NORWEGIAN ENVIRONMENT AGENCY

REPORT

M-911|2017 | 2017

Norwegian Institute for Water Research

Biodegradation of selected offshore chemicals

COLOPHON

Executive institution

Norwegian Institute for Water Research, NIVA — NIVA report 7218-2017

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M-no	Year	Pages	Contract number
M-911|2017	2017	118	17088152

Publisher

Norwegian Environment Agency

The project is funded by

Norwegian Environment Agency

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Title - Norwegian and English

Biodegradation of selected offshore chemicals
Evaluering av nedbrytningsegenskaper for utvalgte offshorekjemikalier

ISBN: 978-82-577-6953-6

Summary - sammendrag

A review of biodegradation data for specific oil field chemicals and chemical groups were performed in order to evaluate if the current categorisation of these were appropriate based on the biodegradation properties. Data were compiled from databases like ECHA and MITI and from the literature. For compounds with limited or inconclusive test data, biodegradation was also estimated by the BIOWIN models, and the EAWAG-BBD pathway prediction system was used to predict plausible biodegradation pathways. A weight of evidence approach was used to assess the compiled information and a conclusion regarding categorisation of the single chemicals and/or chemical groups were performed whenever possible. For most compounds, no clear conclusion on the biodegradability could be drawn. Only two of the investigated compounds, benzotriazole and N-methyldiethanolamine, were assessed to very likely and likely have a biodegradability of less than 20% in seawater.

4 emneord

Nedbrytbarhet, Offshore-kjemikalier, QSAR

4 subject words

Biodegradation, Offshore chemicals, QSAR

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1. Results of the literature search

2. BIOWIN output data

3. EAWAG-BBD Pathway Prediction System

Summary

A review of biodegradation data for specific oil field chemicals and chemical groups were performed to evaluate if the current categorisation of these, according to the Norwegian regulations, were appropriate based on the biodegradation properties. Chemicals used in the petroleum industry are in Norway categorised into black, red, yellow and green environmental categories. Chemicals in the black category are not readily biodegradable, show a high potential for bioaccumulation and have a high acute toxicity. Chemicals in the red category are slowly biodegraded in the marine environment, show potential for bioaccumulation and/or are acutely toxic. Organic chemicals are classified as red when the biodegradation measured as BOD28 (biological oxygen demand after 28 days) is ≤ 20%, or if two of the following three criteria are fulfilled: biodegradation measured as BOD < 60%, log Pow ≥3, acute toxicity ≤ 10 mg/L. Chemicals in the red category can be harmful to the environment and shall be prioritized for substitution with less harmful alternatives. Chemicals in the yellow category are the ones that do not qualify for red or black category and which is not listed on the OSPARs PLONOR-list (pose little or no risk to the environment).

Biodegradation data were compiled from databases such as ECHA and MITI, and supporting information on biodegradation from the literature. Biodegradation was also estimated by the BIOWIN models, and the EAWAG-BBD pathway prediction system was used to predict plausible biodegradation pathways. A weight of evidence approach was used to assess the compiled information and a conclusion regarding categorisation of the single chemicals and/or chemical groups were performed whenever possible. For most compounds, no clear conclusion on the biodegradability could be drawn due to conflicting data or limited amount of relevant data. Only two of the investigated single compounds were assessed to very likely (benzotriazole) and likely (N-methyldiethanolamine) have a biodegradability of less than 20% in seawater in 28 days. For the two compounds polydimethylsiloxan and Di-Epoxide/Oxyalkylated polyglycolan, no relevant biodegradation data were found and both compounds were outside the applicability domain of the BIOWIN model for biodegradation prediction.

The search strategy for information on biodegradation on chemical groups were to search either for single chemical representatives and/or for general observations for the chemical group. A rather large variation in data for chemical group representatives, limited available relevant data and large differences in size of the compounds within a group was found. However, based on the available information and general rules of thumb for biodegradation, large molecules of polyacrylamide and hydrolysed polyacrylamide (<1e^6 DA) are likely to be categorised as red. Quaternary ammonium compounds contain both ready biodegradable and persistent substances and no general conclusion for the group can be drawn. Large polymers of polyacrylate are likely to be categorised as red, however, it is possible to include co-polymers during synthesis to create a more degradable polymer.

Overall, the review of biodegradation test data and predicted data identified two compounds that are likely and very likely to be in the red category. For most of the other single compounds, no clear conclusion could be drawn due to conflicting or limited amount of relevant data. A general evaluation of different chemical groups was challenging due to the different properties and sizes of the chemicals within each group. However, large polymers of polyacrylamide, hydrolysed polyacrylamides and polyacrylates are likely to be in the red category. For most compounds and chemical groups, more information is warranted to evaluate the biodegradation in sea water and thus the assessment of proper categorisation of the chemicals.

Sammendrag

Nedbrytningsdata for spesifikke petroleumskjemikalier og kjemiske grupper ble samlet inn og gjennomgått for å vurdere om den gjeldende kategoriseringen av disse stoffene var passende basert på stoffenes nedbrytningsegenskaper.

I Norge kategoriseres petroleumskjemikalier i svart, rød, gul og grønn miljøkategori. Stoffer i svart kategori er ikke lett nedbrytbare, har et høyt potensial for bioakkumulering og har høy akutt giftighet. Stoffer i rød kategori brytes sakte ned i det marine miljøet, viser potensial for bioakkumulering og/eller er akutt giftige. Organiske stoffer plasseres i rød kategori når nedbrytningen målt som BOD28 (biologisk oksygenforbruk etter 28 dager) er ≤ 20%, eller hvis stoffet oppfyller to av følgende tre kriterier: nedbrytning målt som BOD < 60%, logPow ≥3, akutt giftighet ≤ 10 mg/L. Stoffer i rød kategori kan være skadelige for miljøet og skal prioriteres for erstatning med mindre skadelige alternativer. Stoffer i gul kategori har egenskaper som ikke kvalifiserer til rød eller svart kategori og som ikke er listet opp på OPARs PLONOR-liste (pose little or no risk to the environment).

Nedbrytningsdata ble hentet fra databaser som ECHA og MITI, og støttende informasjon om nedbrytning ble hentet fra vitenskapelig litteratur. Nedbrytning ble også estimert ved bruk av BIOWIN modeller, og «EAWAG-BBD pathway prediction system» ble brukt for å predikere sannsynligheten for ulike nedbrytningsveier. En «weight of evidence» tilnærming ble brukt for å vurdere den innsamlede informasjonen og en konklusjon angående kategoriseringen av stoffene og stoffgruppene ble gjort der dette var mulig. For de fleste stoffene var det ikke mulig å trekke noen klare konklusjoner på grunn av motstridende data eller begrenset mengde med relevante data. Kun to av de vurderte stoffene, benzotriazole and N-methyldiethanolamine ble vurdert til veldig sannsynlig eller sannsynlig å ha en nedbrytning mindre enn 20% i sjøvann iløpet av 28 dager. For de to stoffene polydimetylsiloksan og di-epoxide/oxyalkylated polyglykol ble de ikke funnet noen relevante nedbrytningsdata og begge stoffene var utenfor brukerdomenet til BIOWIN prediksjonsmodellene.

Strategien for litteratursøket for nedbrytningsdata og generell informasjon om nedbrytning av stoffgruppene var å søke på enkeltstoffer som representanter for stoffgruppen og/eller for generelle observasjoner for stoffgruppen. Det var stor variasjon i dataene for representantene for stoffgruppene, begrenset mengde med relevante data og store forskjeller i størrelsen på stoffene innen en stoffgruppe. Basert på den tilgjengelige informasjonen og generelle tommelfingerregler for nedbrytning ble det likevel vurdert dit at store molekyler av polyakrylamid og hydrolysert polyakrylamid (>1e^6 DA) sannsynligvis er i rød kategori. Stoffgruppen kvarternære ammoniumforbindelser består av stoffer som lett nedbrytbare og stoffer som er persistente. Det kan derfor ikke trekkes noen generell konklusjon for denne stoffgruppen. Store polymerer av polyakrylat er sannsynligvis i rød kategori, men det er mulig å inkludere kopolymerer for å øke nedbrytbarheten.

Gjennomgangen og vurderingen av test-data og predikerte data for nedbrytbarhet førte til identifisering av to stoffer som sannsynlig og veldig sannsynlig kan plasseres i rød kategori. For de fleste andre enkeltstoffene kunne det ikke trekkes noen klare konklusjoner på grunn av motstridende data eller begrenset mengde relevante data. En generell vurdering av stoffgruppene var utfordrende på grunn av de ulike egenskapene og størrelsene på stoffene innenfor de enkelte stoffgruppene. Likevel ble det vurdert at store polymerer av polyakrylamid, hydrolysert polyakrylamid og polyakrylater sannsynligvis kan plasseres i rød kategori. For de fleste enkeltstoffer og stoffgrupper trengs det mer informasjon for å evaluere nedbrytningen i sjøvann og deretter gjøre en korrekt kategorisering av stoffene.

1. Background

1.1 Chemicals used in oilfield industries

The convention for the Protection of the Marine Environment of the North-East Atlantic (the 'OSPAR Convention') entered into force in 1998 and was signed by 17 governments and the EU cooperative. The convention contains decisions, recommendations and agreements, also regarding regulations on use of chemicals. The harmonized Offshore Chemical Notification Format (HOCNF) applies to all chemicals used in connection with offshore exploration and production activities in the OSPAR maritime area(1). However, the substances included in HOCNF should also fully comply with the relevant requirements of REACH (registration, evaluation, authorisation and restriction of chemicals) for that substance. There are in addition some extra requirements for the HOCNF, for example that toxicity and biodegradation data should preferably be obtained with marine tests. In addition to these requirements, the Norwegian government has adopted five sets of regulations for health, safety and the environment (HSE) in Norway's offshore petroleum sector. In the activities regulation (2), emissions and discharges to the external environment are regulated, amongst others, based on a categorization of chemicals (Figure 1) based on their possible impact on the environment with the goal to substitute chemicals with high risk to the environment with more environmentally friendly chemicals.

Most organic chemicals, used in the petroleum industry, should be tested for biodegradation in seawater, bioaccumulation potential and acute toxicity for marine organisms (ecotoxicity tests on algae, crustaceans and fish). Based on the results, the chemicals are categorized into black, red, yellow and green environmental categories. Chemicals in the black category are not readily biodegradable, show a high potential for bioaccumulation and have a high acute toxicity. In principle, use and discharge of these chemicals is not permitted unless deemed necessary based on safety- and technical reasons, or it has been documented in special cases that application of these will result in the lowest risk for environmental harm. Chemicals in the red category are slowly biodegraded in the marine environment, show potential for bioaccumulation and/or are acutely toxic. Organic chemicals are classified as red when the biodegradation measured as BOD28 (biological oxygen demand after 28 days) is ≤ 20%, or if the chemicals fulfill two of the following three criteria: biodegradation measured as BOD < 60%, log Pow ≥3, acute toxicity ≤ 10 mg/L. Chemicals in the red category can be harmful to the environment and shall be prioritized for substitution with less harmful alternatives. Approval of use and discharge are given only based on documented safety- and technical reasons. Chemicals in the yellow category are the ones with properties that do not qualify for red or black category and which is not listed on the OSPARs PLONOR-list (pose little or no risk to the environment). The chemicals in yellow category are further divided into sub-categories a to c depending on the biodegradation of the degradation products. Chemicals on the PLONOR list are considered to have no, or very low, effect on the environment.

	Priority list from Stortingsmelding nr. 21 OSPAR List of Chemicals for Priority Action BOD28 < 20% + Kow > 4.5 BOD28 < 20% + (LC50 / EC50 < 10 mg/L) Substances that are genotoxic / reprotoxic	 PB PT
	BOD28 < 20% Or two of the following criteria - BOD28 < 60% - Kow > 3 and Mw < 700 - LC50 or EC50 < 10 mg/L	P P B T
	Doesn't fit in any other categories	
	OSPARs PLONOR-list (pose little or no risk to the environment)	

Figure 1. Categorisation of chemicals used in oilfield industries. P refers to properties that affect persistence, B to properties that affect bioaccumulation and T to properties that affect toxicity.

Biodegradability is the most important property for assessing the environmental fate of chemicals. Therefore, the persistence of the chemical has a large influence of whether a chemical is categorized as red or yellow. Biodegradability of offshore chemicals are tested with the OECD 306 test: "Biodegradability in Seawater". The results for the same chemical can vary due to differences in the raw materials, uncertainties in the analytical methods, and variation in the content of microorganisms in the seawater used in the test (3). The variance could be problematic for organic compounds with biodegradation around 20%, and can make it difficult to make a correct categorization of the chemicals (yellow or red category). Thus, there is a potential for mis-categorization (3).

Due to variation in biodegradation data, and uncertainty in the categorization of substances in the environmental categories, there is a need to evaluate the available biodegradation data for certain offshore chemicals and some chemical groups. An assessment must be carried out to find out whether their current category placement can be justified, if there is a need to change their current category or if more information is needed to draw a sound conclusion on the biodegradation potential. This project focused on chemicals used in offshore petroleum activity that show variation in the test results for biodegradation (around 20% BOD). The selected offshore chemicals and representatives of chemical groups covered by this project are shown in table 2 (section 1.4).

1.2 Factors affecting biodegradation

1.2.1 Definition of biodegradation (4)

Degradation is the loss or transformation of a chemical. When this happens due to biotic or biological activity it is referred to as **biodegradation**. Biodegradation occurs because the microorganisms use the chemical as a source of energy or as building blocks to produce new biomass. **Aerobic biodegradation** is degradation when oxygen is present, while **anaerobic biodegradation** is degradation without oxygen. Primary degradation is the first transformation of a chemical to a new chemical. **Specific chemical analysis** (analysis targeting one chemical) can be used to measure **primary degradation** as loss (dissipation) of the chemical of interest. **Ultimate degradation** is the degradation process that leads to inorganic end products (i.e. CO_2, NH_4, NO_3) and biomass, often referred to as full mineralization. Ultimate degradation is measured by indirect methods, either removal of dissolved organic carbon (DOC), microbial oxygen consumption or CO_2 production. The indirect methods for measuring ultimate biodegradation will usually not measure 100% degradation since some of the chemicals will be incorporated into new biomass.

Testing the potential for a chemical to biodegrade is one of the parameters that help understand the **fate** of the chemical in the environment. Understanding how long a chemical persists in the environment is important when evaluating exposure for environmental risk assessments. A chemical that degrades fast in the environment is referred to as **readily biodegradable**, while a chemical that degrades slowly or not at all is a **persistent chemical**.

1.2.2 Resistance towards biodegradation

Reasons why a substance can be resistant to biodegradation is summarized in Figure 2.(5)

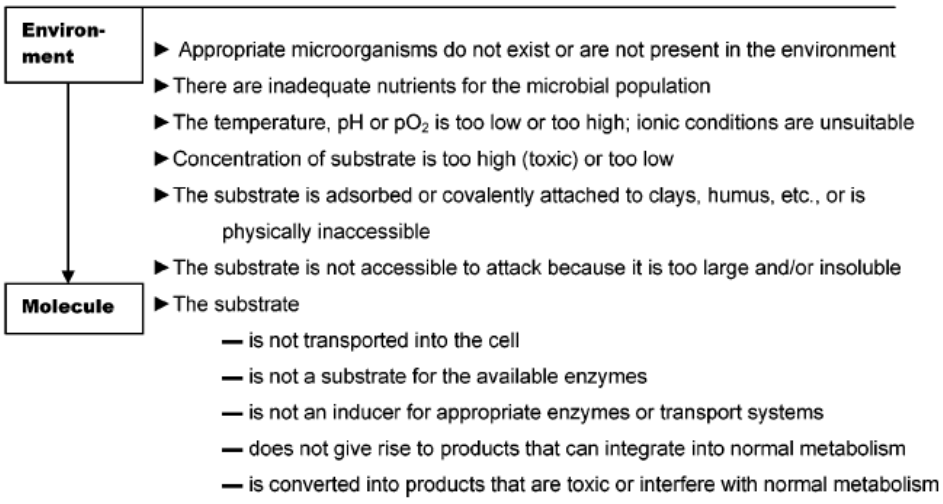


Figure 2. Overview of factors affecting the resistance of a substance to microbial degradation. Modified from (5)

Below follows a description of some of the factors that affect biodegradation of organic molecules in general and factors of relevance to the laboratory tests that are used for determining biodegradability.

