumes
89	AATS1v	Average Broto-Moreau autocorrelation - lag 1 / weighted by van der Waals volumes
90	AATS2v	Average Broto-Moreau autocorrelation - lag 2 / weighted by van der Waals volumes
91	AATS3v	Average Broto-Moreau autocorrelation - lag 3 / weighted by van der Waals volumes
92	AATS4v	Average Broto-Moreau autocorrelation - lag 4 / weighted by van der Waals volumes
93	AATS5v	Average Broto-Moreau autocorrelation - lag 5 / weighted by van der Waals volumes
94	AATS6v	Average Broto-Moreau autocorrelation - lag 6 / weighted by van der Waals volumes
95	AATS7v	Average Broto-Moreau autocorrelation - lag 7 / weighted by van der Waals volumes
96	AATS8v	Average Broto-Moreau autocorrelation - lag 8 / weighted by van der Waals volumes
97	AATS0e	Average Broto-Moreau autocorrelation - lag 0 / weighted by Sanderson electronegativities
98	AATS1e	Average Broto-Moreau autocorrelation - lag 1 / weighted by Sanderson electronegativities
99	AATS2e	Average Broto-Moreau autocorrelation - lag 2 / weighted by Sanderson electronegativities
100	AATS3e	Average Broto-Moreau autocorrelation - lag 3 / weighted by Sanderson electronegativities
101	AATS4e	Average Broto-Moreau autocorrelation - lag 4 / weighted by Sanderson electronegativities
102	AATS5e	Average Broto-Moreau autocorrelation - lag 5 / weighted by Sanderson electronegativities
103	AATS6e	Average Broto-Moreau autocorrelation - lag 6 / weighted by Sanderson electronegativities
104	AATS7e	Average Broto-Moreau autocorrelation - lag 7 / weighted by Sanderson electronegativities
105	AATS8e	Average Broto-Moreau autocorrelation - lag 8 / weighted by Sanderson electronegativities
106	AATS0p	Average Broto-Moreau autocorrelation - lag 0 / weighted by polarizabilities
107	AATS1p	Average Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities
108	AATS2p	Average Broto-Moreau autocorrelation - lag 2 / weighted by polarizabilities
109	AATS3p	Average Broto-Moreau autocorrelation - lag 3 / weighted by polarizabilities
110	AATS4p	Average Broto-Moreau autocorrelation - lag 4 / weighted by polarizabilities
111	AATS5p	Average Broto-Moreau autocorrelation - lag 5 / weighted by polarizabilities
112	AATS6p	Average Broto-Moreau autocorrelation - lag 6 / weighted by polarizabilities
113	AATS7p	Average Broto-Moreau autocorrelation - lag 7 / weighted by polarizabilities
114	AATS8p	Average Broto-Moreau autocorrelation - lag 8 / weighted by polarizabilities
115	AATS0i	Average Broto-Moreau autocorrelation - lag 0 / weighted by first ionization potential
116	AATS1i	Average Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential
117	AATS2i	Average Broto-Moreau autocorrelation - lag 2 / weighted by first ionization potential
118	AATS3i	Average Broto-Moreau autocorrelation - lag 3 / weighted by first ionization potential
119	AATS4i	Average Broto-Moreau autocorrelation - lag 4 / weighted by first ionization potential
120	AATS5i	Average Broto-Moreau autocorrelation - lag 5 / weighted by first ionization potential
121	AATS6i	Average Broto-Moreau autocorrelation - lag 6 / weighted by first ionization potential

122	AATS7i	Average Broto-Moreau autocorrelation - lag 7 / weighted by first ionization potential
123	AATS8i	Average Broto-Moreau autocorrelation - lag 8 / weighted by first ionization potential
124	AATS0s	Average Broto-Moreau autocorrelation - lag 0 / weighted by I-state
125	AATS1s	Average Broto-Moreau autocorrelation - lag 1 / weighted by I-state
126	AATS2s	Average Broto-Moreau autocorrelation - lag 2 / weighted by I-state
127	AATS3s	Average Broto-Moreau autocorrelation - lag 3 / weighted by I-state
128	AATS4s	Average Broto-Moreau autocorrelation - lag 4 / weighted by I-state
129	AATS5s	Average Broto-Moreau autocorrelation - lag 5 / weighted by I-state
130	AATS6s	Average Broto-Moreau autocorrelation - lag 6 / weighted by I-state
131	AATS7s	Average Broto-Moreau autocorrelation - lag 7 / weighted by I-state
132	AATS8s	Average Broto-Moreau autocorrelation - lag 8 / weighted by I-state
133	ATSC0c	Centered Broto-Moreau autocorrelation - lag 0 / weighted by charges
134	ATSC1c	Centered Broto-Moreau autocorrelation - lag 1 / weighted by charges
135	ATSC2c	Centered Broto-Moreau autocorrelation - lag 2 / weighted by charges
136	ATSC3c	Centered Broto-Moreau autocorrelation - lag 3 / weighted by charges
137	ATSC4c	Centered Broto-Moreau autocorrelation - lag 4 / weighted by charges
138	ATSC5c	Centered Broto-Moreau autocorrelation - lag 5 / weighted by charges
139	ATSC6c	Centered Broto-Moreau autocorrelation - lag 6 / weighted by charges
140	ATSC7c	Centered Broto-Moreau autocorrelation - lag 7 / weighted by charges
141	ATSC8c	Centered Broto-Moreau autocorrelation - lag 8 / weighted by charges
142	ATSC0m	Centered Broto-Moreau autocorrelation - lag 0 / weighted by mass
143	ATSC1m	Centered Broto-Moreau autocorrelation - lag 1 / weighted by mass
144	ATSC2m	Centered Broto-Moreau autocorrelation - lag 2 / weighted by mass
145	ATSC3m	Centered Broto-Moreau autocorrelation - lag 3 / weighted by mass
146	ATSC4m	Centered Broto-Moreau autocorrelation - lag 4 / weighted by mass
147	ATSC5m	Centered Broto-Moreau autocorrelation - lag 5 / weighted by mass
148	ATSC6m	Centered Broto-Moreau autocorrelation - lag 6 / weighted by mass
149	ATSC7m	Centered Broto-Moreau autocorrelation - lag 7 / weighted by mass
150	ATSC8m	Centered Broto-Moreau autocorrelation - lag 8 / weighted by mass
151	ATSC0v	Centered Broto-Moreau autocorrelation - lag 0 / weighted by van der Waals volumes
152	ATSC1v	Centered Broto-Moreau autocorrelation - lag 1 / weighted by van der Waals volumes
153	ATSC2v	Centered Broto-Moreau autocorrelation - lag 2 / weighted by van der Waals volumes
154	ATSC3v	Centered Broto-Moreau autocorrelation - lag 3 / weighted by van der Waals volumes
155	ATSC4v	Centered Broto-Moreau autocorrelation - lag 4 / weighted by van der Waals volumes
156	ATSC5v	Centered Broto-Moreau autocorrelation - lag 5 / weighted by van der Waals volumes
157	ATSC6v	Centered Broto-Moreau autocorrelation - lag 6 / weighted by van der Waals volumes
158	ATSC7v	Centered Broto-Moreau autocorrelation - lag 7 / weighted by van der Waals volumes
159	ATSC8v	Centered Broto-Moreau autocorrelation - lag 8 / weighted by van der Waals volumes
160	ATSC0e	Centered Broto-Moreau autocorrelation - lag 0 / weighted by Sanderson electronegativities
161	ATSC1e	Centered Broto-Moreau autocorrelation - lag 1 / weighted by Sanderson electronegativities
162	ATSC2e	Centered Broto-Moreau autocorrelation - lag 2 / weighted by Sanderson electronegativities
163	ATSC3e	Centered Broto-Moreau autocorrelation - lag 3 / weighted by Sanderson electronegativities
164	ATSC4e	Centered Broto-Moreau autocorrelation - lag 4 / weighted by Sanderson electronegativities
165	ATSC5e	Centered Broto-Moreau autocorrelation - lag 5 / weighted by Sanderson electronegativities

166	ATSC6e	Centered Broto-Moreau autocorrelation - lag 6 / weighted by Sanderson electronegativities
167	ATSC7e	Centered Broto-Moreau autocorrelation - lag 7 / weighted by Sanderson electronegativities
168	ATSC8e	Centered Broto-Moreau autocorrelation - lag 8 / weighted by Sanderson electronegativities
169	ATSC0p	Centered Broto-Moreau autocorrelation - lag 0 / weighted by polarizabilities
170	ATSC1p	Centered Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities
171	ATSC2p	Centered Broto-Moreau autocorrelation - lag 2 / weighted by polarizabilities
172	ATSC3p	Centered Broto-Moreau autocorrelation - lag 3 / weighted by polarizabilities
173	ATSC4p	Centered Broto-Moreau autocorrelation - lag 4 / weighted by polarizabilities
174	ATSC5p	Centered Broto-Moreau autocorrelation - lag 5 / weighted by polarizabilities
175	ATSC6p	Centered Broto-Moreau autocorrelation - lag 6 / weighted by polarizabilities
176	ATSC7p	Centered Broto-Moreau autocorrelation - lag 7 / weighted by polarizabilities
177	ATSC8p	Centered Broto-Moreau autocorrelation - lag 8 / weighted by polarizabilities
178	ATSC0i	Centered Broto-Moreau autocorrelation - lag 0 / weighted by first ionization potential
179	ATSC1i	Centered Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential
180	ATSC2i	Centered Broto-Moreau autocorrelation - lag 2 / weighted by first ionization potential
181	ATSC3i	Centered Broto-Moreau autocorrelation - lag 3 / weighted by first ionization potential
182	ATSC4i	Centered Broto-Moreau autocorrelation - lag 4 / weighted by first ionization potential
183	ATSC5i	Centered Broto-Moreau autocorrelation - lag 5 / weighted by first ionization potential
184	ATSC6i	Centered Broto-Moreau autocorrelation - lag 6 / weighted by first ionization potential
185	ATSC7i	Centered Broto-Moreau autocorrelation - lag 7 / weighted by first ionization potential
186	ATSC8i	Centered Broto-Moreau autocorrelation - lag 8 / weighted by first ionization potential
187	ATSC0s	Centered Broto-Moreau autocorrelation - lag 0 / weighted by I-state
188	ATSC1s	Centered Broto-Moreau autocorrelation - lag 1 / weighted by I-state
189	ATSC2s	Centered Broto-Moreau autocorrelation - lag 2 / weighted by I-state
190	ATSC3s	Centered Broto-Moreau autocorrelation - lag 3 / weighted by I-state
191	ATSC4s	Centered Broto-Moreau autocorrelation - lag 4 / weighted by I-state
192	ATSC5s	Centered Broto-Moreau autocorrelation - lag 5 / weighted by I-state
193	ATSC6s	Centered Broto-Moreau autocorrelation - lag 6 / weighted by I-state
194	ATSC7s	Centered Broto-Moreau autocorrelation - lag 7 / weighted by I-state
195	ATSC8s	Centered Broto-Moreau autocorrelation - lag 8 / weighted by I-state
196	AATSC0c	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by charges
197	AATSC1c	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by charges
198	AATSC2c	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by charges
199	AATSC3c	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by charges
200	AATSC4c	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by charges
201	AATSC5c	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by charges
202	AATSC6c	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by charges
203	AATSC7c	Average centered Broto-Moreau autocorrelation - lag 7 / weighted by charges
204	AATSC8c	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by charges
205	AATSC0m	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by mass
206	AATSC1m	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by mass
207	AATSC2m	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by mass
208	AATSC3m	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by mass
209	AATSC4m	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by mass