1.2.3 Microbial factors

Microorganisms uses enzymes for degrading organic matter to be used as source of energy or growth. Not all bacteria can produce all enzymes necessary to break all types of chemical bindings, so it is important with a diverse microbial consortium to be able to degrade organic chemicals. Different environmental niches such as seawater, rivers, wastewater treatment plants, sediments and soil will have different microbial communities, so that biodegradation data from one environmental niche is not directly transferable to another niche (4, 6, 7).

The most important microbial factors that affect the results of biodegradation lab tests are the source, diversity and abundance of microorganisms in the test inoculum (6). The seawater test OECD 306 has often lower concentration of bacteria than the OECD 301 test series, making it a more stringent test (8), while the inherent test OECD 302 uses a higher inoculum concentration than the OECD 301 tests to increase chances of biodegradation. Both increasing concentration of bacteria or using larger test volume is used to increase chances of biodegradation (9).

Another factor is the time the bacteria needs for adapting to a new environment or producing the enzymes they need for biodegradation. This is referred to as the lag-phase. Studies have shown that marine bacteria often show longer lag-phases than freshwater bacteria (7). Changes in test set-up that can influence the lag-phase is acclimatizing (or aging) of test inoculum or pre-exposure of bacteria to the test substance (adaption) (10). Aging of test water up to one week is accepted within the OECD 306 guideline, while adaption of inoculum to test substance is not accepted in any biodegradation tests (4).

The chemical substance can be used as either a source of energy or building blocks. Bacteria need both carbon, nitrogen and phosphorous as key elements for growth (7). Organic chemicals that contain a large portion of nitrogen or phosphorus (i.e. as amines or phosphonates) can be used as nitrogen or phosphorous sources for the bacteria in the environment. However, in laboratory test, inorganic sources of nitrogen and phosphorous is added and is often more available than the organic sources. Nitrogen containing substances can appear to have high (false) biodegradability in tests that use dissolved oxygen as the end point if nitrification is not included in the assessment. Organic nitrogen can be degraded to either ammonia (NH_3) without consuming oxygen, or nitrite (NO_2) or nitrate (NO_3) with the consumption of oxygen. Another factor that differs in the laboratory tests is that the test substance is added as the only carbon source, while in the environment it can be co-degraded together with other substances even if the substance cannot be used as source of energy or for growth (7).

1.2.4 Environmental factors

Biodegradation in water, sediments or soil can be affected by different factors such as transport processes, salinities, dissolved oxygen, pH and temperatures that are specific to that environmental niche (4). Laboratory tests for biodegradation can simulate the environment only to a certain extent. Especially the temperature is most often higher in laboratory tests than in the environment (6). Most biological processes are faster at higher temperature, and the Arrhenius equation can be used to estimate the reaction rates (or degradation rates) at different temperatures (7). However, some microorganisms are adapted to a cold climate (psychrophilic) and will not grow at higher temperatures. Thus, the source of the inoculum should be taken into consideration when choosing the test temperature (7).

The presence or absence of oxygen is decisive for aerobic or anaerobic biodegradation. The aerobic and anaerobic degradation pathway use different enzymes, and results in different end products (methane (CH_4) in anaerobic process and carbon dioxide (CO_2) in aerobic processes). Thus, results from anaerobic and aerobic biodegradation studies are not easily comparable. It is also important that aerobic screening tests using closed bottles is designed so that there is residual dissolved oxygen in the test flasks to prevent anaerobic conditions.

1.2.5 Chemical structure

The structural or chemical factors of a substance can affect the potential for biodegradation by affecting bioavailability, microbial toxicity and/or by the type of chemical bindings in the molecule. Bioavailability is affected by the molecules solubility in water, partition coefficient and also molecular size and tertiary structures. Some substances are toxic or inhibitory to microbial growth and biodegradation of these substances are thus hindered or reduced. Some generalisations regarding biodegradation have been proposed by various sources. For instance, the OSPAR Guidelines for Completing the Harmonised Offshore Chemical Notification Format (HOCNF) states that offshore chemicals being man-made polymers can be assessed as non-biodegradable without the provision of test data if they are not polycationic, surface active or have a functional group equivalent weight equal to or less than 5 000 Da (1). A study of the biodegradation of 43 solvents found that the sterically hindered compounds, cyclic compounds which were not natural and most of the tested tertiary alkanolamines had a biodegradability lower than 20 % (11). Some generalizations can also come from different modeling approaches. In a group contribution model (12) compounds containing quaternary carbons and tertiary amines are assumed to be less biodegradable than compounds having linear carbon chains of four, and primary and secondary amino and hydroxyl groups result in higher biodegradability.

In essence, a large number of generalizations about the effects of chemical structure on biodegradability have emerged, including effects of various substituent groups or substructures, the number and times a given substituent appears in a molecule, substituent position, size, and branching(5). Some of the generalizations have been formulated as “rules of thumb” for biodegradation in a review by Boethling et al.(5) and are given below.

Molecular features that generally increase resistance to aerobic biodegradation includes:
1) Halogens, especially chlorine and fluorine and especially if there are more than three in a small molecule. Highly substituted structures are likely to be less easily biodegraded than much simpler compounds.
2) Extensive chain branching, quaternary carbon is especially problematic.
3) Tertiary amine, nitro, nitroso, azo, and arylamino groups.
4) Polycyclic residues, such as in PAHs, especially when there are more than three fused rings.
5) Heterocyclic residues.
6) Aliphatic ether bonds (except in ethoxylates).

Molecular features that generally increase aerobic biodegradation includes:
1) Groups susceptible to enzymatic hydrolysis like esters and amides.
2) Oxygen atom present in the form of hydroxyl, aldehyde, or carboxylic acid groups and probably also ketone.
3) Unsubstituted linear alkyl chains (especially with ≥ 4 carbons) and phenyl rings.

1.3 Methods for evaluating biodegradation

1.3.1 Standardized tests for biodegradation

Different tests are designed to evaluate ready biodegradability and persistence, and to cover all environmental compartments (fresh and marine water, fresh and marine sediments, soil and sludge/waste water). Tests can be performed both in the presence and absence of oxygen. An overview of guidelines from The Organisation for Economic Co-operation and Development (OECD), International Organization for Standardization (ISO) and Office of Pollution Prevention and Toxics (OPPTS) on tests for biodegradability is presented in: International Guidelines for Assessing Biodegradability (Appendix R.7.9—1). Below follows a short summary of the most relevant tests.

Ready biodegradability tests are also referred to as **screening tests**. They have a simple design (lab test over 28 days, aerobic, incubation in dark) with higher chemical concentration than what is expected in the environment. Microorganisms are added and are normally from activated sludge from waste water treatment plants. These tests are quite stringent because of the high chemical concentration that can be inhibitory to microorganism. A failed test does therefore not rule out a potential for ready biodegradability. **OECD 301** test series (A to F) and the **OECD 310** are used for ready biodegradability testing in freshwater. The different tests use different methods for measuring ultimate biodegradation.

Table 1. Screening tests for ready biodegradability
Freshwater tests

OECD test nr	Test name (alternative guidelines)	Description	Pass level
301 A	DOC die away (ISO 7827)	Open shake flask where DOC is measured. Non-volatile test substance	70% removal of dissolved organic carbon (DOC) within 10-day window
301 B	CO_2 evolution test (ISO 9439, OPPTS 835.3120)	Measures CO_2 production	60% theoretical CO_2 ($ThCO_2$) production within 10-day window
301 C	modified MITI[1]	Test using automatic respirometers measuring O_2 uptake. Subject to interference from nitrification	60% theoretical oxygen demand (ThOD)
301 D	Closed bottle test (ISO 10707)	Manual measurements of dissolved oxygen (DO). Subject to interference from nitrification	60% ThOD within 10-day window
301 E	Modified OECD screening test (ISO 7827)	Test similar to 301 A, but with a lower concentration of microorganisms	70% removal of DOC within 10-day window
301 F	Manometric respirometry test (ISO 9408)	Closed bottle with head space and automatic measurement of air pressure (manometric respirometry)	60% ThOD within 10-day window
310	Headspace test (ISO 14593)	Measures inorganic carbon (IC) in the water phase and head space	60% theoretical IC (ThIC) production within 10-day window

The different methods have different detection limits and thus require different initial concentrations of chemicals, and differ in use with respect to solvability and volatility. The

[1] Ministry of International Trade and Industry, Japan

pass level for ready biodegradability is 70% removal of DOC and 60% of theoretical oxygen demand (ThOD) or theoretical CO_2 ($ThCO_2$) production for respirometric methods. These pass levels must be reached in a 10-day window (except for 301 C MITI test) within the test period of 28 days.

The seawater test OECD 306 is also a screening test and has a similar test set-up to OECD 301 A and E (shake flask DOC die away and closed bottle DO analysis). However, no microorganisms are added to the test water besides the indigenous organisms in the seawater. That is why this test is more stringent than the OECD 301 tests. The test guideline of OECD 306 states that "If the result is positive (<70% DOC removal; <60% ThOD), it may be concluded that there is a potential for biodegradation in the marine environment. However, a negative result does not preclude such a potential but indicated that further study is necessary(..)". The **marine BODIS test** (BOD-test for insoluble substances) is used for chemicals that has low water solubility and is a modification of an ISO test for freshwater BODIS (**ISO 10708**: "Water quality – Evaluation in an aqueous medium of ultimate aerobic biodegradability of organic compounds. – Determination of biochemical oxygen demand in a two-phase closed bottle test") published by OSPAR (appendix 6 of HOCNF).

Modified screening tests are the test describes above, but with lower test concentration than recommended in the guideline because the test substance can be inhibitory to microorganisms, or modification to facilitate testing of substances that are poorly water soluble. These tests are considered valid test for ready biodegradability when modifications are performed according to the recommendations in the guidelines. **Enhanced screening tests** has extended incubation time and/or increased volumes (larger test vessels) to compensate for long lag phases before incubation starts and is mainly used to show that a substance is not persistent. Other enhancements that are not acceptable in REACH regulation include the use of higher concentrations of microorganisms, pre-adaption of microorganisms to the test substance, semi-continuous assessment and use of co-substrate.

Inherent biodegradability tests (OECD 302 A-C) uses a higher concentration of added bacteria **(**inoculum), thus offering a higher chance of enabling biodegradation. Therefore, if the inherent test is negative this could indicate the potential for environmental persistence. According to the guideline, the Inoculum is not allowed to be pre-adapted. Pass criteria for Zahn-Wellens (OECD 302B) is ≥70% mineralization (DOC removal) within 7 days; log phase no longer than 3d; removal before degradation occurs below 15%. Pass criteria for MITI II test (OECD TG 302C) ≥70% mineralisation (O_2 uptake) within 14 days; lag phase no longer than 3 days.

Simulation tests are designed to simulate environmental conditions, including environmentally relevant substance concentrations, and are used to assess persistence. OECD 308 is for aerobic and anaerobic transformation in aquatic sediment systems and OECD 309 is a test for aerobic mineralisation in surface water. They can both be used for marine and freshwater systems. The biodegradation potential in these tests are reported as biodegradation half-lives (time to reach 50% reduction), however, OSPAR allow the use of raw data from these tests to calculate percent biodegradation if certain test criteria are met. Other tests can be used to simulate environmental conditions in soil (OECD 304 and 307), sludge (OECD 311) and waste water (OECD 314).

1.3.2 Using biodegradation data for classification of persistence

Biodegradation tests according to OECD are designed to help the categorisation of chemicals according to REACH (13, 14), where the purpose is to establish if the chemical fall into the category readily biodegradable (screening tests), or if they are persistent (P) or very persistent (vP). Persistence is defined by half lives of the chemicals, preferably derived from test data from OECD 308 or 309 tests

REACH (EC 1907/2006) Annex XIII criteria:

- The degradation half-life in marine water is higher than 60 days, or
- The degradation half-life in fresh- or estuarine water is higher than 40 days, or
- The degradation half-life in marine sediment is higher than 180 days, or
- The degradation half-life in fresh- or estuarine water sediment is higher than 120 days, or
- The degradation half-life in soil is higher than 120 days.

According to OSPAR § 2.2, 57(1): The substance will be considered persistent if:

i. Biodegradation is <20% in OECD 306, Marine BODIS or any other accepted marine protocols or <20% in 28 days freshwater (ready test).
ii. Half-life values derived from aquatic simulation tests (e.g. OECD 308, 309) indicate persistence to REACH (EC 1907/2006) Annex XIII criteria.

However, according to the Norwegian activities regulation (2), a chemical is classified in red or black category if biodegradation is less than 20% BOD28 in a seawater test (OECD 306 or marine BODIS).

The OSPAR and Norwegian regulations, including 20% biodegradation in screening tests as an indicator of persistence, is thus a more stringent requirement than what is described in REACH where a negative screening test does not preclude biodegradation, but means that there is a need for further testing of persistence. A biodegradation of 20% in a screening test can indicate primary degradation, thus, even if a substance is not considered persistent in accordance with REACH, it can still be in the red or black category according to the Norwegian regulation of offshore chemicals (2).

1.3.3 Prediction of biodegradation

An intensive development of and/or improvement of quantitative and qualitative biodegradability models have occurred over the recent years due to application of new and advanced computational and statistical methods and by use of larger data sets for biodegradation data. One of the methods for predicting biodegradation is the group contribution method which is developed to generalize the applicability to a large and structurally diverse sets of chemicals. The group contribution approach allows structurally diverse sets of chemicals to be analyzed but it has the disadvantage of being dependent on the type and number of a priori selected fragments, and the results are therefore strongly affected by the way the molecule is fragmented (15). The Biodegradation Probability Program (BIOWIN) is a well-used group contribution approach that estimates the probability of rapid aerobic biodegradation of organic chemicals in the presence of mixed populations of environmental microorganisms using seven different models:

Biowin1: linear probability model
Biowin2: nonlinear probability model
Biowin3: expert survey ultimate biodegradation model
Biowin4: expert survey primary biodegradation model
Biowin5: MITI linear model

Biowin6: MITI nonlinear model
Biowin7: anaerobic biodegradation model

Biowin1 and 2 provide an indication of biodegradability under aerobic conditions. Biowin3 and 4 estimate the time required to achieve complete ultimate and primary biodegradation in an aquatic environment. Biowin5 and 6 are predictive models for biodegradability in the Japanese MITI (Ministry of International Trade and Industry) ready biodegradability test; i.e. OECD 301C. Biowin7, the anaerobic biodegradation model predicts probability of rapid degradation in the "serum bottle" anaerobic biodegradation screening test (On-Line Biowin™ Users's Guide v4.10). An evaluation of BIOWIN showed that for Biowin1 and 2, the prediction "not readily degradable" is highly accurate whereas the prediction "ready degradable" is frequently not in agreement with experimental data obtained by the MITI test. In a study by Eide-Haugmo et al.(11), 43 solvents were screened for biodegradation and compared with the Biowin prediction. They found that the Biowin model failed to identify compounds with biodegradability below 20%. One of the shortcomings of Biowin is the lack of sophistication required to consider the effects of neighboring substituents and substituent position(5).

Other prediction models for biodegradation have been reviewed and evaluated in Pavan and Worth (2006)(15) and include several expert system approaches. Examples of these are the MultiCASE/META approach that can help assess the biodegradability of industrial organic materials in the ecosystem, and CATABOL which is a mechanistic modelling approach for the quantitative assessment of biodegradability in biodegradation pathways (15).