210	AATSC5m	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by mass
211	AATSC6m	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by mass
212	AATSC7m	Average centered Broto-Moreau autocorrelation - lag 7 / weighted by mass
213	AATSC8m	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by mass
214	AATSC0v	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by van der Waals volumes
215	AATSC1v	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by van der Waals volumes
216	AATSC2v	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by van der Waals volumes
217	AATSC3v	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by van der Waals volumes
218	AATSC4v	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by van der Waals volumes
219	AATSC5v	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by van der Waals volumes
220	AATSC6v	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by van der Waals volumes
221	AATSC7v	Average centered Broto-Moreau autocorrelation - lag 7 / weighted by van der Waals volumes
222	AATSC8v	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by van der Waals volumes
223	AATSC0e	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by Sanderson electronegativities
224	AATSC1e	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by Sanderson electronegativities
225	AATSC2e	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by Sanderson electronegativities
226	AATSC3e	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by Sanderson electronegativities
227	AATSC4e	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by Sanderson electronegativities
228	AATSC5e	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by Sanderson electronegativities
229	AATSC6e	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by Sanderson electronegativities
230	AATSC7e	Average centered Broto-Moreau autocorrelation - lag 7 / weighted by Sanderson electronegativities
231	AATSC8e	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by Sanderson electronegativities
232	AATSC0p	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by polarizabilities
233	AATSC1p	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities
234	AATSC2p	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by polarizabilities
235	AATSC3p	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by polarizabilities
236	AATSC4p	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by polarizabilities
237	AATSC5p	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by polarizabilities
238	AATSC6p	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by polarizabilities
239	AATSC7p	Average centered Broto-Moreau autocorrelation - lag 7 / weighted by polarizabilities
240	AATSC8p	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by polarizabilities
241	AATSC0i	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by first ionization potential
242	AATSC1i	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential
243	AATSC2i	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by first ionization potential
244	AATSC3i	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by first ionization potential
245	AATSC4i	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by first ionization potential
246	AATSC5i	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by first ionization potential
247	AATSC6i	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by first ionization potential
248	AATSC7i	Average centered Broto-Moreau autocorrelation - lag 7 / weighted by first ionization potential
249	AATSC8i	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by first ionization potential
250	AATSC0s	Average centered Broto-Moreau autocorrelation - lag 0 / weighted by I-state
251	AATSC1s	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by I-state
252	AATSC2s	Average centered Broto-Moreau autocorrelation - lag 2 / weighted by I-state
253	AATSC3s	Average centered Broto-Moreau autocorrelation - lag 3 / weighted by I-state

254	AATSC4s	Average centered Broto-Moreau autocorrelation - lag 4 / weighted by I-state
255	AATSC5s	Average centered Broto-Moreau autocorrelation - lag 5 / weighted by I-state
256	AATSC6s	Average centered Broto-Moreau autocorrelation - lag 6 / weighted by I-state
257	AATSC7s	Average centered Broto-Moreau autocorrelation - lag 7 / weighted by I-state
258	AATSC8s	Average centered Broto-Moreau autocorrelation - lag 8 / weighted by I-state
259	MATS1c	Moran autocorrelation - lag 1 / weighted by charges
260	MATS2c	Moran autocorrelation - lag 2 / weighted by charges
261	MATS3c	Moran autocorrelation - lag 3 / weighted by charges
262	MATS4c	Moran autocorrelation - lag 4 / weighted by charges
263	MATS5c	Moran autocorrelation - lag 5 / weighted by charges
264	MATS6c	Moran autocorrelation - lag 6 / weighted by charges
265	MATS7c	Moran autocorrelation - lag 7 / weighted by charges
266	MATS8c	Moran autocorrelation - lag 8 / weighted by charges
267	MATS1m	Moran autocorrelation - lag 1 / weighted by mass
268	MATS2m	Moran autocorrelation - lag 2 / weighted by mass
269	MATS3m	Moran autocorrelation - lag 3 / weighted by mass
270	MATS4m	Moran autocorrelation - lag 4 / weighted by mass
271	MATS5m	Moran autocorrelation - lag 5 / weighted by mass
272	MATS6m	Moran autocorrelation - lag 6 / weighted by mass
273	MATS7m	Moran autocorrelation - lag 7 / weighted by mass
274	MATS8m	Moran autocorrelation - lag 8 / weighted by mass
275	MATS1v	Moran autocorrelation - lag 1 / weighted by van der Waals volumes
276	MATS2v	Moran autocorrelation - lag 2 / weighted by van der Waals volumes
277	MATS3v	Moran autocorrelation - lag 3 / weighted by van der Waals volumes
278	MATS4v	Moran autocorrelation - lag 4 / weighted by van der Waals volumes
279	MATS5v	Moran autocorrelation - lag 5 / weighted by van der Waals volumes
280	MATS6v	Moran autocorrelation - lag 6 / weighted by van der Waals volumes
281	MATS7v	Moran autocorrelation - lag 7 / weighted by van der Waals volumes
282	MATS8v	Moran autocorrelation - lag 8 / weighted by van der Waals volumes
283	MATS1e	Moran autocorrelation - lag 1 / weighted by Sanderson electronegativities
284	MATS2e	Moran autocorrelation - lag 2 / weighted by Sanderson electronegativities
285	MATS3e	Moran autocorrelation - lag 3 / weighted by Sanderson electronegativities
286	MATS4e	Moran autocorrelation - lag 4 / weighted by Sanderson electronegativities
287	MATS5e	Moran autocorrelation - lag 5 / weighted by Sanderson electronegativities
288	MATS6e	Moran autocorrelation - lag 6 / weighted by Sanderson electronegativities
289	MATS7e	Moran autocorrelation - lag 7 / weighted by Sanderson electronegativities
290	MATS8e	Moran autocorrelation - lag 8 / weighted by Sanderson electronegativities
291	MATS1p	Moran autocorrelation - lag 1 / weighted by polarizabilities
292	MATS2p	Moran autocorrelation - lag 2 / weighted by polarizabilities
293	MATS3p	Moran autocorrelation - lag 3 / weighted by polarizabilities
294	MATS4p	Moran autocorrelation - lag 4 / weighted by polarizabilities
295	MATS5p	Moran autocorrelation - lag 5 / weighted by polarizabilities
296	MATS6p	Moran autocorrelation - lag 6 / weighted by polarizabilities
297	MATS7p	Moran autocorrelation - lag 7 / weighted by polarizabilities

298	MATS8p	Moran autocorrelation - lag 8 / weighted by polarizabilities
299	MATS1i	Moran autocorrelation - lag 1 / weighted by first ionization potential
300	MATS2i	Moran autocorrelation - lag 2 / weighted by first ionization potential
301	MATS3i	Moran autocorrelation - lag 3 / weighted by first ionization potential
302	MATS4i	Moran autocorrelation - lag 4 / weighted by first ionization potential
303	MATS5i	Moran autocorrelation - lag 5 / weighted by first ionization potential
304	MATS6i	Moran autocorrelation - lag 6 / weighted by first ionization potential
305	MATS7i	Moran autocorrelation - lag 7 / weighted by first ionization potential
306	MATS8i	Moran autocorrelation - lag 8 / weighted by first ionization potential
307	MATS1s	Moran autocorrelation - lag 1 / weighted by I-state
308	MATS2s	Moran autocorrelation - lag 2 / weighted by I-state
309	MATS3s	Moran autocorrelation - lag 3 / weighted by I-state
310	MATS4s	Moran autocorrelation - lag 4 / weighted by I-state
311	MATS5s	Moran autocorrelation - lag 5 / weighted by I-state
312	MATS6s	Moran autocorrelation - lag 6 / weighted by I-state
313	MATS7s	Moran autocorrelation - lag 7 / weighted by I-state
314	MATS8s	Moran autocorrelation - lag 8 / weighted by I-state
315	GATS1c	Geary autocorrelation - lag 1 / weighted by charges
316	GATS2c	Geary autocorrelation - lag 2 / weighted by charges
317	GATS3c	Geary autocorrelation - lag 3 / weighted by charges
318	GATS4c	Geary autocorrelation - lag 4 / weighted by charges
319	GATS5c	Geary autocorrelation - lag 5 / weighted by charges
320	GATS6c	Geary autocorrelation - lag 6 / weighted by charges
321	GATS7c	Geary autocorrelation - lag 7 / weighted by charges
322	GATS8c	Geary autocorrelation - lag 8 / weighted by charges
323	GATS1m	Geary autocorrelation - lag 1 / weighted by mass
324	GATS2m	Geary autocorrelation - lag 2 / weighted by mass
325	GATS3m	Geary autocorrelation - lag 3 / weighted by mass
326	GATS4m	Geary autocorrelation - lag 4 / weighted by mass
327	GATS5m	Geary autocorrelation - lag 5 / weighted by mass
328	GATS6m	Geary autocorrelation - lag 6 / weighted by mass
329	GATS7m	Geary autocorrelation - lag 7 / weighted by mass
330	GATS8m	Geary autocorrelation - lag 8 / weighted by mass
331	GATS1v	Geary autocorrelation - lag 1 / weighted by van der Waals volumes
332	GATS2v	Geary autocorrelation - lag 2 / weighted by van der Waals volumes
333	GATS3v	Geary autocorrelation - lag 3 / weighted by van der Waals volumes
334	GATS4v	Geary autocorrelation - lag 4 / weighted by van der Waals volumes
335	GATS5v	Geary autocorrelation - lag 5 / weighted by van der Waals volumes
336	GATS6v	Geary autocorrelation - lag 6 / weighted by van der Waals volumes
337	GATS7v	Geary autocorrelation - lag 7 / weighted by van der Waals volumes
338	GATS8v	Geary autocorrelation - lag 8 / weighted by van der Waals volumes
339	GATS1e	Geary autocorrelation - lag 1 / weighted by Sanderson electronegativities
340	GATS2e	Geary autocorrelation - lag 2 / weighted by Sanderson electronegativities
341	GATS3e	Geary autocorrelation - lag 3 / weighted by Sanderson electronegativities