1.4 Chemicals evaluated in the current study

Table 2. Selected chemicals and group representatives

Selected compounds	CAS
Alkyl amino phosphonic acid salt	22036-78-8
Triethyleneamine salt of n-methylbenzenesulphonamido caproic acid	26919-50-6
Nitriloacetic acid	139-13-9
DI-Epoxide/Oxyalkylated polyglycol	68123-18-2*
Triethanolamine	102-71-6
Thioglycolic acid	68-11-1
Dipropylene glycol methyl ether	34590-94-8*
Mercaptoethanol	60-24-2
Polyoxyalkylene glycol	9038-95-3
2-Fluorobenzoic acid	445-29-4*
Benzotriazole	95-14-7
Polydimethylsiloksan (PDMS)	63148-62-9
N-Methyldiethanolamine	105-59-9
Polyacrylamides	9003-05-8
HPAM – partyl hydrolyzed polyacrylamider Flopaam	
Quaternary ammonium compounds	
Alkyl(C12-16)dimethylbenzylammonium chloride	68424-85-1
N-Benzyl-N,N-dimethyl-1-tridecanaminium chloride	8001-54-5
N-Decyl-N,N-dimethyl-1-decanaminium chloride	7173-51-5
Phosphonates	
Diethylene Triamine Penta (Methylene Phosphonic Acid) (DTPMP or DETPMP)	
1-Hydroxyethane-1 1-Diphosphonic Acid (HEDP)	2809-21-4
EO/PO block polymer	
Cross-linked ethylene oxide propylene oxide block polymer	68123-18-2
Polyester	
Polyacrylates	
Sodium polyacrylate 2	2594415
Sodium acrylate	9003-04-7
*Candidate for substitution, OSPAR 2009	

2. Methods

The work flow is outlined in Figure 3 and described below. The chemicals to be evaluated was either defined single chemicals identified with CAS numbers, or groups of chemicals.

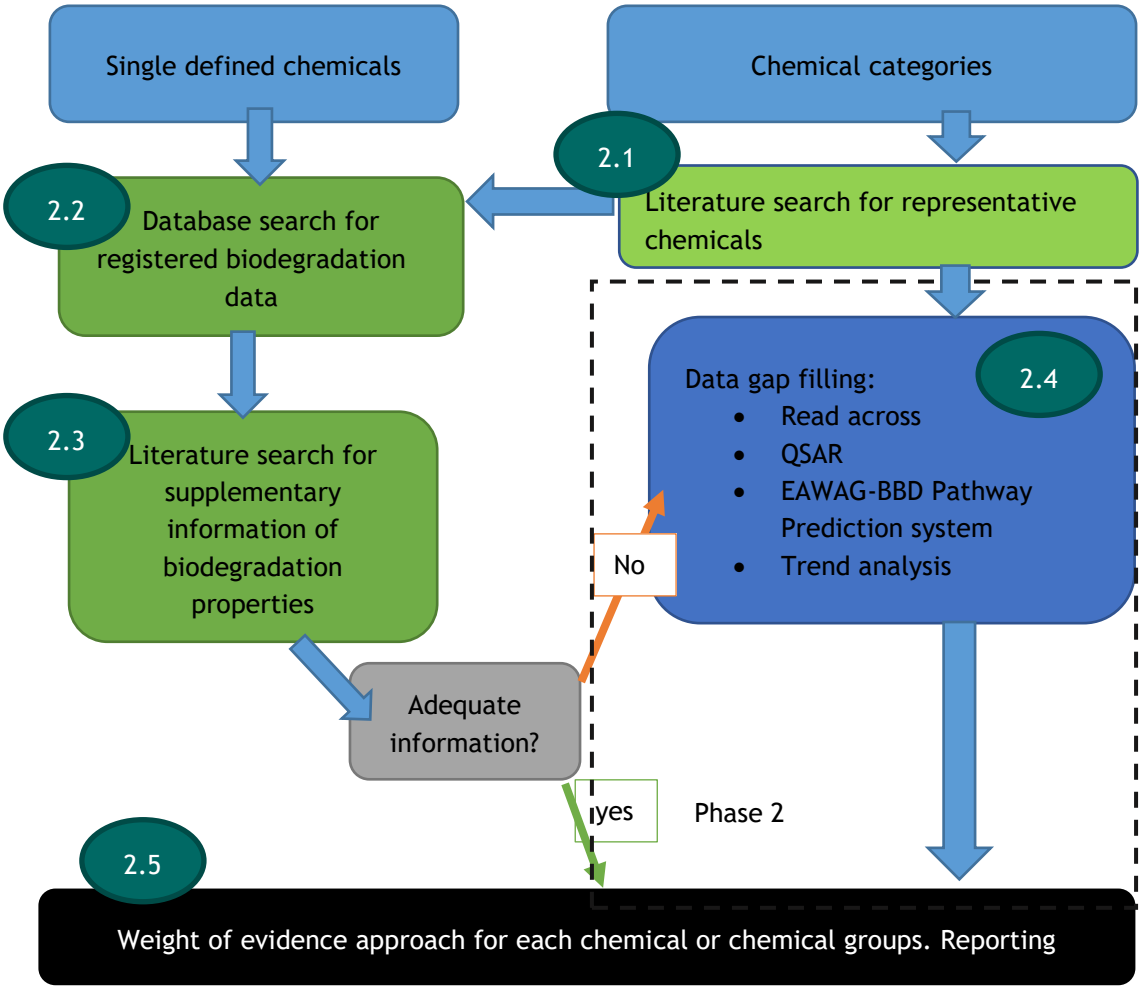


Figure 3: Workflow

2.1 Literature search for representative chemicals

A search for representative chemicals relevant for use in petroleum industry in the following chemical categories was done:

- Polyacrylamides (molecular weight around 1000 and 5000)
- Quaternary ammonium compounds

- Phosphonates
- EO/PO block polymer (molecular weight around 1000, 5000 and 10000)
- Polyesters (molecular weight around 1000, 5000 and 10000)
- Polyacrylates(molecular weight around 1000, 5000 and 10000)

First a search based on typical use was performed in ISI Web of Knowledge with the following search terms:
Scale inhibitor + polymer* +oil*
Emulsion breaker + polymer*
Foam retardant + polymer*

Abstracts were browsed to look for specified chemicals within the above-mentioned categories.

In addition, some chemicals were already mentioned in the previous project report by Stand et al (2014)(16).

2.2 Database search for registered biodegradation data

All chemicals defined by CAS number was entered into the QSAR-Toolbox 4.1 software (version 4.1 released august 2017). A search for experimental data on biodegradation was performed with the built-in function, searching the databases “Biodegradation in soil OASIS”, “Biodegradation NITE” and “ECHA CHEM”.

2.3 Literature search for supplementary information

A literature search was performed with the following search term to find more information of the potential for biodegradation of the chemicals: **(“chemical name” OR “CAS-number”) AND biodeg***, for all compounds in ISI web of knowledge and google scholar. Any duplicates were removed, then the titles and abstracts were browsed to remove non-relevant hits. The final hits were read in full text to extract information of biodegradation testing results, test conditions and quality parameters.

2.4 Data gap filling

2.4.1 Read across

The read across approach were used for a few single compounds where limited data was found. Already registered read across data for these compounds were compiled from the ECHA registered substances database.

For the chemical groups, the read across approach was assessed to be too challenging for the current project due to difficulties in identifying good representatives for all groups, challenges in identifying physico-chemical properties of the representative polymers and limited amount of data for polymers in general.

2.4.2 QSAR-modelling

All substances in table 2 for which a CAS number, smiles or chemical structure was available were analyzed for predicted biodegradation with BIOWIN using the QSAR toolbox and/or the EPI Suite (developed by the EPA's Office of Pollution Prevention Toxics and Syracause Research Corporation, BIOWIN v4.10). All chemicals were checked against the model's applicability domain, herein determined as containing fragments represented in the training set and being within the range of molecular weights of the substances in the training set of the models. Results are only shown for the substances within the applicability domain. Raw data are presented in appendix 2.

The criteria for readily biodegradable being predicted either YES or NO are: if the Biowin3 (ultimate survey model) result is "weeks" or faster and the Biowin5 >= 0.5, then the prediction is YES. If this is not satisfied, the prediction is NO (not readily biodegradable).

The criteria for persistent in the environment are Biowin2 <0.5 or Biowin6 <0.5 and Biowin3 <2.25 (- 2.75), i.e. for substances where Biowin3 indicates a value between 2.25 and 2.75 more degradation relevant information is generally warranted (13).

As a few compounds were outside the applicability domain of the Biowin models, MultiCASE/META was considered as a second QSAR prediction model for biodegradation. This is an expert system that can help assess the biodegradability of industrial organic materials in the ecosystem. However, this is not an open source tool and requires a license. Thus, this model could not be used in the current project. Similarly, a supplier of open source versions of the CATABOL and TOPKAT® tools were not found.

2.4.3 Degradation pathway predictions

Due to limited information on certain compounds and lack of an additional QSAR model for biodegradation, substances were subjected to the EAWAG-BBD Pathway Prediction System which predicts plausible pathways for microbial degradation of chemical compounds. Since the predictions are most accurate for substances that are the sole source of energy, carbon, nitrogen etc. for the microbes in these environments, rather than for substances that are present in trace amounts, the results should be interpreted with caution and only used as supporting information in the context of this report. The tool is available from http://eawag-bbd.ethz.ch/predict/ and the output lists the potential degradation pathways with different colors representing very likely, likely, neutral, unlikely, very unlikely and unknown likelihood for aerobic degradation together with the predicted degradation rule. The list of rules is available at http://eawag-bbd.ethz.ch/servlets/pageservlet?ptype=allrules.

It is important to keep in mind that certain reactions are not predicted in the EAWAG-BBD Pathway Prediction System. These are not predicted, primarily because they are not biodegradation reactions, or they are too difficult to predict. Reactions that are not

predicted includes: 1) Detoxification reactions, 2) Dimerizations, 3) Methylation of hydroxyl groups, 4) Acetylation of primary amines, 5) Formation of intramolecular rings, and 6) Hydroxylation of aliphatic carbon atoms at positions where pure cultures of organisms that metabolize similar compounds do not hydroxylate.

2.4.4 Trend analysis

For substance groups defined by a similar substructure, a substructure search was performed in the QSAR-toolbox. The results were filtered to obtain relevant data and compounds before a trend analysis was performed. The biodegradation data were then plotted against molecular weight and/or logKow to obtain an overall picture of the biodegradation of the specific substance group.

2.5 Weight of evidence approach

Testing data derived from tests performed according to recognized international standards or guidelines by laboratories working in compliance with the current OECD principles of Good Laboratory Practice (GLP) is the preferred source of data for filling in the HOCNF (1). However, other types of information may be sufficient for completing the HOCNF especially when used in a *Weight of Evidence* approach (1). Such information could include:

a. Data from *in vitro* or *in vivo* studies that have not been generated in accordance with the latest adopted/accepted version of the corresponding (validated) test method or to GLP (or equivalent)

b. QSAR model outputs

c. SAR model outputs, read across and category approaches.

The HOCNF guidelines further refer to REACH (4, 13) for how this should be done. A weight of evidence approach including the use of expert judgement should be used to include all relevant information in the assessment of persistence, bioaccumulation and toxicity (PBT) according to REACH Annex XIII:
"[…] A weight-of-evidence determination means that all available information bearing on the identification of a PBT or a vPvB substance is considered together, such as the results of monitoring and modelling, suitable in vitro tests, relevant animal data, information from the application of the category approach (grouping, read-across), (Q)SAR results, human experience such as occupational data and data from accident databases, epidemiological and clinical studies and well documented Case reports and observations. The quality and consistency of the data shall be given appropriate weight. The available results regardless of their individual conclusions shall be assembled together in a single weight-of-evidence determination. […]"

Although the term "weight of evidence" and "expert judgement" is mentioned several times in the ECHA Guidelines Chapter R.7 (4) and R.11(13), there is no approved guideline directly describing how to assign weights to the available information. A suggestion for the workflow is given in Figure R.7.8—2 (4), and the ECHA guideline chapter R.4 (14) gives some guidelines for the overall process, and is the basis for the method used in this report. However, this report has used weight of evidence only to assess the hypothesis "Biodegradation is less than

20% BOD28 in a seawater test (OECD 306 or marine BODIS)", without consideration of bioaccumulation and toxicity. All available data has been assigned a score on reliability and adequacy.

2.5.1 Reliability assessment

The reliability of the information gathered must be assessed before it can be used to draw conclusions of the hypothesis. What is the quality of the study, how are the conclusion drawn, is the purity of the substance reported, is the method valid, is the procedure and results reported completely, are the test controls valid?

The assessment of reliability will follow the method used by ECHA and described in Chapter R.4 (14):
Klimisch et al (1997) (17) developed a scoring system to assess the reliability of data, particularly from toxicological and ecotoxicological studies, that may be extended to physico-chemical and environmental fate and behavior studies:
1 = reliable without restrictions: "studies or data [...] generated according to generally valid and/or internationally accepted testing guidelines (preferably performed according to GLP) or in which the test parameters documented are based on a specific (national) testing guideline [...] or in which all parameters described are closely related/comparable to a guideline method."
2 = reliable with restrictions: "studies or data [...] (mostly not performed according to GLP), in which the test parameters documented do not totally comply with the specific testing guideline, but are sufficient to accept the data or in which investigations are described which cannot be subsumed under a testing guideline, but which are nevertheless, well documented and scientifically acceptable."
3 = not reliable: "studies or data [...] in which there were interferences between the measuring system and the test substance or in which organisms/test systems were used which are not relevant in relation to the exposure (e.g. unphysiological pathways of application) or which were carried out or generated according to a method which is not acceptable, the documentation of which is not sufficient for assessment and which is not convincing for an expert judgment."
4 = not assignable: "studies or data [...] which do not give sufficient experimental details and which are only listed in short abstracts or secondary literature (books, reviews, etc.)."

For the test data retrieved from the ECHA data base, the scores already assigned by ECHA were used. Test data retrieved from the Biodegradation NITE database were given a score of 4 because it has not been possible to control the test data since the database is in Japanese. For test data from the literature and non-test data, an evaluation using this scoring system was used. For QSAR modelling, the score 2 was given if the model was approved and the tested substance was within the applicability domain.

2.5.2 Adequacy

The usefulness (adequacy) of the information for evaluating biodegradability in the marine environment was assessed using the following scoring system:
1 = relevant without restrictions: Test data from OECD 306 tests and marine BODIS
2 = relevant with restrictions: Other seawater tests

3 = relevant with further restrictions: Screening tests, inherent tests and simulation tests for freshwater
4 = relevant for comparison: QSAR modeling using valid models within the applicability domain
5 = little relevance: Test data from sediments, sludge, waste water, soil or anaerobic systems. Test data from single strain bacteria or non-relevant environmental bacteria.

Data that did not fall into any of these categories were only used as supporting information during expert judgement.

2.5.3 Hypothesis testing

The overall question that the weight of evidence approach should answer was:

Q: Is biodegradation less than 20% BOD28 in a seawater test (OECD 306 or marine BODIS)?

As with most hypotheses, it was easier to make a test for the 0-hypothesis:

H1: Biodegradation is more than 20% BOD28 in a seawater test (OECD 306 or marine BODIS)

Only the two tests OECD 306 and marine BODIS gives direct support to this hypothesis, so some assumptions must be made based on expert judgement to also be able to use other types of information. Test data that concluded with persistent or very persistent according to the definition in REACH contradict the hypothesis of "more than 20% BOD28 in a seawater test ", even if it is not the same as the definition of persistence in REACH (as described in chapter 1.3.2).

H2: Substance is persistent (P or vP) according to definition in REACH

Likewise, a test conclusion of ready biodegradable was evaluated as a strong evidence to hypothesis H1.

H3: Substance is ready biodegradable

A review performed by ECETOC(7) concluded that in general, readily biodegradable substances showed similar rates of degradation in marine and freshwater. However, less degradable chemicals exhibited degradation rates approximately four times slower in saline water compared with freshwater. Substances shown to be readily biodegradable in freshwater were also biodegradable in marine environments (7)(ECETOC, 1993).

Information will be considered for either of the three hypotheses as follows:

H1: Test data from OECD 306 tests and marine BODIS
H2: Any test data that provides half-lives of degradation, and QSAR modelling
H3: Test data from screening tests and inherent tests, and QSAR modelling

Data that did not fall into any of these categories were only used as supporting information during expert judgement.

2.5.4 Interpretation of test results

Each information was evaluated separately and filled into one row in the table below (Table 3) for summary of all assessments.

1. Information type: type of test, literature or QSAR
2. Reliability assessment

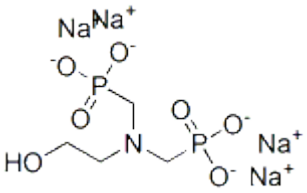
3. Adequacy assessment
4. Answer “yes” or “no” to one of hypothesis H1, H2 or H3
5. Mark the conclusion to Q1 in column representing either:
    a. Yes - *biodegradation is **less than 20%** BOD28 in a seawater test*
    b. *No - biodegradation is **more than 20%** BOD28 in a seawater test*
    c. *Non-conclusive - data is not conclusive to the biodegradation in seawater*

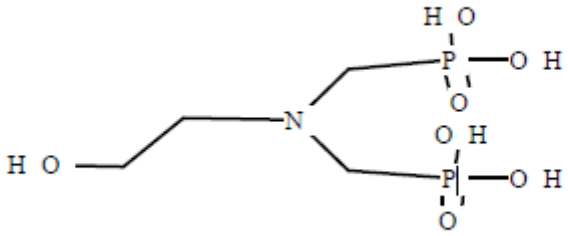
Table 3. Weight of evidence matrix

Information	Reliability [R]	Adequacy [A]	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conclusive
Test data QSAR modelling Literature values	Score from 1 to 4, 1 is most reliable	Score from 1 to 5, 1 is most relevant	Yes or No (applicable for test data from OECD 306 and marine BODIS)	Yes or No (applicable for test derived half-lives data + QSAR)	Yes or No (applicable for ready biodegradation test data + QSAR)	H1 = No H2 = Yes	H1 = Yes H3 = Yes	H2 = No H3 = No

3. Results and Discussion

3.1 Alkyl amino phosphonic acid





CAS: 22036-78-8
Molecular weight: 249.10
Log Kow (estimate): -4.60
Water solubility (estimate): 1*10^6 mg/L

3.1.1 Biodegradation data

No relevant data were found in the databases or in the literature.

3.1.2 Biodegradation predictions

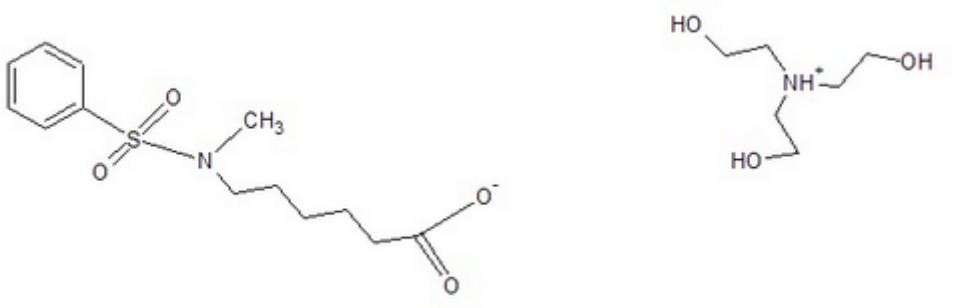
The SMILES: OCCN(CP(O)(O)=O)CP(O)(O)=O), were used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of NO, and a prediction of Persistence of Maybe which indicate that more degradation relevant information might be warranted (see appendix 2 for full BIOWIN output records).

Acetylation of primary amines are not predicted by the EAWAG-BBD Pathway Prediction System. However, two other rules of degradation were **likely** to occur (aerobic likelihood = likely) for primary degradation; the two rules include degradation of tertiary amine to secondary amine and aldehyde or ketone (bt0063), and degradation of primary alcohol to aldehyde (bt0001). The degradation pathway prediction map is shown in appendix 3. The pathway prediction ends at small readily degraded compounds. Thus, degradation of the compound is likely to occur by several pathways. However, the degradation pathway prediction does not provide any information on the speed of degradation.

3.1.3 Summary and conclusion

No conclusion can be drawn due to no available test data for biodegradation and non-conclusive model predictions. The compound is predicted to have a likely degradation pathway, but it is also predicted to not be Ready Biodegradable.

3.2 Triethanolamine salt of n-methylbenzenesulphonamido caproic acid



CAS: 26919-50-6
Molecular weight methylbenzenesulphonamido caproic acid: 285.36
Log Kow (estimate): 2.27
Water solubility (estimate): 430.2 mg/L

3.2.1 Biodegradation data

Table 4. Registered biodegradation test data in databases
Triethanolamine salt of n-methylbenzenesulphonamido caproic acid

Value (%)	Duration (days)	Initial conc. (mg/L)	Data-base	GLP comp-liance	Reliability	Test guideline	Ref
76,84% ThCO2 / 72,03% DOC - failed 10d window	28d	Read across: 6-[(p-tosyl)amino]hexanoic acid, compound with 2, 2', 2"-nitrilotriethanol 11,99 mg/L	ECHA	Yes	2	Read across OECD 301B	Report 2013
Half-life: 0.02-0.18 days	Not specified	818 mg/L	ECHA	Not specified	2	No guideline: half-life of biodegradation in activated sludge	Publication 1996

3.2.2 Biodegradation predictions

The SMILES: CN(CCCCCC([O-])=O)S(=O)(=O)c1ccccc1, were used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of NO, and a prediction of Persistence of NO (see appendix 2 for full BIOWIN output records).

Only one rule was **likely** to occur for primary degradation of this compound, including degradation of fatty acid (n) to fatty acid (n-2) (Bt0337). The full predicted degradation pathway can be found in the appendix 3. The predicted degradation pathway to reach small readily degraded compounds involved steps marked as neutral aerobic likelihood and no pathway involving only likely aerobic degradation steps were seen.

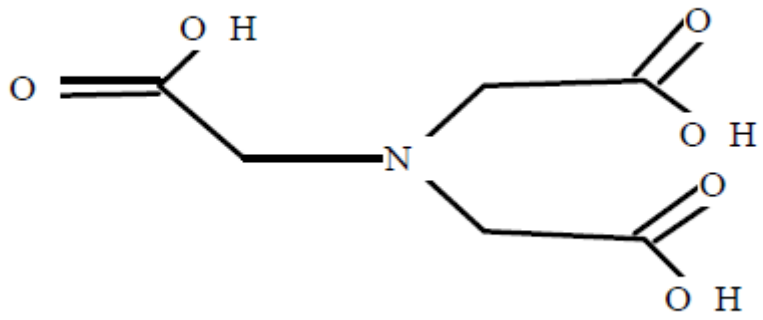
3.2.3 Summary and conclusion

Table 5. Weight of evidence matrix
Triethanolamine salt of n-methylbenzenesulphonamido caproic acid

Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
Read across from 301B: **76,84% ThCO2 / 72,03% DOC, failed 10d**	2	4			no	X		
Half-life (no guideline): 0.02-0.18 days	2	5		no				x
BIOWIN Ready test	2	4			no			x
BIOWIN persistence	2	4		no				x

There is only one study with a conclusion that can be used for evaluation of biodegradability in seawater, and it supports that triethyleneamine salt of n-methylbenzenesulphonamido caproic acid is less than 20% biodegradable in seawater, thus in the red category. The QSAR data indicate not ready biodegradable and not persistent and cannot be used as support either for or against 20% biodegradation in seawater, however, the degradation pathway prediction had no “very likely” degradation pathways, indicating an uncertain degradation. Overall, the lack of relevant data indicate that the substance should be subject to future evaluations.

3.3 Nitriloacetic acid



CAS: 139-13-9
Molecular weight: 191.14
Log Kow (estimate): -3.81
Water solubility (measured value): 1.28*10^3 mg/L

3.3.1 Biodegradation data

Table 6. Registered biodegradation test data in databases
Nitriloacetic acid

Value (%)	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Ref.
89 ThCO2	14	60	ECHA CHEM	no	2 (Key)	OECD 301 B	report 2009
<10 DOC	59	52 (20 DOC)	ECHA CHEM	not specified	2	ISO 16221 (Marine Environment)	report 2010
>95 DOC	28	40 DOC	ECHA CHEM	no	2	The combined CO2/DOC test	(18)
1 ThOD	28		Biodegradation NITE	not specified	4	OECD 301C	Record ID 811
100 DOC	14	Trisodium nitriloacetate (Trilon A 92) 70 (20 DOC)	ECHA CHEM	No	2	Read across OECD 301 E	Report 1983
90-100 DOC	7	Trisodium nitriloacetate (Trilon A 92) 70 (20 DOC)	ECHA CHEM	No	2	Read across OECD 301 E	Report 1983
75-90 DOC	12	Trisodium nitriloacetate (Trilon A 92) 140 (40 DOC)	ECHA CHEM	No	2	Read across OECD 301 E Adapted inoculum	Report 1983
75-90 ThCO2	9	Trisodium nitriloacetate (Trilon A 92) 10-20	ECHA CHEM	No	2	Read across Sturm Test (based on CO2 evolution)	Report 1983
96 ThCO2	28	Trisodium nitriloacetate (Trilon A 92) 1400 (400 DOC)	ECHA CHEM	No	2	Read across OECD 302 B	Report 1983

Three studies were reported in the ECHA database and one in the NITE database. The only test with a marine inoculum showed less than 10% degradation. However, the source of the bacteria was a filter for a marine aquarium and in addition artificial seawater was used, so the relevance can be questioned. Only two references were found relevant in the literature search: Enzymes used for degradation of nitriloacetic acid (NTA) in a bacterial strain (*Chelatobacter heintzii*) has been documented (19). Because of observed variance in biodegradation, NTA was considered as possible reference substance for biodegradation testing representing intermediate biodegradation (Half-lives >15 days) (20).

3.3.2 Biodegradation predictions

The SMILES: O=C(O)CN(CC(=O)O)CC(=O)O, were used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of YES, and a prediction of Persistence of NO (see appendix 2 for full BIOWIN output records).

One rule was **likely** for primary degradation of this compound; degradation of tertiary amine to secondary amine and aldehyde or ketone (Bt0063). The degradation pathway prediction ends at small readily degraded compounds with all degradation steps being **likely**, and is shown in appendix 3.

3.3.3 Summary and conclusion

Table 7. Weight of evidence matrix
Nitriloacetic acid

Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
ISO 16221 <10% DOC 59d	2	2	no			x		
combined CO2/DOC test >95% DOC 28d	2	3			yes		x	
OECD 301B: 89% $ThCO_2$ 14d	2	3			yes		x	
OECD 301C <1% BOD, 28d	4	3			no			x
Read across OECD 301E 100% DOC 14d	2	4			Yes		X	
Read across OECD 301E 90-100% DOC 7d	2	4			Yes		X	
Read across Adapted inoculum 75-90% DOC 12d	2	5			Yes		X	
Read across Sturm Test 75-90% $ThCO_2$ 9d	2	4			Yes		X	
Read across OECD 302B 96% $ThCO_2$ 28d	2	4			Non conclusive			X
BIOWIN Ready test	2	4			yes		x	
BIOWIN persistence	2	4		no				x

The most relevant study supports the hypothesis that nitriloacetic acid is less than 20% biodegradable in seawater, however, the test was not according to OECD 306 and did not use natural seawater. There are also reliable results (with restrictions) indicating ready biodegradability in freshwater. These conflicting results indicate that the substance should be subject to future evaluations.

3.4 Di-epoxide/Oxylalkylated polyglycol

CAS: 68123-18-2
Molecular weight: multiconstituent compound

3.4.1 Biodegradation data

No data of biodegradation was found in either databases or literature search, however, the info card in ECHA states that the substance is: “According to the classification provided by companies to ECHA in CLP notifications this substance is toxic to aquatic life with long lasting effects”.

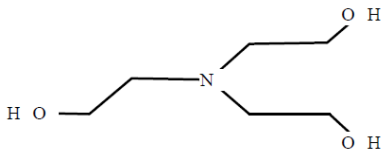
3.4.2 Biodegradation predictions

The compound was not suitable for predictions in BIOWIN or EAWAG-BBD Pathway Prediction System due to being a multi-constituent polymer, and due to lack of SMILES that represented the polymer.

3.4.3 Summary and conclusions

No data available

3.5 Triethanolamine



CAS: 102-71-6
Molecular weight: 149.19
Log Kow (Exper. Database match): -1.00
Water solubility (Exper. Database match): 1*10^6 mg/L

3.5.1 Biodegradation data

Table 8. Registered biodegradation test data in databases Triethanolamine

Value (%)	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Ref
ca 100 specific analysis	1-5	> 0.6 - < 5.7	ECHA CHEM	not specified	2 (Key study)	no guideline followed CO2 evolution test	(21)
96 DOC	19	20	ECHA CHEM	no	2	OECD 301 E	(22)
19,6 ThOD	28	2	ECHA CHEM	no	2	OECD 306 marine	(11)
halflife 133d, K=0,0052	2	2	disregarded ECHA	no	4	OECD 306 marine	(23)
0 ThOD	14	unknown	Biodegradation NITE	unknown	4	OECD 301C	

Triethanolamine (TEA) has shown readily biodegradability properties in activated sludge solids from a municipal wastewater treatment plants (WWTP) (21), in a test using activated sludge from a WWTP (22), and biofilm bacteria obtained from an aged oil-based metalworking fluid (MWF) bioreactor (24). Bacterial isolates that can degrade TEA has been identified in metal working fluid (25), sewage sludge (26) and laboratory scale activated sludge plant (27), and their biodegradation pathway identified. Another study showed that TEA had an inhibitory effect on bacteria isolated from contaminated metal working fluids. The inhibition of bacteria occurred at increasing concentration of TEA and increasing pH of the water: inhibitory concentration of 400 mM at pH 7.2 to between 50-100 mM at pH 9.1 (28). The lowest inhibitory concentration of 50 mM (4.5 g/L) is much higher than typical test concentrations for biodegradability testing (5-40 mg/L). TEA is included in the ring test for the modified OECD 306 test by Newcastle University and CEFIC (8). The report from the ring test is under preparation, however, the results from one lab (NIVA) showed 23% biodegradation at day 28 and 22%[2] at day 60 of the closed bottle test according to OECD 306, not performed according to GLP.

3.5.2 Biodegradation predictions

The SMILES: OCCN(CCO)CCO, were used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of YES, and a prediction of Persistence of NO (see appendix 2 for full BIOWIN output records).

Two rules were **likely** for primary degradation of this compound, including degradation of tertiary amine to secondary amine and aldehyde or ketone (Bt0063) and degradation of primary alcohol to aldehyde (bt0001). The degradation pathway prediction ends at small readily degraded compounds with all steps having a likely aerobic likelihood, and is shown in appendix 3.

[2] Preliminary results. Not subjected to QA by Newcastle University

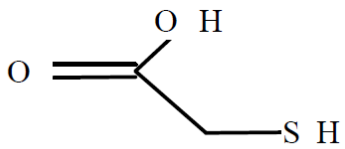
3.5.3 Summary and conclusions

Table 9. Weight of evidence matrix
Triethanolamine

Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
OECD 306 19,6% ThOD 28d	2	1	No			x		
OECD 306 23% ThOD 28d	2	1	yes				x	
OECD 306 **half-life 133d**	4	2		yes		x		
CO2 evolution test ca 100% $ThCO_2$ 5d	2	3			yes		x	
OECD 301E 96% DOC 19d	2	3			yes		x	
OECD 301C 0%ThOD 14d	4	3			No			x
BIOWIN Ready test	2	4			Yes		x	
BIOWIN persistence	2	4		No				x
Literature several types of environment or industrial applications	4	5			yes		x	

The most relevant study submitted to ECHA is the OECD 306 test with 19.6% ThOD in 28 days, which is close to the limit of 20% biodegradation in seawater. The other OECD 306 test is part of a ring test (8) (results from one test, report in prep.) had a result of 23% ThOD reduction in 28 days, just above the 20% -limit. There are also reliable results (with restrictions) and supplementary information with indication of ready biodegradability in freshwater. These conflicting results indicate that the substance should be subject to future evaluations.