342	GATS4e	Geary autocorrelation - lag 4 / weighted by Sanderson electronegativities
343	GATS5e	Geary autocorrelation - lag 5 / weighted by Sanderson electronegativities
344	GATS6e	Geary autocorrelation - lag 6 / weighted by Sanderson electronegativities
345	GATS7e	Geary autocorrelation - lag 7 / weighted by Sanderson electronegativities
346	GATS8e	Geary autocorrelation - lag 8 / weighted by Sanderson electronegativities
347	GATS1p	Geary autocorrelation - lag 1 / weighted by polarizabilities
348	GATS2p	Geary autocorrelation - lag 2 / weighted by polarizabilities
349	GATS3p	Geary autocorrelation - lag 3 / weighted by polarizabilities
350	GATS4p	Geary autocorrelation - lag 4 / weighted by polarizabilities
351	GATS5p	Geary autocorrelation - lag 5 / weighted by polarizabilities
352	GATS6p	Geary autocorrelation - lag 6 / weighted by polarizabilities
353	GATS7p	Geary autocorrelation - lag 7 / weighted by polarizabilities
354	GATS8p	Geary autocorrelation - lag 8 / weighted by polarizabilities
355	GATS1i	Geary autocorrelation - lag 1 / weighted by first ionization potential
356	GATS2i	Geary autocorrelation - lag 2 / weighted by first ionization potential
357	GATS3i	Geary autocorrelation - lag 3 / weighted by first ionization potential
358	GATS4i	Geary autocorrelation - lag 4 / weighted by first ionization potential
359	GATS5i	Geary autocorrelation - lag 5 / weighted by first ionization potential
360	GATS6i	Geary autocorrelation - lag 6 / weighted by first ionization potential
361	GATS7i	Geary autocorrelation - lag 7 / weighted by first ionization potential
362	GATS8i	Geary autocorrelation - lag 8 / weighted by first ionization potential
363	GATS1s	Geary autocorrelation - lag 1 / weighted by I-state
364	GATS2s	Geary autocorrelation - lag 2 / weighted by I-state
365	GATS3s	Geary autocorrelation - lag 3 / weighted by I-state
366	GATS4s	Geary autocorrelation - lag 4 / weighted by I-state
367	GATS5s	Geary autocorrelation - lag 5 / weighted by I-state
368	GATS6s	Geary autocorrelation - lag 6 / weighted by I-state
369	GATS7s	Geary autocorrelation - lag 7 / weighted by I-state
370	GATS8s	Geary autocorrelation - lag 8 / weighted by I-state
371	SpAbs_DzZ	Graph energy from Barysz matrix / weighted by atomic number
372	SpMax_DzZ	Leading eigenvalue from Barysz matrix / weighted by atomic number
373	SpDiam_DzZ	Spectral diameter from Barysz matrix / weighted by atomic number
374	SpAD_DzZ	Spectral absolute deviation from Barysz matrix / weighted by atomic number
375	SpMAD_DzZ	Spectral mean absolute deviation from Barysz matrix / weighted by atomic number
376	EE_DzZ	Estrada-like index from Barysz matrix / weighted by atomic number (ln(1+x))
377	SM1_DzZ	Spectral moment of order 1 from Barysz matrix / weighted by atomic number
378	VE1_DzZ	Coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number
379	VE2_DzZ	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number
380	VE3_DzZ	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by atomic number
381	VR1_DzZ	Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number
382	VR2_DzZ	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number
383	VR3_DzZ	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by atomic number
384	SpAbs_Dzm	Graph energy from Barysz matrix / weighted by mass
385	SpMax_Dzm	Leading eigenvalue from Barysz matrix / weighted by mass

386	SpDiam_Dzm	Spectral diameter from Barysz matrix / weighted by mass
387	SpAD_Dzm	Spectral absolute deviation from Barysz matrix / weighted by mass
388	SpMAD_Dzm	Spectral mean absolute deviation from Barysz matrix / weighted by mass
389	EE_Dzm	Estrada-like index from Barysz matrix / weighted by mass (ln(1+x))
390	SM1_Dzm	Spectral moment of order 1 from Barysz matrix / weighted by mass
391	VE1_Dzm	Coefficient sum of the last eigenvector from Barysz matrix / weighted by mass
392	VE2_Dzm	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by mass
393	VE3_Dzm	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by mass
394	VR1_Dzm	Randic-like eigenvector-based index from Barysz matrix / weighted by mass
395	VR2_Dzm	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by mass
396	VR3_Dzm	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by mass
397	SpAbs_Dzv	Graph energy from Barysz matrix / weighted by van der Waals volumes
398	SpMax_Dzv	Leading eigenvalue from Barysz matrix / weighted by van der Waals volumes
399	SpDiam_Dzv	Spectral diameter from Barysz matrix / weighted by van der Waals volumes
400	SpAD_Dzv	Spectral absolute deviation from Barysz matrix / weighted by van der Waals volumes
401	SpMAD_Dzv	Spectral mean absolute deviation from Barysz matrix / weighted by van der Waals volumes
402	EE_Dzv	Estrada-like index from Barysz matrix / weighted by van der Waals volumes (ln(1+x))
403	SM1_Dzv	Spectral moment of order 1 from Barysz matrix / weighted by van der Waals volumes
404	VE1_Dzv	Coefficient sum of the last eigenvector from Barysz matrix / weighted by van der Waals volumes
405	VE2_Dzv	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by van der Waals volumes
406	VE3_Dzv	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by van der Waals volumes
407	VR1_Dzv	Randic-like eigenvector-based index from Barysz matrix / weighted by van der Waals volumes
408	VR2_Dzv	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by van der Waals volumes
409	VR3_Dzv	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by van der Waals volumes
410	SpAbs_Dze	Graph energy from Barysz matrix / weighted by Sanderson electronegativities
411	SpMax_Dze	Leading eigenvalue from Barysz matrix / weighted by Sanderson electronegativities
412	SpDiam_Dze	Spectral diameter from Barysz matrix / weighted by Sanderson electronegativities
413	SpAD_Dze	Spectral absolute deviation from Barysz matrix / weighted by Sanderson electronegativities
414	SpMAD_Dze	Spectral mean absolute deviation from Barysz matrix / weighted by Sanderson electronegativities
415	EE_Dze	Estrada-like index from Barysz matrix / weighted by Sanderson electronegativities (ln(1+x))
416	SM1_Dze	Spectral moment of order 1 from Barysz matrix / weighted by Sanderson electronegativities
417	VE1_Dze	Coefficient sum of the last eigenvector from Barysz matrix / weighted by Sanderson electronegativities
418	VE2_Dze	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by Sanderson electronegativities
419	VE3_Dze	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by Sanderson electronegativities
420	VR1_Dze	Randic-like eigenvector-based index from Barysz matrix / weighted by Sanderson electronegativities
421	VR2_Dze	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by Sanderson electronegativities
422	VR3_Dze	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by Sanderson electronegativities
423	SpAbs_Dzp	Graph energy from Barysz matrix / weighted by polarizabilities
424	SpMax_Dzp	Leading eigenvalue from Barysz matrix / weighted by polarizabilities
425	SpDiam_Dzp	Spectral diameter from Barysz matrix / weighted by polarizabilities
426	SpAD_Dzp	Spectral absolute deviation from Barysz matrix / weighted by polarizabilities
427	SpMAD_Dzp	Spectral mean absolute deviation from Barysz matrix / weighted by polarizabilities