3.6 Thioglycolic acid



CAS: 68-11-1
Molecular weight:
Log Kow (Measured): 0.09
Water solubility (Measured): >1*10^6 mg/L

3.6.1 Biodegradation data

Table 10. Registered biodegradation test data in databases
Thioglycolic acid

Value (%)	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Ref.
67 ThOD	28	not specified	ECHA CHEM	not specified	2 (key)	OECD 301 D	(29)
21 DOC	28	153	ECHA CHEM	yes	2	OECD 301 A (new Version)	report 1994
Ready biodegradable	28	not specified	ECHA CHEM	not specified	2	Several tests done by several labs, see table below	(30)
Based on Weight of evidence							

Tests	% passed	n
Modified Zahn Wellens	67	6
Sturm	60	5
MITI 2	60	10
MITI 1	40	10
Modified OECD	13	16
Closed Bottle	0	7

Average n=26: 43 ThOD	28	not specified	ECHA CHEM	not specified	2	EU Method C.4-F (MITI Test) Ringtest 26 labs	grey literature 1985
100 BOD	28	30	ECHA CHEM		4	OECD 302C	report 1978

Thioglycolic acid (TGA) showed variable biodegradation in different tests systems in the studies reported in the ECHA database, and none of the tests has been done with marine bacteria. No recent literature was found to help evaluate the potential for biodegradation in the marine environment. The only study found was an isolation of a soil bacteria (*Alcaligenes xylosoxydans* subsp. *denitrificans* TD1) that can degrade thiodiglycol and TGA(31).

3.6.2 Biodegradation predictions

The SMILES: O=C(O)CS, was used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of YES, and a prediction of Persistence of NO (see appendix 2 for full BIOWIN output records).

No **likely** rules for primary degradation were predicted. The predicted degradation pathway is shown in appendix 3.

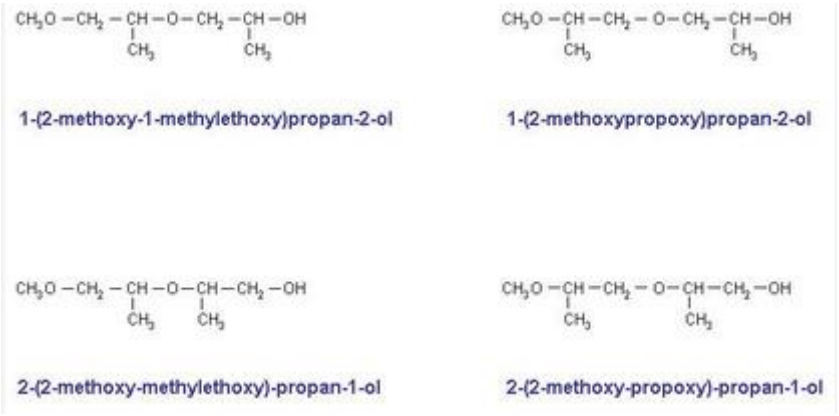
3.6.3 Summary and conclusions

Table 11. Weight of evidence matrix
Thioglycolic acid

Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
OECD 301D 67% ThOD	2	3			yes		X	
OECD 301A 21% DOC	2	3			no			X
Several test OECD 301 and 302: ready biodegradable	2	3			yes		X	
MITI test **n=26: 43 ThOD**	2	3			No, variable results			X
OECD 302C 100% BOD	4	3			yes		X	
BIOWIN Ready test	2	4			yes		x	
BIOWIN persistence	2	4		no				x

The weight of evidence suggests that tioglycolic acid (mercaptoacetic acid) is biodegradable, but with variable results in freshwater with respect to the definition of ready biodegradability. No information from seawater tests were available, indicating that the substance should be subject to future evaluations.

3.7 Dipropylene glycol methyl ether



CAS: 34590-94-8
Molecular weight: 148.20
Log KoW (estimated): -0.35
Water solubility (measured): 1*10^6 mg/L

3.7.1 Biodegradation data

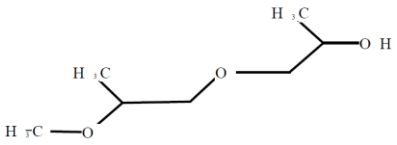
Table 12. Registered biodegradation test data in databases
Dipropylene glycol methyl ether

Value (%)	Duration (days)	Initial conc. (mg/L)	Data-base	GLP compliance	Reliability	Test guideline	Ref.
76 ThCO2 (75 ThOD 10d window)	28	79.5	ECHA CHEM	yes	1 (Key)	OECD 301 F	Report 1998 + (32)
72,9 DOC	28	17	ECHA CHEM	Yes	1	OECD 301 E	report 1993
34 ThCO2	28	10-20	ECHA CHEM	yes	2	OECD 301 B	report 1990 + (32)
94 DOC 73 DOC	13 8	740	ECHA CHEM	No	2	OECD 302 B	report 1981 + (32)
10 (CO2 and methane gas)	81	51	ECHA CHEM	yes	2	OECD 311 (anaerobe)	Report 1998

Most of the recorded biodegradation data in the ECHA CHEM database for dipropylene glycol methyl ether (DGME) conclude with ready biodegradable, except for one of the OECD 301B test (34%), and an anaerobic test OECD 311 (10%). No relevant data was found in the literature search.

3.7.2 Biodegradation predictions

The SMILES: COC(C)COCC(C)O, structure:



was used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of NO, and a prediction of Persistence of NO (see appendix 2 for full BIOWIN output records).

No likely or very likely degradation pathways for primary degradation was predicted for this compound. All pathways for primary degradation were predicted to be neutral.

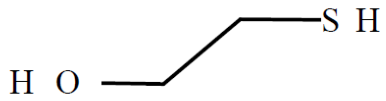
3.7.3 Summary and conclusion

Table 13. Weight of evidence matrix
Dipropylene glycol methyl ether

Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
OECD 301F 76% ThCO2 28d	1	3			yes		X	
OECD 301E 73% DOC 28d	1	3			yes		X	
OECD 301B **34% ThCO2 28d**	2	3			no			X
OECD 302B 73% DOC d8	2	3			Possibly (no d7 data)			x
OECD 311 10% gas 81d	2	5			no			x
BIOWIN Ready test	2	4			no			x
BIOWIN persistence	2	4		no				x

The weight of evidence suggests that dipropylene glycol methyl ether is biodegradable in freshwater. No information from seawater tests were available, indicating that the substance should be subject to future evaluations.

3.8 Mercaptoethanol



CAS: 60-24-2
Molecular weight: 78.13
Log Kow (measured): -0.056
Water solubility: M: 1*10^6 mg/L

3.8.1 Biodegradation data

Table 14. Registered biodegradation test data in databases
Mercaptoethanol

Value (%)	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Ref.
69 TIC	60	20	ECHA CHEM	yes	1 (key)	OECD 310	study report 2011
<10 DOC	28	70.7	ECHA CHEM	yes	1	OECD 301 A	study report 1994
90 TOC	28	not specified	ECHA CHEM	not specified	2	OECD 302 C	MITI Japan 1992
29 COD	55	1000	ECHA CHEM	no	2	No guideline followed	(33)
≥15 ≤21 ThOD	28	100	ECHA CHEM	not specified	2	OECD 301 C	MITI Japan 1992
19 ThOD	28	not specified	Biodegradation NITE	not specified	4	OECD 301C	1997

Mercaptoethanol is used in DNA-extractions, so there were many genetic and enzymatic studies in literature databases, but none were relevant for evaluation of the potential for biodegradation of mercaptoethanol in marine waters.

3.8.2 Biodegradation predictions

The SMILES: OCCS, was used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of YES, and a prediction of Persistence of NO (see appendix 2 for full BIOWIN output records).

The only likely degradation pathway for primary degradation was transformation of primary Alcohol to Aldehyde (bt0001). The predicted degradation pathway to reach the small readily degraded compounds involved steps marked as neutral aerobic likelihood and no pathway involving only likely degradation steps were seen.

3.8.3 Summary and conclusion

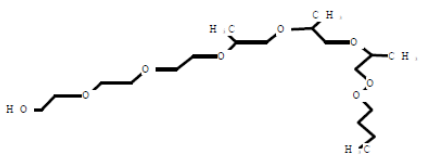
Table 15. Weight of evidence matrix
Mercaptoethanol

Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
OECD 310 69% TIC 60d	1	3			No			X
OECD 301A <10% DOC 28d	1	3			No			X
OECD 302C 90% TOC 28d	2	3			No data on d14			X
OECD 301C ≥15 ≤21% ThOD 28d	2	3			no			x
OECD 301C 19% ThOD 28d	4	3			no			x
No guideline 29% COD 55d	2	5			x			x
BIOWIN Ready test	2	4			Yes		X	
BIOWIN persistence	2	4		No				x

Weight of evidence suggest that mercaptoethanol is not ready biodegradable in freshwater. Due to expected lower biodegradation in seawater than in freshwater, it is possible that the substance is in the red category. The substance should be subject to future evaluations since no information from seawater tests or other supporting information was available for this hypothesis.

3.9 Polyoxylalkylene glycol

CAS: 9038-95-3
Molecular weight: 396.53
Log Kow (estimated): 1.1
Water solubility: 1188 mg/L



3.9.1 Biodegradation data

No data of biodegradation was found in either databases or literature search. The info card in ECHA states: “According to the classification provided by companies to ECHA in CLP notifications this substance is (…), may cause long lasting harmful effects to aquatic life and (…).”

3.9.2 Biodegradation predictions

The SMILES: OCCOCCOCCOC(C)COC(C)COC(C)COOCCCC, was used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of YES, and a prediction of Persistence of Maybe (indicating that more degradation relevant information might be warranted, see appendix 2 for full BIOWIN output records).

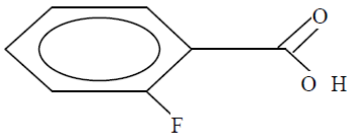
The only likely degradation pathway predicted for primary degradation was transformation of primary Alcohol to Aldehyde (bt0001). The predicted degradation pathway to reach the small readily degraded compounds involved steps marked as neutral aerobic likelihood and no pathway involving only likely degradation steps were seen.

3.9.3 Summary and conclusion

Since there are no available test data for biodegradation and non-conclusive model predictions, no conclusions can be drawn. According to predictions, polyoxylalkylene glycol has a likely or neutral degradation pathway, is predicted to not be Ready Biodegradable, and might be persistent.

3.10 2-Fluorobenzoic acid

CAS: 445-29-4
Molecular weight:140.11
Log Kow (measured): 1.77
Water solubility (measured): 7.2*10^3 mg/L



3.10.1 Biodegradation data

No data of biodegradation was found in either databases or literature search.

3.10.2 Biodegradation predictions

The SMILES: O=C(O)c(c(F)ccc1)c1, was used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of NO, and a prediction of Persistence of Maybe (indicating that more degradation relevant information might be warranted, see appendix 2 for full BIOWIN output records).

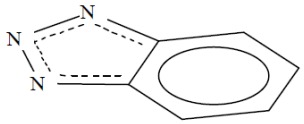
No likely or very likely degradation pathways for primary degradation was predicted.

3.10.3 Summary and conclusion

Because there was no available test date for biodegradation it is not possible to conclude on the biodegradability in seawater. Modelling data suggest that the substance is not easily biodegradable.

3.11 Benzotriazole

CAS: 95-14-7
Molecular weight: 119.13
Log Kow (Exper database match):1.44
Water solubility (Exper database match): 1.98*10^4 mg/L



3.11.1 Biodegradation data

Table 16. Registered biodegradation test data in databases
Benzotriazole

Value (%)	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Ref.
0 ThOD	28	1000	ECHA CHEM	Yes	2 (key)	OECD 301 D	Report 1991
0.8 DOC	30	20	ECHA CHEM	Yes	2 (key)	OECD302 A	Report 1994
-1 DOC	29	10	ECHA CHEM	Yes	2	OECD 301 B	Report 1994
4 DOC	29	10					
2 ThOD	28		Biodegradation NITE	not specified		OECD 301C	

All the submitted reports to ECHA CHEM and NITE suggested that benzotriazole (BTril) is non-biodegradable in water.

Considerable literature was found on BTril, as it is widely used both as corrosion inhibitor, in de-icing fluids for aircrafts and in detergents, and it is also widely studied when it comes to biodegradation or persistence in the environment. Only one study following a biodegradation test guideline was found during literature search. That study concluded that triazoles are not readily biodegradable according to the OECD 301 D test guideline, with an incubation time of 28 days (34). Another controlled experiment used two bacterial strains isolated from

activated sludge and a test concentration of 10mg/L and found a primary biodegradation of BTril of 10-19% (35).

Several studies investigated the removal (primary degradation) of BTril in different forms of sludge bioreactors, and compared removal in aerobic and anaerobic conditions: Activated sludge communities eliminated up to 30 mg/L BTril under aerobic conditions within 21-49 days (or 7 days after acclimation), but not under anoxic or anaerobic conditions (36); half-life of 1H-Benzotriazole of 1 day in activated sludge confirmed partial persistence in conventional wastewater treatment(37); shortest half-life for BTril was 114 days under anaerobic conditions, while the longest was 315 days under sulphate reducing conditions in microcosm studies at test concentration of 1 mg/L with sludge from a WWTP(38); half-life values in activated sludge batch experiments ranged between 23 and 45 h(39); in a sequence batch reactor the biodegradation of BTril was less than 1%, while it was between 75-100% in the aerobic/anoxic reactor probably due to increased reaction time(40); Tham and Kenedy did not observe any evidence for anaerobic degradation of BTril in batch or continuously fed anaerobic systems (41); a comparison between lab-scale membrane bioreactor and conventional activated sludge-treatment showed 61 and 31% removal(42).

Other treatment systems include biofilm reactors, biofilters, nitrifying trickling filters, constructed wet-lands: a laboratory hybrid moving bed biofilm reactor showed average removal of five benzotriazoles including BTril between 41 and 88% (43); a pilot-scale biofilter with natural manganese oxides as carrier material removed 91% BTril from secondary effluent after adaption(44); removal of BTril in a nitrifying trickling filter was poor in the presence of exogenous organic carbon (20,20%) (45), but better without added organic carbon or increased nitrification (42,8%) (46); BTril from raw waste water (initial concentration between 0.2 to 2.2.µg/L) was removed in the range 65-70% and 89-93% in conventional WWTP and constructed wetlands, respectively (47); batch experiments with the duckweed *Lemna minor* gave full elimination of BTril up to the end of the experiment (day36), and the kinetic constant of plant uptake were by far higher than the kinetic constants for hydrolysis or photodegradation (48).

Removal of BTril under aquifer condition in a column experiment had a lag-time of approximately 30-60 days and a biodegradation half-live of 29±2 days (49). In a microcosm with fresh groundwater and aquifer sediment materials, BTril degraded more rapidly under aerobic conditions (half-life of 43±4.8 days) compared to anaerobic conditions (half-life 57±5,8 days) (50).

Another interesting factor affecting biodegradation of BTril is its inhibitory properties as documented for soil bacteria: Microbial growth yields were severely reduced with increasing concentration of BTril (51, 52). More than 50% reduction of growth yield at a concentration of 400 mg/L BTril (51).

3.11.2 Biodegradation predictions

The SMILES: c1ccc2[nH]nnc2c1, was used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. The Biowin predictions were not valid for this compound.

The only likely degradation pathway predicted for primary degradation was transformation of *vic*-unsubstituted Aromatic to *vic*-Dihydroxyaromatic (bt0005). The predicted degradation pathway to reach the small readily degraded compounds involved steps marked as neutral aerobic likelihood and no pathway involving only likely degradation steps were seen.