428	EE_Dzp	Estrada-like index from Barysz matrix / weighted by polarizabilities (ln(1+x))
429	SM1_Dzp	Spectral moment of order 1 from Barysz matrix / weighted by polarizabilities
430	VE1_Dzp	Coefficient sum of the last eigenvector from Barysz matrix / weighted by polarizabilities
431	VE2_Dzp	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by polarizabilities
432	VE3_Dzp	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by polarizabilities
433	VR1_Dzp	Randic-like eigenvector-based index from Barysz matrix / weighted by polarizabilities
434	VR2_Dzp	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by polarizabilities
435	VR3_Dzp	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by polarizabilities
436	SpAbs_Dzi	Graph energy from Barysz matrix / weighted by first ionization potential
437	SpMax_Dzi	Leading eigenvalue from Barysz matrix / weighted by first ionization potential
438	SpDiam_Dzi	Spectral diameter from Barysz matrix / weighted by first ionization potential
439	SpAD_Dzi	Spectral absolute deviation from Barysz matrix / weighted by first ionization potential
440	SpMAD_Dzi	Spectral mean absolute deviation from Barysz matrix / weighted by first ionization potential
441	EE_Dzi	Estrada-like index from Barysz matrix / weighted by first ionization potential (ln(1+x))
442	SM1_Dzi	Spectral moment of order 1 from Barysz matrix / weighted by first ionization potential
443	VE1_Dzi	Coefficient sum of the last eigenvector from Barysz matrix / weighted by first ionization potential
444	VE2_Dzi	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by first ionization potential
445	VE3_Dzi	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by first ionization potential
446	VR1_Dzi	Randic-like eigenvector-based index from Barysz matrix / weighted by first ionization potential
447	VR2_Dzi	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by first ionization potential
448	VR3_Dzi	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by first ionization potential
449	SpAbs_Dzs	Graph energy from Barysz matrix / weighted by I-state
450	SpMax_Dzs	Leading eigenvalue from Barysz matrix / weighted by I-state
451	SpDiam_Dzs	Spectral diameter from Barysz matrix / weighted by I-state
452	SpAD_Dzs	Spectral absolute deviation from Barysz matrix / weighted by I-state
453	SpMAD_Dzs	Spectral mean absolute deviation from Barysz matrix / weighted by I-state
454	EE_Dzs	Estrada-like index from Barysz matrix / weighted by I-state (ln(1+x))
455	SM1_Dzs	Spectral moment of order 1 from Barysz matrix / weighted by I-state
456	VE1_Dzs	Coefficient sum of the last eigenvector from Barysz matrix / weighted by I-state
457	VE2_Dzs	Average coefficient sum of the last eigenvector from Barysz matrix / weighted by I-state
458	VE3_Dzs	Logarithmic coefficient sum of the last eigenvector from Barysz matrix / weighted by I-state
459	VR1_Dzs	Randic-like eigenvector-based index from Barysz matrix / weighted by I-state
460	VR2_Dzs	Normalized Randic-like eigenvector-based index from Barysz matrix / weighted by I-state
461	VR3_Dzs	Logarithmic Randic-like eigenvector-based index from Barysz matrix / weighted by I-state
462	nBase	Number of basic groups. The list of basic groups is defined by this SMARTS "[$([NH2]-[CX4])]", "[$([NH](-[CX4])-[CX4])]", "[$(N(-[CX4])(-[CX4])-[CX4])]", "[$([*;+;!$(*~[*;-])])]", "[$(N=C-N)]", and "[$(N-C=N)]" originally presented in JOELib
463	BCUTw-1l	nhigh lowest atom weighted BCUTS
464	BCUTw-1h	nlow highest atom weighted BCUTS
465	BCUTc-1l	nhigh lowest partial charge weighted BCUTS
466	BCUTc-1h	nlow highest partial charge weighted BCUTS
467	BCUTp-1l	nhigh lowest polarizability weighted BCUTS
468	BCUTp-1h	nlow highest polarizability weighted BCUTS
469	nBonds	Number of bonds (excluding bonds with hydrogen)

470	nBonds2	Total number of bonds (including bonds to hydrogens)
471	nBondsS	Number of single bonds (including bonds with hydrogen)
472	nBondsS2	Total number of single bonds (including bonds to hydrogens, excluding aromatic bonds)
473	nBondsS3	Total number of single bonds (excluding bonds to hydrogens and aromatic bonds)
474	nBondsD	Number of double bonds
475	nBondsD2	Total number of double bonds (excluding bonds to aromatic bonds)
476	nBondsT	Number of triple bonds
477	nBondsM	Total number of bonds that have bond order greater than one (aromatic bonds have bond order 1.5).
478	bpol	Sum of the absolute value of the difference between atomic polarizabilities of all bonded atoms in the molecule (including implicit hydrogens)
479	SpMax1_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative mass
480	SpMax2_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative mass
481	SpMax3_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative mass
482	SpMax4_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative mass
483	SpMax5_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative mass
484	SpMax6_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative mass
485	SpMax7_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative mass
486	SpMax8_Bhm	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative mass
487	SpMin1_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative mass
488	SpMin2_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative mass
489	SpMin3_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative mass
490	SpMin4_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative mass
491	SpMin5_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative mass
492	SpMin6_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative mass
493	SpMin7_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative mass
494	SpMin8_Bhm	Smallest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative mass
495	SpMax1_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative van der Waals volumes
496	SpMax2_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative van der Waals volumes
497	SpMax3_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative van der Waals volumes
498	SpMax4_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative van der Waals volumes
499	SpMax5_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative van der Waals volumes
500	SpMax6_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative van der Waals volumes
501	SpMax7_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative van der Waals volumes
502	SpMax8_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative van der Waals volumes
503	SpMin1_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative van der Waals volumes
504	SpMin2_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative van der Waals volumes
505	SpMin3_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative van der Waals volumes
506	SpMin4_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative van der Waals volumes
507	SpMin5_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative van der Waals volumes
508	SpMin6_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative van der Waals volumes
509	SpMin7_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative van der Waals

		volumes
510	SpMin8_Bhv	Smallest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative van der Waals volumes
511	SpMax1_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative Sanderson electronegativities
512	SpMax2_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative Sanderson electronegativities
513	SpMax3_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative Sanderson electronegativities
514	SpMax4_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative Sanderson electronegativities
515	SpMax5_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative Sanderson electronegativities
516	SpMax6_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative Sanderson electronegativities
517	SpMax7_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative Sanderson electronegativities
518	SpMax8_Bhe	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative Sanderson electronegativities
519	SpMin1_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative Sanderson electronegativities
520	SpMin2_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative Sanderson electronegativities
521	SpMin3_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative Sanderson electronegativities
522	SpMin4_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative Sanderson electronegativities
523	SpMin5_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative Sanderson electronegativities
524	SpMin6_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative Sanderson electronegativities
525	SpMin7_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative Sanderson electronegativities
526	SpMin8_Bhe	Smallest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative Sanderson electronegativities
527	SpMax1_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative polarizabilities
528	SpMax2_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative polarizabilities
529	SpMax3_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative polarizabilities
530	SpMax4_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative polarizabilities
531	SpMax5_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative polarizabilities
532	SpMax6_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative polarizabilities
533	SpMax7_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative polarizabilities
534	SpMax8_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative polarizabilities
535	SpMin1_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative polarizabilities
536	SpMin2_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative polarizabilities
537	SpMin3_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative polarizabilities
538	SpMin4_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative polarizabilities
539	SpMin5_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative polarizabilities
540	SpMin6_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative polarizabilities
541	SpMin7_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative polarizabilities
542	SpMin8_Bhp	Smallest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative polarizabilities
543	SpMax1_Bhi	Largest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative first ionization potential
544	SpMax2_Bhi	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative first ionization potential
545	SpMax3_Bhi	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative first ionization potential
546	SpMax4_Bhi	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative first ionization potential

547	SpMax5_Bhi	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative first ionization potential
548	SpMax6_Bhi	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative first ionization potential
549	SpMax7_Bhi	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative first ionization potential
550	SpMax8_Bhi	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative first ionization potential
551	SpMin1_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative first ionization potential
552	SpMin2_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative first ionization potential
553	SpMin3_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative first ionization potential
554	SpMin4_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative first ionization potential
555	SpMin5_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative first ionization potential
556	SpMin6_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative first ionization potential
557	SpMin7_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative first ionization potential
558	SpMin8_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative first ionization potential
559	SpMax1_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative I-state
560	SpMax2_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative I-state
561	SpMax3_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative I-state
562	SpMax4_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative I-state
563	SpMax5_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative I-state
564	SpMax6_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative I-state
565	SpMax7_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative I-state
566	SpMax8_Bhs	Largest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative I-state
567	SpMin1_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 1 / weighted by relative I-state
568	SpMin2_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative I-state
569	SpMin3_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 3 / weighted by relative I-state
570	SpMin4_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 4 / weighted by relative I-state
571	SpMin5_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 5 / weighted by relative I-state
572	SpMin6_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 6 / weighted by relative I-state
573	SpMin7_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 7 / weighted by relative I-state
574	SpMin8_Bhs	Smallest absolute eigenvalue of Burden modified matrix - n 8 / weighted by relative I-state
575	C1SP1	Triply bound carbon bound to one other carbon
576	C2SP1	Triply bound carbon bound to two other carbons
577	C1SP2	Doubly bound carbon bound to one other carbon
578	C2SP2	Doubly bound carbon bound to two other carbons
579	C3SP2	Doubly bound carbon bound to three other carbons
580	C1SP3	Singly bound carbon bound to one other carbon
581	C2SP3	Singly bound carbon bound to two other carbons
582	C3SP3	Singly bound carbon bound to three other carbons
583	C4SP3	Singly bound carbon bound to four other carbons
584	SCH-3	Simple chain, order 3
585	SCH-4	Simple chain, order 4
586	SCH-5	Simple chain, order 5
587	SCH-6	Simple chain, order 6

588	SCH-7	Simple chain, order 7
589	VCH-3	Valence chain, order 3
590	VCH-4	Valence chain, order 4
591	VCH-5	Valence chain, order 5
592	VCH-6	Valence chain, order 6
593	VCH-7	Valence chain, order 7
594	SC-3	Simple cluster, order 3
595	SC-4	Simple cluster, order 4
596	SC-5	Simple cluster, order 5
597	SC-6	Simple cluster, order 6
598	VC-3	Valence cluster, order 3
599	VC-4	Valence cluster, order 4
600	VC-5	Valence cluster, order 5
601	VC-6	Valence cluster, order 6
602	SPC-4	Simple path cluster, order 4
603	SPC-5	Simple path cluster, order 5
604	SPC-6	Simple path cluster, order 6
605	VPC-4	Valence path cluster, order 4
606	VPC-5	Valence path cluster, order 5
607	VPC-6	Valence path cluster, order 6
608	SP-0	Simple path, order 0
609	SP-1	Simple path, order 1
610	SP-2	Simple path, order 2
611	SP-3	Simple path, order 3
612	SP-4	Simple path, order 4
613	SP-5	Simple path, order 5
614	SP-6	Simple path, order 6
615	SP-7	Simple path, order 7
616	ASP-0	Average simple path, order 0
617	ASP-1	Average simple path, order 1
618	ASP-2	Average simple path, order 2
619	ASP-3	Average simple path, order 3
620	ASP-4	Average simple path, order 4
621	ASP-5	Average simple path, order 5
622	ASP-6	Average simple path, order 6
623	ASP-7	Average simple path, order 7
624	VP-0	Valence path, order 0
625	VP-1	Valence path, order 1
626	VP-2	Valence path, order 2
627	VP-3	Valence path, order 3
628	VP-4	Valence path, order 4
629	VP-5	Valence path, order 5
630	VP-6	Valence path, order 6
631	VP-7	Valence path, order 7

632	AVP-0	Average valence path, order 0
633	AVP-1	Average valence path, order 1
634	AVP-2	Average valence path, order 2
635	AVP-3	Average valence path, order 3
636	AVP-4	Average valence path, order 4
637	AVP-5	Average valence path, order 5
638	AVP-6	Average valence path, order 6
639	AVP-7	Average valence path, order 7
640	Sv	Sum of atomic van der Waals volumes (scaled on carbon atom)
641	Sse	Sum of atomic Sanderson electronegativities (scaled on carbon atom)
642	Spe	Sum of atomic Pauling electronegativities (scaled on carbon atom)
643	Sare	Sum of atomic Allred-Rochow electronegativities (scaled on carbon atom)
644	Sp	Sum of atomic polarizabilities (scaled on carbon atom)
645	Si	Sum of first first ionization potentials (scaled on carbon atom)
646	Mv	Mean atomic van der Waals volumes (scaled on carbon atom)
647	Mse	Mean atomic Sanderson electronegativities (scaled on carbon atom)
648	Mpe	Mean atomic Pauling electronegativities (scaled on carbon atom)
649	Mare	Mean atomic Allred-Rochow electronegativities (scaled on carbon atom)
650	Mp	Mean atomic polarizabilities (scaled on carbon atom)
651	Mi	Mean first first ionization potentials (scaled on carbon atom)
652	CrippenLogP	Crippen's LogP
653	CrippenMR	Crippen's molar refractivity
654	SpMax_Dt	Leading eigenvalue from detour matrix
655	SpDiam_Dt	Spectral diameter from detour matrix
656	SpAD_Dt	Spectral absolute deviation from detour matrix
657	SpMAD_Dt	Spectral mean absolute deviation from detour matrix
658	EE_Dt	Estrada-like index from detour matrix
659	VE1_Dt	Coefficient sum of the last eigenvector from detour matrix
660	VE2_Dt	Average coefficient sum of the last eigenvector from detour matrix
661	VE3_Dt	Logarithmic coefficient sum of the last eigenvector from detour matrix
662	VR1_Dt	Randic-like eigenvector-based index from detour matrix
663	VR2_Dt	Normalized Randic-like eigenvector-based index from detour matrix
664	VR3_Dt	Logarithmic Randic-like eigenvector-based index from detour matrix
665	ECCEN	A topological descriptor combining distance and adjacency information
666	nHBd	Count of E-States for (strong) Hydrogen Bond donors
667	nwHBd	Count of E-States for weak Hydrogen Bond donors
668	nHBa	Count of E-States for (strong) Hydrogen Bond acceptors
669	nwHBa	Count of E-States for weak Hydrogen Bond acceptors
670	nHBint2	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 2
671	nHBint3	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 3
672	nHBint4	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 4
673	nHBint5	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 5
674	nHBint6	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 6
675	nHBint7	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 7

676	nHBint8	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 8
677	nHBint9	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 9
678	nHBint10	Count of E-State descriptors of strength for potential Hydrogen Bonds of path length 10
679	nHsOH	Count of atom-type H E-State: -OH
680	nHsNH2	Count of atom-type H E-State: -NH2
681	nHssNH	Count of atom-type H E-State: -NH-
682	nHaaNH	Count of atom-type H E-State: :NH:
683	nHsNH3p	Count of atom-type H E-State: -NH3+
684	nHssNH2p	Count of atom-type H E-State: -NH2-+
685	nHtCH	Count of atom-type H E-State: #CH
686	nHdCH2	Count of atom-type H E-State: =CH2
687	nHdsCH	Count of atom-type H E-State: =CH-
688	nHaaCH	Count of atom-type H E-State: :CH:
689	nHCHnX	Count of atom-type H E-State: CHnX
690	nHCsats	Count of atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb
691	nHCsatu	Count of atom-type H E-State: H on C sp3 bonded to unsaturated C
692	nHAvin	Count of atom-type H E-State: H on C vinyl bonded to C aromatic
693	nHother	Count of atom-type H E-State: H on aaCH, dCH2 or dsCH
694	nsCH3	Count of atom-type E-State: -CH3
695	ndCH2	Count of atom-type E-State: =CH2
696	nssCH2	Count of atom-type E-State: -CH2-
697	ntCH	Count of atom-type E-State: #CH
698	ndsCH	Count of atom-type E-State: =CH-
699	naaCH	Count of atom-type E-State: :CH:
700	nsssCH	Count of atom-type E-State: >CH-
701	nddC	Count of atom-type E-State: =C=
702	ntsC	Count of atom-type E-State: #C-
703	ndssC	Count of atom-type E-State: =C<
704	naasC	Count of atom-type E-State: :C:-
705	naaaC	Count of atom-type E-State: ::C:
706	nssssC	Count of atom-type E-State: >C<
707	nsNH3p	Count of atom-type E-State: -NH3+
708	nsNH2	Count of atom-type E-State: -NH2
709	nssNH2p	Count of atom-type E-State: -NH2-+
710	nssNH	Count of atom-type E-State: -NH-
711	naaNH	Count of atom-type E-State: :NH:
712	ntN	Count of atom-type E-State: #N
713	ndsN	Count of atom-type E-State: =N-
714	naaN	Count of atom-type E-State: :N:
715	nsssN	Count of atom-type E-State: >N-
716	naasN	Count of atom-type E-State: :N:-
717	nssssNp	Count of atom-type E-State: >N<+
718	nsOH	Count of atom-type E-State: -OH
719	ndO	Count of atom-type E-State: =O

720	nssO	Count of atom-type E-State: -O-
721	naaO	Count of atom-type E-State: :O:
722	nsOm	Count of atom-type E-State: -O-
723	nsF	Count of atom-type E-State: -F
724	nssssSi	Count of atom-type E-State: >Si<
725	ndsssP	Count of atom-type E-State: ->P=
726	ndS	Count of atom-type E-State: =S
727	nssS	Count of atom-type E-State: -S-
728	naaS	Count of atom-type E-State: aSa
729	ndssS	Count of atom-type E-State: >S=
730	nddssS	Count of atom-type E-State: >S==
731	nsCl	Count of atom-type E-State: -Cl
732	nssssSn	Count of atom-type E-State: >Sn<
733	SHBd	Sum of E-States for (strong) hydrogen bond donors
734	SwHBd	Sum of E-States for weak hydrogen bond donors
735	SHBa	Sum of E-States for (strong) hydrogen bond acceptors
736	SwHBa	Sum of E-States for weak hydrogen bond acceptors
737	SHBint2	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 2
738	SHBint3	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 3
739	SHBint4	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 4
740	SHBint5	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 5
741	SHBint6	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 6
742	SHBint7	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 7
743	SHBint8	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 8
744	SHBint9	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 9
745	SHBint10	Sum of E-State descriptors of strength for potential hydrogen bonds of path length 10
746	SHsOH	Sum of atom-type H E-State: -OH
747	SHsNH2	Sum of atom-type H E-State: -NH2
748	SHssNH	Sum of atom-type H E-State: -NH-
749	SHaaNH	Sum of atom-type H E-State: :NH:
750	SHsNH3p	Sum of atom-type H E-State: -NH3+
751	SHssNH2p	Sum of atom-type H E-State: -NH2-+
752	SHtCH	Sum of atom-type H E-State: #CH
753	SHdCH2	Sum of atom-type H E-State: =CH2
754	SHdsCH	Sum of atom-type H E-State: =CH-
755	SHaaCH	Sum of atom-type H E-State: :CH:
756	SHCHnX	Sum of atom-type H E-State: CHnX
757	SHCsats	Sum of atom-type H E-State: H on C sp3 bonded to saturated C
758	SHCsatu	Sum of atom-type H E-State: H on C sp3 bonded to unsaturated C
759	SHAvin	Sum of atom-type H E-State: H on C vinyl bonded to C aromatic
760	SHother	Sum of atom-type H E-State: H on aaCH, dCH2 or dsCH
761	SsCH3	Sum of atom-type E-State: -CH3
762	SdCH2	Sum of atom-type E-State: =CH2
763	SssCH2	Sum of atom-type E-State: -CH2-

764	StCH	Sum of atom-type E-State: #CH
765	SdsCH	Sum of atom-type E-State: =CH-
766	SaaCH	Sum of atom-type E-State: :CH:
767	SsssCH	Sum of atom-type E-State: >CH-
768	SddC	Sum of atom-type E-State: =C=
769	StsC	Sum of atom-type E-State: #C-
770	SdssC	Sum of atom-type E-State: =C<
771	SaasC	Sum of atom-type E-State: :C:-
772	SaaaC	Sum of atom-type E-State: ::C:
773	SssssC	Sum of atom-type E-State: >C<
774	SsNH3p	Sum of atom-type E-State: -NH3+
775	SsNH2	Sum of atom-type E-State: -NH2
776	SssNH2p	Sum of atom-type E-State: -NH2-+
777	SssNH	Sum of atom-type E-State: -NH-
778	SaaNH	Sum of atom-type E-State: :NH:
779	StN	Sum of atom-type E-State: #N
780	SdsN	Sum of atom-type E-State: =N-
781	SaaN	Sum of atom-type E-State: :N:
782	SsssN	Sum of atom-type E-State: >N-
783	SaasN	Sum of atom-type E-State: :N:-
784	SssssNp	Sum of atom-type E-State: >N<+
785	SsOH	Sum of atom-type E-State: -OH
786	SdO	Sum of atom-type E-State: =O
787	SssO	Sum of atom-type E-State: -O-
788	SaaO	Sum of atom-type E-State: :O:
789	SsOm	Sum of atom-type E-State: -O-
790	SsF	Sum of atom-type E-State: -F
791	SssssSi	Sum of atom-type E-State: >Si<
792	SdsssP	Sum of atom-type E-State: ->P=
793	SdS	Sum of atom-type E-State: =S
794	SssS	Sum of atom-type E-State: -S-
795	SaaS	Sum of atom-type E-State: aSa
796	SdssS	Sum of atom-type E-State: >S=
797	SddssS	Sum of atom-type E-State: >S==
798	SsCl	Sum of atom-type E-State: -Cl
799	SssssSn	Sum of atom-type E-State: >Sn<
800	minHBd	Minimum E-States for (strong) Hydrogen Bond donors
801	minwHBd	Minimum E-States for weak Hydrogen Bond donors
802	minHBa	Minimum E-States for (strong) Hydrogen Bond acceptors
803	minwHBa	Minimum E-States for weak Hydrogen Bond acceptors
804	minHBint2	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 2
805	minHBint3	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 3
806	minHBint4	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 4
807	minHBint5	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 5