3.11.3 Summary and conclusion

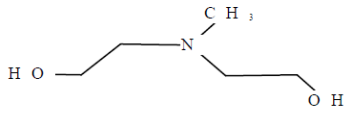
Table 17. Weight of evidence matrix
Benzotriazole

Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
OECD 301D 0% ThOD 28d	2	3			No			X
OECD 302A 0.8% DOC 30d	2	3			No			X
OECD 301B -1-4% DOC 29d	2	3			No			X
OECD 301C 2% ThOD 28d	4	3			No			X

All the available test data suggest that benzotriazole is not ready biodegradable in water, and since they all are below 20%, it is also likely that it is non-biodegradable in water. The data from the literature suggest that benzotriazole can be at least partly degraded in optimized (treatment) systems. This is probably due to adaption, but that in most cases degradation is slow, only partly and/or have a long lag phase. There is a weight of evidence supporting that benzotriazole is less than 20% biodegradable in seawater, thus in the red category.

3.12 N-methyldiethanolamine

CAS: 105-59-9
Molecular weight: 119.16
Log Kow (measured): -1.08
Water solubility (measured): 1*10^6 mg/L



3.12.1 Biodegradation data

Table 18. Registered biodegradation test data in databases
N-methyldiethanolamine

Value (%)	Endpoint	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Reference
96	DOC removal	10	41 (20 DOC)	ECHA CHEM	no	2 (Key)	OECD 301 A (new Version)	Report 1994
95	DOC removal	14	400	ECHA CHEM	no	2	OECD 302 B	Report 1988
-1	O_2 consumption	28	2	ECHA CHEM	no	2	OECD 306 (marine)	Eide-Haugmo(11)
23	TOC removal	28	100	ECHA CHEM	not specified	2	OECD 301 C	unnamed publication 2005
0	O_2 consumption	28	1,49	ECHA CHEM	Yes (incl. certificate)	1	OECD 306 (marine)	Report 2011
15		63						
>95	CO_2 evolution / DOC removal	15	85 (42.9 DOC)	ECHA CHEM	no	2	ISO DIS 9439	Report 1994
7	BOD	28		Biodegradation NITE	not specified	4	OECD 301C	Record ID 999

The result of a study that compared aerobic biodegradation of MDEA in a batch and continuous flow experiment indicated that MDEA-solution was non-biodegradable during the test period of 28 days, whereas the continuous flow experiments showed biodegradation of more than 96% based on TOC-measurements. This was probably due to the adaptation of the microorganisms to this particular wastewater contamination during continuous flow experiment (53).

3.12.2 Biodegradation predictions

The SMILES: OCCN(CCO)C, was used as input for prediction with the BIOWIN models and the EAWAG-BBD Pathway Prediction System. BIOWIN gave a Ready Biodegradability Prediction of YES, and a prediction of Persistence of NO (see appendix 2 for full BIOWIN output records).

Two rules for primary degradation was likely for this compound, including transformation of primary alcohol to aldehyde (bt0001) and tertiary amine to secondary amine and aldehyde or ketone (bt0063). The degradation pathway prediction ends at small readily degraded compounds with likely degradation steps.

3.12.3 Summary and conclusion

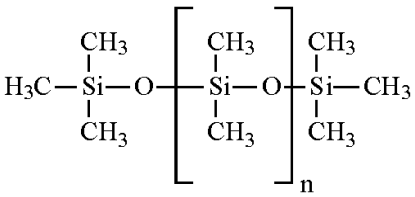
Table 19. Weight of evidence matrix
N-methyldietahanolamine

Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
OECD 306 15% ThOD 63d (0% ThOD 28d)	1	1	no			X		
OECD 306 -1% ThOD 28d	2	1	no			X		
OECD 301A 96% DOC 10d	2	3			yes		X	
OECD 302B 95% DOC 14d	2	3			yes		X	
OECD 301C 7% ThOD, 23% TOC 28d	2	3			no			X
ISO DIS 9439 >95% DOC 15d	2	3			yes		X	
OECD 301C 7% ThOD 28d	4	3			No			X
BIOWIN Ready test	2	4			Yes		X	
BIOWIN persistence	2	4		No				X

When only reliability is assessed, the overall information of the results are conflicting. However, considering the relevance of the studies, there is a weight of evidence supporting that N-Methyldiethanolamine is less than 20% biodegradable in seawater, thus in the red category.

3.13 Polydimethylsiloxan

CAS: 63148-62-9
Molecular weight: 310.69
Log Kow (Exper. Database match): 8.21
Water solubility (Exper. database match):0.00674 mg/L



3.13.1 Biodegradation data

No data were found beside the data compiled and reported by Stang et al.(16). The compound has low solubility and high affinity to particles (54). The compound has been

observed to degrade in soil in lab and field-tests (55), but no information regarding biodegradation in seawater was found.

3.13.2 Biodegradation predictions

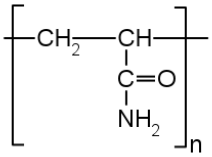
The Biowin predictions were not valid for this compound and the compound could not be entered into the EAWAG-BBD Pathway Prediction System as Si was not a valid atom in the model.

3.13.3 Summary and conclusion

No conclusion can be drawn as no data for biodegradation in water was available. The compound was outside the applicability domain for both biodegradation predictions with Biowin and for the EAWAG-BBD pathway prediction system.

3.14 Polyacrylamides

CAS: 9003-05-8
Molecule formula: $(C_3H_5NO)_n$
Molecular weight monomer: 71.08



3.14.1 Biodegradation data

The commercial product named “Flopaam” followed by different numbers, contain different types of partly hydrolyzed polyacrylamides (HPAM) (56).

HPAM (FLOPAAM™ 3230 S) is included in the ring test for modified OECD 306 test by Newcastle University and CEFIC(8). The report from the ring test is under preparation, however, the results from one lab (NIVA) showed 4%[3] degradation at day 28 and -18% (negative due to respiration in blank control) at day 60 of the closed bottle test according to OECD 306, not performed to GLP.

A review (57) of degradation of polyacrylamide (PAM) flocculants from 2015 concluded that there is a lack of detailed data about the behaviour and fate of PAM-based flocculants in the environment. The molecular weight of the PAM described in the review varied between $3x10^6$ to $2x10^7$. Most studies of biodegradation were from agricultural application where PAM is generally resistant to microbial degradation. However, several bacteria species have been isolated from soil that can use PAM as sole nitrogen and or carbon source. Degradation rates were in the range 15 to 20% in these studies. Several bacterial strains that demonstrated abilities of degrading hydrolysed PAM have also been isolated during oil recovery processes

[3] Preliminary results. Not subjected to QA by Newcastle University

with degradation rates in the range 30 to 70% for the different strains. The studies presented in this review demonstrated that PAM can be subjected to microbial degradation, and that PAM could be used as nitrogen source by hydrolysis of the amine group from the polymer. The biodegradation of PAM induced changes in the structure of the polymer (reduction of molecular weight), but no evidence of release of acrylamide monomer was found (57).

A strain of *Pseudomonas aeruginosa* was isolated from hydrolysed polyacrylamide (HPAM)-containing wastewater and achieved removal efficiency of 41.6% when pH was 7 at 35°C measured with an optical density method (Starch-cadmium iodide method). HPAM had an average molecular weight as about $1.5\text{-}3x10^6$ and it was 24.14% hydrolysed (58).
Two HPAM-degrading strains of Bacillus were isolated from produced water of polymer flooding and tested for their ability to degrade HPAM in aerobic conditions. They used the amide group of HPAM as nitrogen source and the carbon backbone of HPAM could be partly utilized (59).

Combined anaerobic and aerobic biological treatment processes was assessed for the removal of HPAM. The average molecular weight of the HPAM was about 2.2×10^7 and it was 10% hydrolysed. The test concentration was 500 mg/L, and added glucose as a co-additives of carbon source. Two bacterial strains isolated from oilfield production water were used in the bioreactors. Removal rate of amide group from HPAM (measured by starch-cadmium iodine method) in anaerobe reactor was 48.1% (24h retention time) and 41.8% in aerobic aeration tank (48h retention time). Combined anaerobic and aerobic treatment resulted in HPAM removal of TOC of 32.9%. Analysis with HPLC showed additional peaks to the original HPAM molecule, indicating a HPAM fragment with lower molecular weight as biodegradation product, but no monomer acrylamide (60). In a follow-up study using an anaerobic and aerobic activated sludge biochemical treatment system, the maximum rate of biodegradation of HPAM was explored by optimizing the nutrient proportions. Aerobic conditions gave better biodegradation rates than anaerobic conditions (61).

An evaluation of biodegradation of polyacrylamide was performed by Stang et al. (16) and according to the available information, they do not expect that polyacrylamides larger than a molecular weight of 1000 will be biodegraded in standard seawater tests (16).

3.14.2 Biodegradation prediction

The predicted biodegradation for different sizes of polyacrylamides are presented in table 20.

Table 20. BIOWIN prediction of biodegradability
Polyacrylamides

CAS rn	Acrylamide monomer, C=CC(=O)N	Acrylamide, dimer, C(N)(=O)C(C)CCC(N)=O	Acrylamide trimer C(N)(=O)C(C)CC(C(N)=O)CCC(N)=O	Acrylamide (7 monomers) C(N)(=O)C(C)CC(C(N)=O)CC(C(N)=O)CC(C(N)=O)CC(C(N)=O)CCC(N)=O	polyacrylamide (10 monomers) C(N)(=O)C(C)CC(C(N)=O)CC(C(N)=O)CC(C(N)=O)CC(C(N)=O)CC(C(N)=O)CC(C(N)=O)CC(C(N)=O)CCC(N)=O
Ready Biodegradability Prediction	YES	YES	NO	NO	NO
Persistence (if B2 or B6 is <0.5 and B3 is <2.25 (-2.75)	NO	NO	NO	YES	YES

3.14.3 Summary and conclusions

Table 21. Weight of evidence matrix
Polyakrylamides

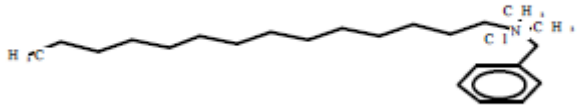
Information	R	A	H1: >20%BOD	H2: Persistent	H3: Ready biodegradable	Conclusion for Q1:		
						yes < 20%	No > 20%	Non conc
OECD 306 4% ThOD 24d (-18% ThOD 60d)	2	1	no			X		
BIOWIN Ready test mono	2	4			Yes		X	
BIOWIN Ready test -di	2	4			Yes		X	
BIOWIN Ready test -tri	2	4			No			X
BIOWIN Ready test - hepta	2	4			No			X
BIOWIN Ready test - deca	2	4			No			X
BIOWIN persistence mono	2	4		No				X
BIOWIN persistence -di	2	4		No				X
BIOWIN persistence - tri	2	4		No				X
BIOWIN persistence - hepta	2	4		Yes		X		
BIOWIN persistence - deca	2	4		Yes		X		

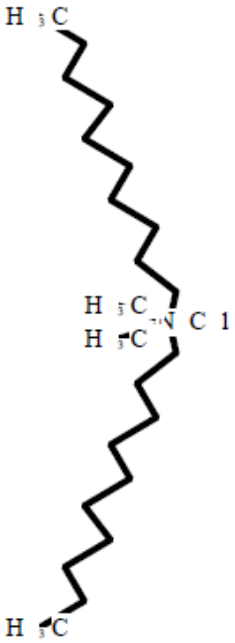
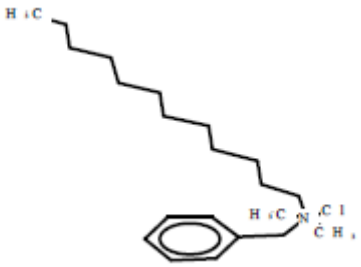
The information found in the literature describe PAM or HPAM as large molecules (Mw >10^6 g/mol), and conclude that a partial biodegradation is possible. However, high biodegradation rates in the environment is unlikely. There is a weight of evidence supporting that high molecular weight PAM or HPAM is less than 20% biodegradable in seawater, thus in the red category.

When it comes to PAM with molecular weight in the range 500 to 1000, no test data was found. Modelling data suggest that the monomer and dimer of acrylamide are ready biodegradable (molecular weight 71 – 142 g/mol), whereas longer oligomers and polymers are not readily biodegradable. The monomer, dimer and trimer are not predicted to be persistent, whereas the longer polyacrylamides (7 and 10 monomers: 500 and 700 g/mol) are predicted to be persistent.

3.15 Quaternary ammonium compounds

Representative chemicals:

<table>
<tr>
<td>benzyl-C12-16-alkyldimethyl, chlorides
CAS 68424-85-1
  </td>
<td rowspan="2">Didecyldimethylammonium chloride

CAS 7173-51-5
  </td>
</tr>
<tr>
<td>Benzalkonium Chloride
CAS: 8001-54-5
  </td>
</tr>
</table>

3.15.1 Biodegradation data

Table 22. Registered biodegradation of Quaternary ammonium compounds in databases
Didecyldimethylammonium chloride CAS 7173-51-5

Value (%)	Endpoint	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Reference
69	COD	28	4	ECHA CHEM	Yes	1	OECD 301D	Report 1996
67-71	ThCO2	28	10	ECHA CHEM	Yes	1	OECD 301B	Report 2006
80	DOC	28	162 DOC	ECHA CHEM	no	2	Zahn-Wellens Test	Report 1982

No data was found in databases for benzyl-C12-16-alkyldimethyl chlorides or benzalkonium chloride.

Literature search of the same representatives gave no relevant results. However, in a review study of surfactants in the marine environment included ditallow dimethyl ammonium chloride (DTDMAC), a quaternary ammonium compound that is a historically commonly used cationic surfactant and is now on the Norwegian priority list (http://www.miljostatus.no/tema/kjemikalier/prioritetslisten/). Even if the use of these compounds is reduced, the concentrations found in marine sediments were still high (0.0048 mg/kg to >25 mg/kg) probably due to their persistent nature. No marine biodegradation data was however found in the literature (62).

Structural element search in QSAR Toolbox was done for quaternary ammonium with the SMILE for a quaternary ammonium compound:

Biodegradation screening test results were collected (automated database search), and only substances with available data were included (13 linear and 1 cyclic quaternary compound) (see table 23). The relevance of the chemicals towards use in oilfield where checked with a search in google. There was no correlation between biodegradation data and molecular weight or log Kow for these molecules (see figure 4). The substances that did not contain halogens were all biodegradable, however, the substances that contained chlorine or bromide could either be ready biodegradable or not biodegradable, and for two of the substances (CAS 57-09-0 and CAS 7173-51-5) there were conflicting test results, where the data from NITE database concluded with non-biodegradable, while data from ECHA database concluded with ready biodegradable.

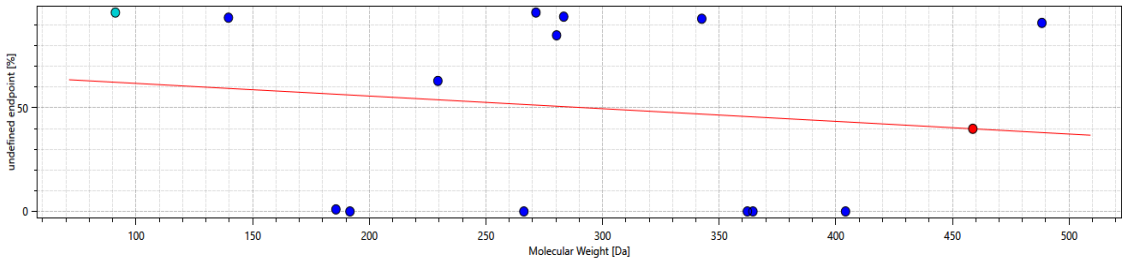


Figure 4: Trend analysis for percent biodegradation in screening tests with test data registered in either the NITE or ECHA database plotted against molecular weight (Da) for quaternary ammonium compounds. Based on 14 values.