808	minHBint6	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 6
809	minHBint7	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 7
810	minHBint8	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 8
811	minHBint9	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 9
812	minHBint10	Minimum E-State descriptors of strength for potential Hydrogen Bonds of path length 10
813	minHsOH	Minimum atom-type H E-State: -OH
814	minHsNH2	Minimum atom-type H E-State: -NH2
815	minHssNH	Minimum atom-type H E-State: -NH-
816	minHaaNH	Minimum atom-type H E-State: :NH:
817	minHsNH3p	Minimum atom-type H E-State: -NH3+
818	minHssNH2p	Minimum atom-type H E-State: -NH2-+
819	minHtCH	Minimum atom-type H E-State: #CH
820	minHdCH2	Minimum atom-type H E-State: =CH2
821	minHdsCH	Minimum atom-type H E-State: =CH-
822	minHaaCH	Minimum atom-type H E-State: :CH:
823	minHCHnX	Minimum atom-type H E-State: CHnX
824	minHCsats	Minimum atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb
825	minHCsatu	Minimum atom-type H E-State: H on C sp3 bonded to unsaturated C
826	minHAvin	Minimum atom-type H E-State: H on C vinyl bonded to C aromatic
827	minHother	Minimum atom-type H E-State: H on aaCH, dCH2 or dsCH
828	minsCH3	Minimum atom-type E-State: -CH3
829	mindCH2	Minimum atom-type E-State: =CH2
830	minssCH2	Minimum atom-type E-State: -CH2-
831	mintCH	Minimum atom-type E-State: #CH
832	mindsCH	Minimum atom-type E-State: =CH-
833	minaaCH	Minimum atom-type E-State: :CH:
834	minsssCH	Minimum atom-type E-State: >CH-
835	minddC	Minimum atom-type E-State: =C=
836	mintsC	Minimum atom-type E-State: #C-
837	mindssC	Minimum atom-type E-State: =C<
838	minaasC	Minimum atom-type E-State: :C:-
839	minaaaC	Minimum atom-type E-State: ::C:
840	minssssC	Minimum atom-type E-State: >C<
841	minsNH3p	Minimum atom-type E-State: -NH3+
842	minsNH2	Minimum atom-type E-State: -NH2
843	minssNH2p	Minimum atom-type E-State: -NH2-+
844	minssNH	Minimum atom-type E-State: -NH-
845	minaaNH	Minimum atom-type E-State: :NH:
846	mintN	Minimum atom-type E-State: #N
847	mindsN	Minimum atom-type E-State: =N-
848	minaaN	Minimum atom-type E-State: :N:
849	minsssN	Minimum atom-type E-State: >N-
850	minaasN	Minimum atom-type E-State: :N:-
851	minssssNp	Minimum atom-type E-State: >N<+

852	minsOH	Minimum atom-type E-State: -OH
853	mindO	Minimum atom-type E-State: =O
854	minssO	Minimum atom-type E-State: -O-
855	minaaO	Minimum atom-type E-State: :O:
856	minsOm	Minimum atom-type E-State: -O-
857	minsF	Minimum atom-type E-State: -F
858	minssssSi	Minimum atom-type E-State: >Si<
859	mindsssP	Minimum atom-type E-State: ->P=
860	mindS	Minimum atom-type E-State: =S
861	minssS	Minimum atom-type E-State: -S-
862	minaaS	Minimum atom-type E-State: aSa
863	mindssS	Minimum atom-type E-State: >S=
864	minddssS	Minimum atom-type E-State: >S==
865	minsCl	Minimum atom-type E-State: -Cl
866	minssssSn	Minimum atom-type E-State: >Sn<
867	maxHBd	Maximum E-States for (strong) Hydrogen Bond donors
868	maxwHBd	Maximum E-States for weak Hydrogen Bond donors
869	maxHBa	Maximum E-States for (strong) Hydrogen Bond acceptors
870	maxwHBa	Maximum E-States for weak Hydrogen Bond acceptors
871	maxHBint2	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 2
872	maxHBint3	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 3
873	maxHBint4	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 4
874	maxHBint5	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 5
875	maxHBint6	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 6
876	maxHBint7	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 7
877	maxHBint8	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 8
878	maxHBint9	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 9
879	maxHBint10	Maximum E-State descriptors of strength for potential Hydrogen Bonds of path length 10
880	maxHsOH	Maximum atom-type H E-State: -OH
881	maxHsNH2	Maximum atom-type H E-State: -NH2
882	maxHssNH	Maximum atom-type H E-State: -NH-
883	maxHaaNH	Maximum atom-type H E-State: :NH:
884	maxHsNH3p	Maximum atom-type H E-State: -NH3+
885	maxHssNH2p	Maximum atom-type H E-State: -NH2-+
886	maxHtCH	Maximum atom-type H E-State: #CH
887	maxHdCH2	Maximum atom-type H E-State: =CH2
888	maxHdsCH	Maximum atom-type H E-State: =CH-
889	maxHaaCH	Maximum atom-type H E-State: :CH:
890	maxHCHnX	Maximum atom-type H E-State: CHnX
891	maxHCsats	Maximum atom-type H E-State: H bonded to B, Si, P, Ge, As, Se, Sn or Pb
892	maxHCsatu	Maximum atom-type H E-State: H on C sp3 bonded to unsaturated C
893	maxHAvin	Maximum atom-type H E-State: H on C vinyl bonded to C aromatic
894	maxHother	Maximum atom-type H E-State: H on aaCH, dCH2 or dsCH
895	maxsCH3	Maximum atom-type E-State: -CH3

896	maxdCH2	Maximum atom-type E-State: =CH2
897	maxssCH2	Maximum atom-type E-State: -CH2-
898	maxtCH	Maximum atom-type E-State: #CH
899	maxdsCH	Maximum atom-type E-State: =CH-
900	maxaaCH	Maximum atom-type E-State: :CH:
901	maxsssCH	Maximum atom-type E-State: >CH-
902	maxddC	Maximum atom-type E-State: =C=
903	maxtsC	Maximum atom-type E-State: #C-
904	maxdssC	Maximum atom-type E-State: =C<
905	maxaasC	Maximum atom-type E-State: :C:-
906	maxaaaC	Maximum atom-type E-State: ::C:
907	maxssssC	Maximum atom-type E-State: >C<
908	maxsNH3p	Maximum atom-type E-State: -NH3+
909	maxsNH2	Maximum atom-type E-State: -NH2
910	maxssNH2p	Maximum atom-type E-State: -NH2-+
911	maxssNH	Maximum atom-type E-State: -NH-
912	maxaaNH	Maximum atom-type E-State: :NH:
913	maxtN	Maximum atom-type E-State: #N
914	maxdsN	Maximum atom-type E-State: =N-
915	maxaaN	Maximum atom-type E-State: :N:
916	maxsssN	Maximum atom-type E-State: >N-
917	maxaasN	Maximum atom-type E-State: :N:-
918	maxsssNp	Maximum atom-type E-State: >N<+
919	maxsOH	Maximum atom-type E-State: -OH
920	maxdO	Maximum atom-type E-State: =O
921	maxssO	Maximum atom-type E-State: -O-
922	maxaaO	Maximum atom-type E-State: :O:
923	maxsOm	Maximum atom-type E-State: -O-
924	maxsF	Maximum atom-type E-State: -F
925	maxdS	Maximum atom-type E-State: =S
926	maxsCl	Maximum atom-type E-State: -Cl
927	sumI	Sum of the intrinsic state values I
928	meanI	Mean intrinsic state values I
929	hmax	Maximum H E-State
930	gmax	Maximum E-State
931	hmin	Minimum H E-State
932	gmin	Minimum E-State
933	LipoaffinityIndex	Lipoaffinity index
934	MAXDN	Maximum negative intrinsic state difference in the molecule (related to the nucleophilicity of the molecule). Using deltaV = (Zv-maxBondedHydrogens) /(atomicNumber-Zv-1). Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.
935	MAXDP	Maximum positive intrinsic state difference in the molecule (related to the electrophilicity of the molecule). Using deltaV = (Zv-maxBondedHydrogens) /(atomicNumber-Zv-1). Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.
936	DELS	Sum of all atoms intrinsic state differences (measure of total charge transfer in the molecule). Using deltaV = (Zv-maxBondedHydrogens) /(atomicNumber-Zv-1). Gramatica, P., Corradi, M., and Consonni,