Table 23. Compounds in QSAR Toolbox with biodegradation data from screening tests.
Quaternary ammonium compounds

Biodegradable	CAS	Name and relevance to oilfield	SMILE
No	1941-30-6	Tetrapropylammonium bromide – not oilfiled	[Br-].CCC[N+](CCC)(CCC)CCC
Yes	2082-84-0	decyltrimethylammonium bromide – maybe oilfiled	[Br-].CCCCCCCCCC[N+](C)(C)C
No NITE, Yes literature	57-09-0	cetrimonium bromide – maybe oilfiled	[Br-].CCCCCCCCCCCCCCCC[N+](C)(C)C
No	56-93-9	Benzyltrimethylammonium chloride - oilfiled	[Cl-].C[N+](C)(C)Cc1ccccc1 (cyclic)
Yes	67-48-1	Choline chloride - oilfield	[Cl-].C[N+](C)(C)CCO
no NITE yes ECHA	7173-51-5	Didecyldimethylammonium chloride – biocide oilfiled	[Cl-].CCCCCCCCCC[N+](C)(C)CCCCCCCCCC
No	17301-53-0	docosyltrimethylammonium chloride – not oilfield	[Cl-].CCCCCCCCCCCCCCCCCCCCCC[N+](C)(C)C
No	1892-57-5	N'-(ethylcarbonimidoyl)-N,N-dimethylpropane-1,3-diamine - uncertain	[Cl-].CCN=C=NCCC[N+H](C)C
Yes	75-59-2	Tetramethylammonium hydroxide chloride - oilfield	[O-H].C[N+](C)(C)C
Yes	987-78-0	Citicoline – not oilfield	C[N+](C)(C)CCOP([O-])(=O)OP(O)(=O)OCC1OC(C(O)C1O)N1C=CC(N)=NC1=O
Yes	4292-10-8	Cocamidopropyl betaine - oilfiled	CCCCCCCCCCCC(=O)NCCC[N+](C)(C)CC([O-])=O
Yes	1643-20-5	dodecyldimethylamine oxide -oilfield	CCCCCCCCCCCC[N+](C)(C)[O-]
Yes	683-10-3	[dodecyl(dimethyl)ammonio]acetate - oilfield	CCCCCCCCCCCC[N+](C)(C)CC([O-])=O
Yes	6891-44-7	Choline, methyl sulfate, methacrylate – not oilfield	COS([O-])(=O)=O.CC(=C)C(=O)OCC[N+](C)(C)C

3.15.2 Biodegradation predictions

The BIOWIN prediction for Ready Biodegradability and Persistence for three quaternary ammonium compounds are shown in table 24.

Table 24. BIOWIN prediction of biodegradability
Quarternary ammonium compounds

CAS rn	68424-85-1	8001-54-5	7173-51-5
Ready Biodegradability Prediction	NO	NO	YES
Persistence (if B2 or B6 is <0.5 and B3 is <2.25 (-2.75)	Maybe More degradation relevant information might be warranted	NO	NO

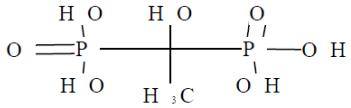
3.15.3 Summary and conclusions

This group contain both ready biodegradable substances and persistent substances. More details are needed to predict which compounds are likely in red category.

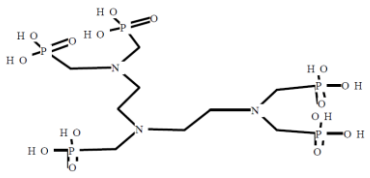
3.16 Phosphonates

Phosphonates are anthropogenic complexing agents containing one or more C-PO(OH)$_2$ groups. In oil fields, phosphonates are used to inhibit scale formation, e.g. bariumsulfate or calcium carbonate precipitation. Based on total industrial use worldwide, HEDP (1-hydroxyethane(1,1-diylbisphosphonicacid) and DTPMP (Diethylenetriaminepentakis (methylenephosphonic acid)) are the most important ones (63). Phosphonates adsorb very strongly onto almost all mineral surfaces, and adsorption of chelating agents by surfaces has been shown to decrease the biodegradability (63).

Representatives with CAS numbers:



CAS: 2809-21-4, HEDP



CAS 15827-60-8, DTPMP

3.16.1 Biodegradation data

Data on biodegradability of the group representatives for phosphonates were searched through the ECHA registered substances database and were only found for two of the selected representatives. Two studies for DTPMP (or DETPMP, CAS No. 15827-60-8 [2-4]) have been submitted to ECHA, whereof one is processed. The preliminary conclusion is: Not inherently biodegradable (100%). For 1HEDP, (CAS No. 2809-21-4(64)), eight studies have been submitted to ECHA but none have been processed.

Table 25. Registered biodegradation of Phosphonates in databases
CAS: 2809-21-4, HEDP

Value (%)	Endpoint	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Reference
23% (calculated)	BOD5	5	120	ECHA CHEM	yes	1	OECD 301D	Report 1992
0-10	BOD	30	Not specified	ECHA CHEM	no	4	Closed Bottle Test	review(65)
10.17 ± 1.95 **6.97 ± 3.58**	Not specified	24-hour cycle; 72-hour cycle	Not specified	ECHA CHEM	no	2	Not specified	Report 1978
0	Not specified	30	5	ECHA CHEM	no	4	EU Method C.4-E - Closed Bottle Test	Review (65)
33	DOC	Not specified	500	ECHA CHEM	no	4	Modified Zahn-Wellens-Test	Review (65)
<10	ThCO2	Not specified	Not specified	ECHA CHEM	no	4	Sturm Test	Review(66)
Ca 10	Not specified	28	Not specified	ECHA CHEM	no	2	Modified Screening (ready test	review(67)
23	Not specified	Not specified	500	ECHA CHEM	no	4	Zahn-Wellens Test	Review (65)

Table 26. Registered biodegradation of Phosphonates in databases
CAS 15827-60-8, DTPMP

Value (%)	Endpoint	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Reference
17 **7**	BOD	7 28	6.72 16.79	ECHA CHEM	no	2	Read across OECD 301D modifications*	Report 2006
3.51 **0.87**	Radiochemical measurment	24h 72h	Not specified	ECHA CHEM	no	2	Modified SCAS Test	Report 1978

* Preadapted inoculum was used, and inorganic phosphate was left out of the nutrient medium.

Biodegradation data for pentaphosphonate sodium salt were previously compiled by Stang et al., (2014)(16) and are shown in table 27.

Table 27. Registered biodegradation of phosphonate sodium salt
CAS nr: 22042-96-2

Value (%)	Endpoint	Duration (days)	Initial conc. (mg/L)	Database	GLP compliance	Reliability	Test guideline	Reference
17	O2 consumption	28		ECHA	No		OECD 301 D	(16)
0	DOC consumption	28		ECHA	Yes		OECD 301 E	(16)
0		28		ECHA	Yes		OECD 302 B	(16)
68		56		ECHA	No		ISO 11734:1995	(16)

The literature search for the phosphonate group representatives resulted in 4 hits for full text evaluation and only one of these were considered relevant. Due to the limited amount of information found by searching the group representatives, a search in google scholar with the following search terms was performed; phosphonate* and (oil OR petroleum) and biodeg*, resulting in 54 hits, whereof none appeared to be relevant (based on the title). A google search with the search term “biodegradation of phosphonate*” was then performed and resulted in an additional two relevant references. No available biodegradation data from the OECD 301 or OECD 306 tests were found, however, several references show that phosphonates can be degraded by microorganisms (63, 68, 69). The polyphosphonate DTPMP was shown to be biodegraded by cell-free extracts from cyanobacterial cells of the strain CCALA 007 of *Anabaena variabilis* grown in the absence of any phosphonate (68).

Bacteria have evolved the ability to metabolize phosphonates as phosphorous nutrient sources due to presence of natural phosphonates. However, the industrial polyphosphonates can differ greatly from natural phosphonates. A review of the environmental chemistry of phosphonates showed that biodegradation tests of HEDP and NTMP

(nitrilotris(methylenephosphonic acid)) with sludge from municipal sewage treatment plants gave no indication for any degradation based on CO_2 formation. Also, an investigation of HEDP, NTMP, EDTMP (1,2-diaminoethanetetrakis(methylenephosphonic acid) and DTPMP in standard biodegradation tests failed to identify any biodegradation. In summary, little or no biodegradation of phosphonates are observed in natural systems but microorganisms capable of degrading phosphonates have been isolated from these environments (63).

3.16.2 Biodegradation predictions

The BIOWIN prediction for Ready Biodegradation and Persistence for two phosphonates are shown in table 28.

Table 28. BIOWIN prediction of biodegradability
Phosphonates

	HEDP, CAS: 2809-21-4	DTPMP, CAS: 15827-60-8
Ready Biodegradability Prediction	NO	NO
Persistence (if B2 or B6 is <0.5 and B3 is <2.25 (-2.75)	Maybe More degradation relevant information might be warranted	YES

3.16.3 Summary and conclusions

Little or no biodegradation of phosphonates are observed in natural systems but microorganisms capable of degrading phosphonates have been isolated. Based on test data and literature on the phosphonate representatives, these substances are assumed not readily biodegradable and are likely in the red category. This is supported by the Biowin modelling results and that phosphonates adsorb very strongly onto almost all mineral surfaces, which has been shown to decrease the biodegradability. Some uncertainty regarding the OECD screening tests of phosphonates are due to the use of mineral supplements of phosphorous in these tests. Microorganisms are likely to utilize the more accessible added phosphorous before trying to use phosphonates as a source for phosphorous.

3.17 EO/PO block polymer

3.17.1 Biodegradation data

No data for biodegradation of EO/PO block polymers were found in the searched databases. The literature search for block polymers was challenging due to the fact that block polymers were often identified by listing the two polymers that were used to form the block polymer and not the block polymer itself. No relevant information was found by the literature search for cross-linked ethylene oxide propylene oxide block polymer (CAS nr 68123-18-2). A search in google scholar using the term "block polymer" AND (oil OR petroleum) AND biodeg* was therefore performed and resulted in seven hits, whereof none was considered relevant. A broader search in google scholar resulted in one relevant hit.

PO-polymers are known to break down slowly in the environment whereas poly(ethylene glycol)s biodegrade at a reasonable rate provided that the molecular weight is not too high.

The biodegradation rate of EO-PO block copolymers depends on the EO to PO ratio. However, also the high EO copolymers show a biodegradation rate of < 60% (70).

3.17.2 Biodegradation prediction

No biodegradation predictions were performed with BIOWIN as polymers with molecular weight larger than ~700 and ~900 are outside the range of the chemicals included in the training set of the models.

3.17.3 Summary and conclusions

No conclusion can be drawn regarding the biodegradation of EO/PO block polymers as no relevant data was found, the actual structure and identity of the block polymers are difficult to find, and the biodegradation potential depends on the composition of the block polymer. It is possible to enhance the biodegradation potential of a block polymer by a designing the chemical in a way that it contains sites that are easily accessible for biodegradation along the polymer.

3.18 Polyesters

3.18.1 Biodegradation data

No relevant biodegradation data were found in the searched data-bases. Two partly relevant papers were found for polyesters in the literature review. One study investigated the biodegradability of 21 samples of biosynthetic and chemosynthetic polyester films in river water, and the other investigated the biodegradation of eight aliphatic polyester films in natural water. Polyester films are not believed to be a proper representative for polyesters used in the oil field industry but is included here to provide some information on polyesters as a group. In both studies, biodegradation was tested by a modified version of the MITI test under aerobic conditions in a temperature controlled (25 degrees C) BOD reactor for 28 days. The rate of biodegradation of aliphatic polyesters in river water was strongly dependent on the chemical structure of polyester, and the biodegradability of aliphatic polyesters decreased in the following order: poly(ethylene succinate) > poly(ethylene adipate) > poly(butylene adipate) > poly(butylene sebacate) > poly(ethylene sebacate) = poly(butylene succinate) = poly(hexylene succinate) (71). For most of the eight tested aliphatic polyesters, the biodegradation appeared to be lower in seawater than in freshwater (72). The biodegradability of polyester films in sea water varied from 1% to 84% (BOD) (72).

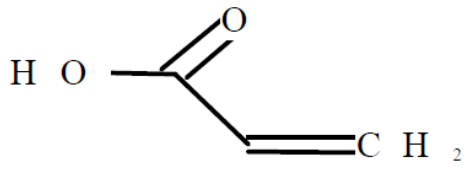
3.18.2 Biodegradation prediction

No biodegradation prediction using Biowin was performed for this group of compounds.

3.18.3 Summary and conclusions

No conclusion can be drawn as no specific polyester representatives for oil field industry was identified and limited general information regarding biodegradability of polyesters was obtained. A more comprehensive literature review or identification of specific polyesters are warranted to further investigate the biodegradability of polyesters used in oil filed industry.

3.19 Polyacrylates



Acrylate, CAS: 9003-04-7

3.19.1 Biodegradation data

Data on biodegradability of the group representatives for polyacrylate were searched through the ECHA registered substances database and no test data was submitted.

Several studies on biodegradation of sodium polyacrylates were found in the literature.

Two studies using bacteria isolated from soil investigated the effect of molecular weight of poly(sodium acrylate) (PSA) on biodegradability (73, 74). The first study used increasing sizes of the oligomers and found from 36 to 80% degradations with decreasing biodegradation with increasing numbers of monomers up to heptamer (7 monomers), however, the octamer (8 monomers) did not degrade in two weeks (74). In another study with two different strains, using 0.2% poly(sodium acrylate) as nutrient source, polymers having average molecular weight of 1000, 1500, and 4000 were degraded to extents of 73%, 49%, and 20%, respectively, in 2 weeks (73).

The degradation path way of PSA was investigated in another study: A consortium of several bacteria degraded PSA with average molecular weight of 2100 g/mol. The proposed degradation pathway of PSA involves (i) oxidation of a methylene group to a carbonyl group next to the terminus, (ii) decarboxylation to form an aldehyde group and dehydrogenation to form a double bond between the terminal unit and the next unit, and (iii) oxidation of the aldehyde group to a carboxyl group followed by elimination of an acetic acid (75).

Two studies looked at design of biodegradable functional polymers: poly[(sodium acrylate)-co-(vinyl alcohol)] [P(SA-co-VA)] (76) and poly[(sodium acrylate)-co-(4-vinylpyridine)] [P(SA-co-4VP)] (77). Matsumura found that: “the acrylate copolymers having more than 80 mol-% vinyl alcohol content showed biodegradability. That is, P(SA-co-VA) having a vinyl alcohol chain length of more than about 5-6 is cleaved by PVA-degrading microbes. This indicates that the vinyl alcohol blocks, which act as biodegradable segments, should be incorporated into the polymer chain in such a manner that they are accepted as substrates by the PVA-degrading enzyme” (76). Peng found that: “the biodegradation of P(SA-co-4VP) was more conspicuous when content of the 4-vinylpyridine in the copolymer was larger. This indicates that the 4-vinylpyridine, which acts as biodegradable segments, should be incorporated into the polymer main chain in such a manner that they are digested by activated sludge” (77).

3.19.2 Biodegradation predictions

Polymers are not fit for BIOWIN predictions if molecular weight is higher than ~700-g/mol for biowin 1-4 and higher than ~900 for biowin5-7. Therefore, only acrylate was predicted with BIOWIN. Acrylate has a Ready Biodegradability Prediction of YES and a Persistence prediction of NO (see appendix 2 for full BIOWIN output).

3.19.3 Summary and conclusions

Biodegradability of substances generally decrease with size. In addition, man-made polymers can be assessed as non-biodegradable without the provision of test data if they are not polycationic, surface active or have a functional group equivalent weight less or equal to 5 000 Da (1). However, it is possible to design polymers that are more biodegradable by including certain co-polymers.