937	MAXDN2	V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777. Maximum negative intrinsic state difference in the molecule (related to the nucleophilicity of the molecule). Using deltaV = Zv-maxBondedHydrogens. Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.
938	MAXDP2	Maximum positive intrinsic state difference in the molecule (related to the electrophilicity of the molecule). Using deltaV = Zv-maxBondedHydrogens. Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.
939	DELS2	Sum of all atoms intrinsic state differences (measure of total charge transfer in the molecule). Using deltaV = Zv-maxBondedHydrogens. Gramatica, P., Corradi, M., and Consonni, V. (2000). Modelling and prediction of soil sorption coefficients of non-ionic organic pesticides by molecular descriptors. Chemosphere 41, 763-777.
940	ETA_Alpha	Sum of alpha values of all non-hydrogen vertices of a molecule
941	ETA_AlphaP	Sum of alpha values of all non-hydrogen vertices of a molecule relative to molecular size
942	ETA_dAlpha_A	A measure of count of non-hydrogen heteroatoms
943	ETA_dAlpha_B	A measure of count of hydrogen bond acceptor atoms and/or polar surface area
944	ETA_Epsilon_1	A measure of electronegative atom count
945	ETA_Epsilon_2	A measure of electronegative atom count
946	ETA_Epsilon_3	A measure of electronegative atom count
947	ETA_Epsilon_4	A measure of electronegative atom count
948	ETA_Epsilon_5	A measure of electronegative atom count
949	ETA_dEpsilon_A	A measure of contribution of unsaturation and electronegative atom count
950	ETA_dEpsilon_B	A measure of contribution of unsaturation
951	ETA_dEpsilon_C	A measure of contribution of electronegativity
952	ETA_dEpsilon_D	A measure of contribution of hydrogen bond donor atoms
953	ETA_Psi_1	A measure of hydrogen bonding propensity of the molecules and/or polar surface area
954	ETA_dPsi_A	A measure of hydrogen bonding propensity of the molecules
955	ETA_dPsi_B	A measure of hydrogen bonding propensity of the molecules
956	ETA_Shape_P	Shape index P
957	ETA_Shape_Y	Shape index Y
958	ETA_Shape_X	Shape index X
959	ETA_Beta	A measure of electronic features of the molecule
960	ETA_BetaP	A measure of electronic features of the molecule relative to molecular size
961	ETA_Beta_s	A measure of electronegative atom count of the molecule
962	ETA_BetaP_s	A measure of electronegative atom count of the molecule relative to molecular size
963	ETA_Beta_ns	A measure of electron-richness of the molecule
964	ETA_BetaP_ns	A measure of electron-richness of the molecule relative to molecular size
965	ETA_dBeta	A measure of relative unsaturation content
966	ETA_dBetaP	A measure of relative unsaturation content relative to molecular size
967	ETA_Beta_ns_d	A measure of lone electrons entering into resonance
968	ETA_BetaP_ns_d	A measure of lone electrons entering into resonance relative to molecular size
969	ETA_Eta	Composite index Eta
970	ETA_EtaP	Composite index Eta relative to molecular size
971	ETA_Eta_R	Composite index Eta for reference alkane
972	ETA_Eta_F	Functionality index EtaF
973	ETA_EtaP_F	Functionality index EtaF relative to molecular size
974	ETA_Eta_L	Local index Eta_local

975	ETA_EtaP_L	Local index Eta_local relative to molecular size
976	ETA_Eta_R_L	Local index Eta_local for reference alkane
977	ETA_Eta_F_L	Local functionality contribution EtaF_local
978	ETA_EtaP_F_L	Local functionality contribution EtaF_local relative to molecular size
979	ETA_Eta_B	Branching index EtaB
980	ETA_EtaP_B	Branching index EtaB relative to molecular size
981	ETA_Eta_B_RC	Branching index EtaB (with ring correction)
982	ETA_EtaP_B_RC	Branching index EtaB (with ring correction) relative to molecular size
983	FMF	Complexity of a molecule
984	fragC	Complexity of a system
985	nHBAcc	Number of hydrogen bond acceptors (using CDK HBondAcceptorCountDescriptor algorithm)
986	nHBAcc2	Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge <= 0) except a non-aromatic nitrogen that is adjacent to an oxygen and aromatic ring, or an aromatic nitrogen with a hydrogen atom in a ring, or an aromatic nitrogen with 3 neighouring atoms in a ring, or a nitrogen with total bond order >=4; any fluorine)
987	nHBAcc3	Number of hydrogen bond acceptors (any oxygen; any nitrogen where the formal charge of the nitrogen is non-positive (i.e. formal charge <= 0) except a non-aromatic nitrogen that is adjacent to an oxygen and aromatic ring, or an aromatic nitrogen with a hydrogen atom in a ring, or an aromatic nitrogen with 3 neighouring atoms in a ring, or a nitrogen with total bond order >=4, or a nitrogen in an amide bond; any fluorine)
988	nHBAcc_Lipinski	Number of hydrogen bond acceptors (using Lipinski's definition: any nitrogen; any oxygen)
989	nHBDon	Number of hydrogen bond donors (using CDK HBondDonorCountDescriptor algorithm)
990	nHBDon_Lipinski	Number of hydrogen bond donors (using Lipinski's definition: Any OH or NH. Each available hydrogen atom is counted as one hydrogen bond donor)
991	HybRatio	Fraction of sp3 carbons to sp2 carbons
992	IC0	Information content index (neighborhood symmetry of 0-order)
993	IC1	Information content index (neighborhood symmetry of 1-order)
994	IC2	Information content index (neighborhood symmetry of 2-order)
995	IC3	Information content index (neighborhood symmetry of 3-order)
996	IC4	Information content index (neighborhood symmetry of 4-order)
997	IC5	Information content index (neighborhood symmetry of 5-order)
998	TIC0	Total information content index (neighborhood symmetry of 0-order)
999	TIC1	Total information content index (neighborhood symmetry of 1-order)
1000	TIC2	Total information content index (neighborhood symmetry of 2-order)
1001	TIC3	Total information content index (neighborhood symmetry of 3-order)
1002	TIC4	Total information content index (neighborhood symmetry of 4-order)
1003	TIC5	Total information content index (neighborhood symmetry of 5-order)
1004	SIC0	Structural information content index (neighborhood symmetry of 0-order)
1005	SIC1	Structural information content index (neighborhood symmetry of 1-order)
1006	SIC2	Structural information content index (neighborhood symmetry of 2-order)
1007	SIC3	Structural information content index (neighborhood symmetry of 3-order)
1008	SIC4	Structural information content index (neighborhood symmetry of 4-order)
1009	SIC5	Structural information content index (neighborhood symmetry of 5-order)
1010	CIC0	Complementary information content index (neighborhood symmetry of 0-order)
1011	CIC1	Complementary information content index (neighborhood symmetry of 1-order)
1012	CIC2	Complementary information content index (neighborhood symmetry of 2-order)
1013	CIC3	Complementary information content index (neighborhood symmetry of 3-order)
1014	CIC4	Complementary information content index (neighborhood symmetry of 4-order)

1015	CIC5	Complementary information content index (neighborhood symmetry of 5-order)
1016	BIC0	Bond information content index (neighborhood symmetry of 0-order)
1017	BIC1	Bond information content index (neighborhood symmetry of 1-order)
1018	BIC2	Bond information content index (neighborhood symmetry of 2-order)
1019	BIC3	Bond information content index (neighborhood symmetry of 3-order)
1020	BIC4	Bond information content index (neighborhood symmetry of 4-order)
1021	BIC5	Bond information content index (neighborhood symmetry of 5-order)
1022	MIC0	Modified information content index (neighborhood symmetry of 0-order)
1023	MIC1	Modified information content index (neighborhood symmetry of 1-order)
1024	MIC2	Modified information content index (neighborhood symmetry of 2-order)
1025	MIC3	Modified information content index (neighborhood symmetry of 3-order)
1026	MIC4	Modified information content index (neighborhood symmetry of 4-order)
1027	MIC5	Modified information content index (neighborhood symmetry of 5-order)
1028	ZMIC0	Z-modified information content index (neighborhood symmetry of 0-order)
1029	ZMIC1	Z-modified information content index (neighborhood symmetry of 1-order)
1030	ZMIC2	Z-modified information content index (neighborhood symmetry of 2-order)
1031	ZMIC3	Z-modified information content index (neighborhood symmetry of 3-order)
1032	ZMIC4	Z-modified information content index (neighborhood symmetry of 4-order)
1033	ZMIC5	Z-modified information content index (neighborhood symmetry of 5-order)
1034	Kier1	First kappa shape index
1035	Kier2	Second kappa shape index
1036	Kier3	Third kappa (κ) shape index
1037	nAtomLC	Number of atoms in the largest chain
1038	nAtomP	Number of atoms in the largest pi system
1039	nAtomLAC	Number of atoms in the longest aliphatic chain
1040	MLogP	Mannhold LogP
1041	McGowan_Volume	McGowan characteristic volume
1042	MDEC-11	Molecular distance edge between all primary carbons
1043	MDEC-12	Molecular distance edge between all primary and secondary carbons
1044	MDEC-13	Molecular distance edge between all primary and tertiary carbons
1045	MDEC-14	Molecular distance edge between all primary and quaternary carbons
1046	MDEC-22	Molecular distance edge between all secondary carbons
1047	MDEC-23	Molecular distance edge between all secondary and tertiary carbons
1048	MDEC-24	Molecular distance edge between all secondary and quaternary carbons
1049	MDEC-33	Molecular distance edge between all tertiary carbons
1050	MDEC-34	Molecular distance edge between all tertiary and quaternary carbons
1051	MDEC-44	Molecular distance edge between all quaternary carbons
1052	MDEO-11	Molecular distance edge between all primary oxygens
1053	MDEO-12	Molecular distance edge between all primary and secondary oxygens
1054	MDEO-22	Molecular distance edge between all secondary oxygens
1055	MDEN-11	Molecular distance edge between all primary nitrogens
1056	MDEN-12	Molecular distance edge between all primary and secondary nitrogens
1057	MDEN-13	Molecular distance edge between all primary and tertiary niroqens
1058	MDEN-22	Molecular distance edge between all secondary nitroqens

1059	MDEN-23	Molecular distance edge between all secondary and tertiary nitrogens
1060	MDEN-33	Molecular distance edge between all tertiary nitrogens
1061	MLFER_A	Overall or summation solute hydrogen bond acidity
1062	MLFER_BH	Overall or summation solute hydrogen bond basicity
1063	MLFER_BO	Overall or summation solute hydrogen bond basicity
1064	MLFER_S	Combined dipolarity/polarizability
1065	MLFER_E	Excessive molar refraction
1066	MLFER_L	Solute gas-hexadecane partition coefficient
1067	MPC2	Molecular path count of order 2
1068	MPC3	Molecular path count of order 3
1069	MPC4	Molecular path count of order 4
1070	MPC5	Molecular path count of order 5
1071	MPC6	Molecular path count of order 6
1072	MPC7	Molecular path count of order 7
1073	MPC8	Molecular path count of order 8
1074	MPC9	Molecular path count of order 9
1075	MPC10	Molecular path count of order 10
1076	TPC	Total path count (up to order 10)
1077	piPC1	Conventional bond order ID number of order 1 (ln(1+x)
1078	piPC2	Conventional bond order ID number of order 2 (ln(1+x)
1079	piPC3	Conventional bond order ID number of order 3 (ln(1+x)
1080	piPC4	Conventional bond order ID number of order 4 (ln(1+x)
1081	piPC5	Conventional bond order ID number of order 5 (ln(1+x)
1082	piPC6	Conventional bond order ID number of order 6 (ln(1+x)
1083	piPC7	Conventional bond order ID number of order 7 (ln(1+x)
1084	piPC8	Conventional bond order ID number of order 8 (ln(1+x)
1085	piPC9	Conventional bond order ID number of order 9 (ln(1+x)
1086	piPC10	Conventional bond order ID number of order 10 (ln(1+x)
1087	TpiPC	Total conventional bond order (up to order 10) (ln(1+x))
1088	R_TpiPCTPC	Ratio of total conventional bond order (up to order 10) with total path count (up to order 10)
1089	PetitjeanNumber	Petitjean number
1090	nRing	Number of rings
1091	n3Ring	Number of 3-membered rings
1092	n4Ring	Number of 4-membered rings
1093	n5Ring	Number of 5-membered rings
1094	n6Ring	Number of 6-membered rings
1095	n7Ring	Number of 7-membered rings
1096	n8Ring	Number of 8-membered rings
1097	n10Ring	Number of 10-membered rings
1098	n12Ring	Number of 12-membered rings
1099	nG12Ring	Number of >12-membered rings
1100	nFRing	Number of fused rings
1101	nF6Ring	Number of 6-membered fused rings
1102	nF7Ring	Number of 7-membered fused rings

1103	nF8Ring	Number of 8-membered fused rings
1104	nF9Ring	Number of 9-membered fused rings
1105	nF10Ring	Number of 10-membered fused rings
1106	nF11Ring	Number of 11-membered fused rings
1107	nF12Ring	Number of 12-membered fused rings
1108	nFG12Ring	Number of >12-membered fused rings
1109	nTRing	Number of rings (includes counts from fused rings)
1110	nT4Ring	Number of 4-membered rings (includes counts from fused rings)
1111	nT5Ring	Number of 5-membered rings (includes counts from fused rings)
1112	nT6Ring	Number of 6-membered rings (includes counts from fused rings)
1113	nT7Ring	Number of 7-membered rings (includes counts from fused rings)
1114	nT8Ring	Number of 8-membered rings (includes counts from fused rings)
1115	nT9Ring	Number of 9-membered rings (includes counts from fused rings)
1116	nT10Ring	Number of 10-membered rings (includes counts from fused rings)
1117	nT11Ring	Number of 11-membered rings (includes counts from fused rings)
1118	nT12Ring	Number of 12-membered rings (includes counts from fused rings)
1119	nTG12Ring	Number of >12-membered rings (includes counts from fused rings)
1120	nHeteroRing	Number of rings containing heteroatoms (N, O, P, S, or halogens)
1121	n3HeteroRing	Number of 3-membered rings containing heteroatoms (N, O, P, S, or halogens)
1122	n4HeteroRing	Number of 4-membered rings containing heteroatoms (N, O, P, S, or halogens)
1123	n5HeteroRing	Number of 5-membered rings containing heteroatoms (N, O, P, S, or halogens)
1124	n6HeteroRing	Number of 6-membered rings containing heteroatoms (N, O, P, S, or halogens)
1125	n7HeteroRing	Number of 7-membered rings containing heteroatoms (N, O, P, S, or halogens)
1126	n8HeteroRing	Number of 8-membered rings containing heteroatoms (N, O, P, S, or halogens)
1127	n10HeteroRing	Number of 10-membered rings containing heteroatoms (N, O, P, S, or halogens)
1128	n12HeteroRing	Number of 12-membered rings containing heteroatoms (N, O, P, S, or halogens)
1129	nG12HeteroRing	Number of >12-membered rings containing heteroatoms (N, O, P, S, or halogens)
1130	nF7HeteroRing	Number of 7-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1131	nF8HeteroRing	Number of 8-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1132	nF9HeteroRing	Number of 9-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1133	nF10HeteroRing	Number of 10-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1134	nF11HeteroRing	Number of 11-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1135	nF12HeteroRing	Number of 12-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1136	nFG12HeteroRing	Number of >12-membered fused rings containing heteroatoms (N, O, P, S, or halogens)
1137	nT4HeteroRing	Number of 4-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1138	nT5HeteroRing	Number of 5-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1139	nT6HeteroRing	Number of 6-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1140	nT7HeteroRing	Number of 7-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1141	nT8HeteroRing	Number of 8-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1142	nT9HeteroRing	Number of 9-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1143	nT10HeteroRing	Number of 10-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1144	nT11HeteroRing	Number of 11-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)

1145	nT12HeteroRing	Number of 12-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1146	nTG12HeteroRing	Number of >12-membered rings (includes counts from fused rings) containing heteroatoms (N, O, P, S, or halogens)
1147	nRotB	Number of rotatable bonds, excluding terminal bonds
1148	RotBFrac	Fraction of rotatable bonds, excluding terminal bonds
1149	nRotBt	Number of rotatable bonds, including terminal bonds
1150	RotBtFrac	Fraction of rotatable bonds, including terminal bonds
1151	LipinskiFailures	Number failures of the Lipinski's Rule Of 5
1152	topoRadius	Topological radius (minimum atom eccentricity)
1153	topoDiameter	Topological diameter (maximum atom eccentricity)
1154	topoShape	Petitjean topological shape index
1155	GGI1	Topological charge index of order 1
1156	GGI2	Topological charge index of order 2
1157	GGI3	Topological charge index of order 3
1158	GGI4	Topological charge index of order 4
1159	GGI5	Topological charge index of order 5
1160	GGI6	Topological charge index of order 6
1161	GGI7	Topological charge index of order 7
1162	GGI8	Topological charge index of order 8
1163	GGI9	Topological charge index of order 9
1164	GGI10	Topological charge index of order 10
1165	JGI1	Mean topological charge index of order 1
1166	JGI2	Mean topological charge index of order 2
1167	JGI3	Mean topological charge index of order 3
1168	JGI4	Mean topological charge index of order 4
1169	JGI5	Mean topological charge index of order 5
1170	JGI6	Mean topological charge index of order 6
1171	JGI7	Mean topological charge index of order 7
1172	JGI8	Mean topological charge index of order 8
1173	JGI9	Mean topological charge index of order 9
1174	JGI10	Mean topological charge index of order 10
1175	JGT	Global topological charge index
1176	SpMax_D	Leading eigenvalue from topological distance matrix
1177	SpDiam_D	Spectral diameter from topological distance matrix
1178	SpAD_D	Spectral absolute deviation from topological distance matrix
1179	SpMAD_D	Spectral mean absolute deviation from topological distance matrix
1180	EE_D	Estrada-like index from topological distance matrix
1181	VE1_D	Coefficient sum of the last eigenvector from topological distance matrix
1182	VE2_D	Average coefficient sum of the last eigenvector from topological distance matrix
1183	VE3_D	Logarithmic coefficient sum of the last eigenvector from topological distance matrix
1184	VR1_D	Randic-like eigenvector-based index from topological distance matrix
1185	VR2_D	Normalized Randic-like eigenvector-based index from topological distance matrix
1186	VR3_D	Logarithmic Randic-like eigenvector-based index from topological distance matrix
1187	TopoPSA	Topological polar surface area
1188	VABC	Van der Waals volume calculated using the method proposed in [Zhao, Yuan H. and Abraham, Michael

		H. and Zissimos, Andreas M., Fast Calculation of van der Waals Volume as a Sum of Atomic and Bond Contributions and Its Application to Drug Compounds, The Journal of Organic Chemistry, 2003, 68:7368-7373]
1189	VAdjMat	Vertex adjacency information (magnitude)
1190	MWC2	Molecular walk count of order 2 (ln(1+x)
1191	MWC3	Molecular walk count of order 3 (ln(1+x)
1192	MWC4	Molecular walk count of order 4 (ln(1+x)
1193	MWC5	Molecular walk count of order 5 (ln(1+x)
1194	MWC6	Molecular walk count of order 6 (ln(1+x)
1195	MWC7	Molecular walk count of order 7 (ln(1+x)
1196	MWC8	Molecular walk count of order 8 (ln(1+x)
1197	MWC9	Molecular walk count of order 9 (ln(1+x)
1198	MWC10	Molecular walk count of order 10 (ln(1+x)
1199	TWC	Total walk count (up to order 10)
1200	SRW2	Self-returning walk count of order 2 (ln(1+x)
1201	SRW3	Self-returning walk count of order 3 (ln(1+x)
1202	SRW4	Self-returning walk count of order 4 (ln(1+x)
1203	SRW5	Self-returning walk count of order 5 (ln(1+x)
1204	SRW6	Self-returning walk count of order 6 (ln(1+x)
1205	SRW7	Self-returning walk count of order 7 (ln(1+x)
1206	SRW8	Self-returning walk count of order 8 (ln(1+x)
1207	SRW9	Self-returning walk count of order 9 (ln(1+x)
1208	SRW10	Self-returning walk count of order 10 (ln(1+x)
1209	TSRW	Total self-return walk count (up to order 10) (ln(1+x))
1210	MW	Molecular weight
1211	AMW	Average molecular weight (Molecular weight / Total number of atoms)
1212	WTPT-1	Molecular ID
1213	WTPT-2	Molecular ID / number of atoms
1214	WTPT-3	Sum of path lengths starting from heteroatoms
1215	WTPT-4	Sum of path lengths starting from oxygens
1216	WTPT-5	Sum of path lengths starting from nitrogens
1217	WPATH	Weiner path number
1218	WPOL	Weiner polarity number
1219	XLogP	XLogP
1220	Zagreb	Sum of the squares of atom degree over all heavy atoms i