3.20 Summary conclusions

Table 29. Summary for all chemicals and groups
Conclusion on classification in red category: less than 20% BOD28 in seawater

Selected compounds (CAS no)	Conclusions
Alkyl amino phosphonic acid salt (22036-78-8)	No conclusion can be drawn due to no available test data for biodegradation and non-conclusive model predictions. The compound is predicted to have a likely degradation pathway, but it is also predicted to not be Ready Biodegradable.
Triethyleneamine salt of n-methylbenzenesulphonamido caproic acid (26919-50-6)	Weak evidence of red category. The lack of relevant data indicate that the substance should be subject to future evaluations.
Nitriloacetic acid (139-13-9)	Conflicting information, not enough evidence to conclude.
DI-Epoxide/Oxyalkylated polyglycol (68123-18-**2)**	No data available, not applicable for QSAR modeling.
Triethanolamine (102-71-6)	Biodegradation in seawater is likely to be close to 20%, but might be both above and below. More information will be available within few months (ringtest data (8)).
Thioglycolic acid (68-11-1)	Biodegradable with variation in freshwater, no seawater data. Not enough evidence to conclude.
Dipropylene glycol methyl ether (34590-94-8)	Biodegradable in freshwater, no seawater data. Not enough evidence to conclude.
Mercaptoethanol (60-24-2)	Not ready biodegradable. Not enough evidence to conclude on biodegradability in seawater.
Polyoxyalkylene glycol (9038-95-3)	Not enough data.
2-Fluorobenzoic acid (445-29-4)	Modelling data suggest that the substance is not easily biodegradable. Not enough data for conclusions
Benzotriazole (95-14-7)	Very likely in red category
N-Methyldiethanolamine (105-59-9)	Likely in red category
Polydimethylsiloksan (PDMS) (63148-62-9)	No data available, not applicable for QSAR modeling.
Polyacrylamides	Large molecules of polyacrylamide and hydrolysed polyacrylamide (>1e6 DA) are likely in red category
Quaternary ammonium compounds	This group contain both ready biodegradable substances and persistent substances. More details are needed to predict which compounds are likely in red category
Phosphonates	Large range of biodegradability. More details are needed to predict which compounds are likely in red category
EO/PO block polymer	biodegradation is linked to EO to PO ratio.
Polyester	Not enough data
Polyacrylates	Large polymers are likely to be in red category, but it is possible to include co-polymers to increase biodegradation

4. References

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Appendix

1. Results of the literature search

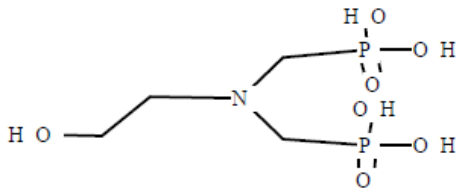
Table A1. Overview of numbers of included and excluded studies

Compound name (CAS)	Hits in ISI	Hits in Google scholar	Hits after removal of duplicates	Relevant hits	Full texts for review
Alkyl amino phosphonic acid salt (22036-78-8)	0	0	0	0	0
Triethyleneamine salt of n-methylbenzenesulphonamido caproic acid (26919-50-6)	0	0	0	0	0
Nitriloacetic acid (139-13-9)	3	14	17	15	2
DI-Epoxide/Oxyalkylated polyglycol (68123-18-2)	0	0			
Triethanolamine (102-71-6)	42	61	100	92	7 (8)
Thioglycolic acid (68-11-1)	15	31	46	45	1
Dipropylene glycol methyl ether (34590-94-8)	0	4	4	4	0
Mercaptoethanol (60-24-2)	38	112	149	148	1
Polyoxyalkylene glycol (9038-95-3)	10	0	10	10	0
2-Fluorobenzoic acid (445-29-4)	0	6	6	6	0
Benzotriazole (95-14-7)	70	52	119	99	20
N-Methyldiethanolamine (105-59-9)	13	1	14	13	1
Polyacrylamides					
HPAM - partly hydrolysed polyacrylamides, Flopaam	12	6	18	6	
Quaternary ammonium compounds					
Alkyl(C12-16)dimethylbenzylammonium chloride (68424-85-1)	0	2	2	1	
N-Benzyl-N,N-dimethyl-1-tridecanaminium chloride (8001-54-5)	0	4	4	0	0
N-Decyl-N,N-dimethyl-1-decanaminium chloride (7173-51-5)	0	3	3	0	0
Phosphonates					
Diethylene Triamine Penta (Methylene Phosphonic Acid) (DTPMP or DETPMP) (15827-60-8)	2 (diethylene…)+ 6 (DTMP)	4	12	1	1
OMPHT	0	1	1	0	0
Sodium Salt of Triethylene-tetramine Hexmethanephonic Acid (TETHMP	0	0	0	0	0
HMTPMP	0	0	0	0	0
1-Hydroxyethane-1 1-Diphosphonic Acid (HEDP) (2809-21-4)	1 + 6 (HEDP)	4 + 10 (HEDP)	21	3	

1,6-diaminohexane-1,1,6,6-tetrayl)tetraphosphonic acid (BP-7)	3	11	14	0	0
Ethylenediamine-tetrakis(methylenephosphonic acid) (EDTMP)	1	2	3	0	0
hexamethylenediamine-tetrakis(methylenephosphonic acid) (HDTMP)	0	0	0	0	0
octamethylenediamine-tetrakis-(methylenephosphonic acid) (ODTMP)	0	0	0	0	0
dodecamethylenediamine-tetrakis(methylenephosphonic acid) (DDTMP	0	0	0	0	0
EO/PO block polymer (1000, 5000 and 10 000 g/mol)					
Cross-linked ethylene oxide propylene oxide block polymer (68123-18-2)	0	0	0	0	0
block copolymer of poly(ethylene oxide-b-propylene oxide)—COP1 (Dow Química, Brazil), cationic polyacrylamide-PAMC (CYTEC) and poly(sodium acrylate)-PAS (Oxiteno, Brazil) were used. Another block copolymer of poly (ethylene oxide-b-propylene oxide) — COP2 (Dow Química, Brazil)[9]					
([OMBP3], [OMBP4], and [OMBP5], respectively). The OM adduct was reacted with [BP4] in presence of lauryl alcohol (LA) and triethylenetetramine (TETA) to produce [(OMBP4)LA] and [(OMBP4)-TETA], respectively.					
Polyesters	0	2	2	1	1
Polyacrylates					
Sodium polyacrylate (2594415)	6	3	9	0	0
Sodium acrylate (9003-04-7)	17	16		10	
Copolymer of acrylic acid and mono-/diacrylate ester derived from mixed ethylene oxide/propylene oxide block copolymer (70857-15-7)	0	0	0	0	0
PDMS (polydimethylsiloksan) (63148-62-9)	153	72	Refined with OECD 301 OR OECD 306 = 2	0	0

2. BIOWIN output data

Alkyl amino phosphonic acid salt



SMILES : OCCN(CP(O)(O)=O)CP(O)(O)=O
CHEM :
MOL FOR: C4 H13 N1 O7 P2
MOL WT : 249.10

---------- BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks
Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable
Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1587	0.1587
Frag	1	Tertiary amine	-0.2053	-0.2053
MolWt	*	Molecular Weight Parameter		-0.1186
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.5824

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	1.1178	1.1178
Frag	1	Tertiary amine	-2.2229	-2.2229
MolWt	*	Molecular Weight Parameter		-3.5372
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.1633

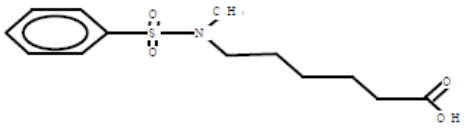
A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1600	0.1600
Frag	1	Tertiary amine	-0.2548	-0.2548
MolWt	*	Molecular Weight Parameter		-0.5505
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.5539

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1294	0.1294
Frag	1	Tertiary amine	-0.2880	-0.2880
MolWt	*	Molecular Weight Parameter		-0.3594
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.3298

```
 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1611 |  0.1611
 Frag |  1  |  Tertiary amine                         | -0.0848 | -0.0848
 Frag |  4  |  -CH2-  [linear]                        |  0.0494 |  0.1977
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.7411
 Const|  *  |  Equation Constant                      |         |  0.7121
============+=========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)|         |  0.2450
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  1.0041 |  1.0041
 Frag |  1  |  Tertiary amine                         | -0.8396 | -0.8396
 Frag |  4  |  -CH2-  [linear]                        |  0.4295 |  1.7180
 MolWt|  *  |  Molecular Weight Parameter             |         | -7.1912
============+=========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.0582
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1328 |  0.1328
 Frag |  1  |  Tertiary amine                         | -1.0749 | -1.0749
 Frag |  4  |  -CH2-  [linear]                        |  0.0260 |  0.1040
 Const|  *  |  Equation Constant                      |         |  0.8361
============+=========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)|         | -0.0020
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
 Criteria for the YES or NO prediction:  If the Biowin3 (ultimate survey
 model) result is "weeks" or faster (i.e. "days", "days to weeks", or
 "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
 the prediction is YES (readily biodegradable).  If this condition is not
 satisfied, the prediction is NO (not readily biodegradable).  This method
 is based on application of Bayesian analysis to ready biodegradation data
 (see Help).  Biowin5 and 6 also predict ready biodegradability, but for
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.
```

N-methylbenzenesulphonamido caproic acid



SMILES : CN(CCCCCC(=O)(O))S(=O)(=O)c1ccccc1
CHEM :
MOL FOR: C13 H19 N1 O4 S1
MOL WT : 285.36

---------- BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks
Biowin4 (Primary Biodegradation Timeframe): Days
Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable
Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable
Biowin7 (Anaerobic Model Prediction): Biodegrades Fast
Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	0.0727	0.0727
Frag	1	Unsubstituted phenyl group (C6H5-)	0.1281	0.1281
MolWt	*	Molecular Weight Parameter		-0.1359
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.8125

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	0.6431	0.6431
Frag	1	Unsubstituted phenyl group (C6H5-)	1.7991	1.7991
MolWt	*	Molecular Weight Parameter		-4.0521
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.8020

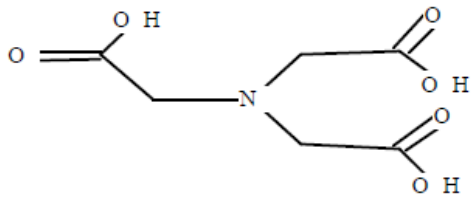
A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	0.3646	0.3646
Frag	1	Unsubstituted phenyl group (C6H5-)	0.0220	0.0220
MolWt	*	Molecular Weight Parameter		-0.6306
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.9552

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	0.3856	0.3856
Frag	1	Unsubstituted phenyl group (C6H5-)	0.0049	0.0049
MolWt	*	Molecular Weight Parameter		-0.4117
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.8265

```
 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.1812 |  0.1812
 Frag |  5  |  Aromatic-H                               |  0.0082 |  0.0411
 Frag |  1  |  Methyl  [-CH3]                           |  0.0004 |  0.0004
 Frag |  5  |  -CH2-  [linear]                          |  0.0494 |  0.2471
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.8489
 Const|  *  |  Equation Constant                        |         |  0.7121
============+===========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability) |         |  0.3329
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  1.1346 |  1.1346
 Frag |  5  |  Aromatic-H                               |  0.1201 |  0.6007
 Frag |  1  |  Methyl  [-CH3]                           |  0.0194 |  0.0194
 Frag |  5  |  -CH2-  [linear]                          |  0.4295 |  2.1475
 MolWt|  *  |  Molecular Weight Parameter               |         | -8.2380
============+===========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.1406
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.1868 |  0.1868
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)       |  0.2182 |  0.2182
 Frag |  5  |  Aromatic-H                               | -0.0954 | -0.4772
 Frag |  1  |  Methyl  [-CH3]                           | -0.0796 | -0.0796
 Frag |  5  |  -CH2-  [linear]                          |  0.0260 |  0.1299
 Const|  *  |  Equation Constant                        |         |  0.8361
============+===========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)  |         |  0.8143
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
 Criteria for the YES or NO prediction:  If the Biowin3 (ultimate survey
 model) result is "weeks" or faster (i.e. "days", "days to weeks", or
 "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
 the prediction is YES (readily biodegradable).  If this condition is not
 satisfied, the prediction is NO (not readily biodegradable).  This method
 is based on application of Bayesian analysis to ready biodegradation data
 (see Help).  Biowin5 and 6 also predict ready biodegradability, but for
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.
```

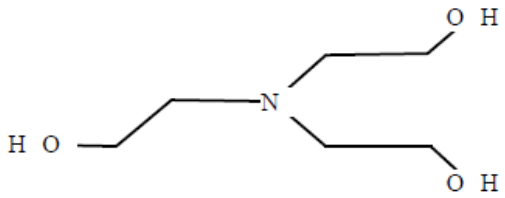
Nitriloacetic acid



```
SMILES : O=C(O)CN(CC(=O)O)CC(=O)O
CHEM   :
MOL FOR: C6 H9 N1 O6
MOL WT : 191.14
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Days-Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Hours-Days
   Biowin5 (MITI Linear Model Prediction)     :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  YES

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic acid   [-C(=O)-OH]           |  0.0727 |  0.2181
 Frag |  1  |  Tertiary amine                         | -0.2053 | -0.2053
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.0910
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.6694
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic acid   [-C(=O)-OH]           |  0.6431 |  1.9293
 Frag |  1  |  Tertiary amine                         | -2.2229 | -2.2229
 MolWt|  *  |  Molecular Weight Parameter             |         | -2.7142
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.5002
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic acid   [-C(=O)-OH]           |  0.3646 |  1.0938
 Frag |  1  |  Tertiary amine                         | -0.2548 | -0.2548
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.4224
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  3.6158
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic acid   [-C(=O)-OH]           |  0.3856 |  1.1567
 Frag |  1  |  Tertiary amine                         | -0.2880 | -0.2880
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2758
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|         |  4.4407
============+=========================================+=========+=========
```

```
 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic acid   [-C(=O)-OH]           |  0.1812 |  0.5435
 Frag |  1  |  Tertiary amine                         | -0.0848 | -0.0848
 Frag |  3  |  -CH2-  [linear]                        |  0.0494 |  0.1482
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.5686
 Const|  *  |  Equation Constant                      |         |  0.7121
============+=========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)|         |  0.7504
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic acid   [-C(=O)-OH]           |  1.1346 |  3.4038
 Frag |  1  |  Tertiary amine                         | -0.8396 | -0.8396
 Frag |  3  |  -CH2-  [linear]                        |  0.4295 |  1.2885
 MolWt|  *  |  Molecular Weight Parameter             |         | -5.5180
============+=========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.7027
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic acid   [-C(=O)-OH]           |  0.1868 |  0.5603
 Frag |  1  |  Tertiary amine                         | -1.0749 | -1.0749
 Frag |  3  |  -CH2-  [linear]                        |  0.0260 |  0.0780
 Const|  *  |  Equation Constant                      |         |  0.8361
============+=========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)|         |  0.3995
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
 Criteria for the YES or NO prediction:  If the Biowin3 (ultimate survey
 model) result is "weeks" or faster (i.e. "days", "days to weeks", or
 "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
 the prediction is YES (readily biodegradable).  If this condition is not
 satisfied, the prediction is NO (not readily biodegradable).  This method
 is based on application of Bayesian analysis to ready biodegradation data
 (see Help).  Biowin5 and 6 also predict ready biodegradability, but for
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.
```

Triethanolamine




```
SMILES : OCCN(CCO)CCO
CHEM   :
MOL FOR: C6 H15 N1 O3
MOL WT : 149.19
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)    :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)    :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  YES

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic alcohol  [-OH]               |  0.1587 |  0.4762
 Frag |  1  |  Tertiary amine                         | -0.2053 | -0.2053
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.0710
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.9474
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic alcohol  [-OH]               |  1.1178 |  3.3534
 Frag |  1  |  Tertiary amine                         | -2.2229 | -2.2229
 MolWt|  *  |  Molecular Weight Parameter             |         | -2.1185
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.8830
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic alcohol  [-OH]               |  0.1600 |  0.4799
 Frag |  1  |  Tertiary amine                         | -0.2548 | -0.2548
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.3297
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  3.0946
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Aliphatic alcohol  [-OH]               |  0.1294 |  0.3883
 Frag |  1  |  Tertiary amine                         | -0.2880 | -0.2880
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2152
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|         |  3.7328
============+=========================================+=========+=========
```

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aliphatic alcohol [-OH]	0.1611	0.4834
Frag	1	Tertiary amine	-0.0848	-0.0848
Frag	6	-CH2- [linear]	0.0494	0.2965
MolWt	*	Molecular Weight Parameter		-0.4438
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.9634

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aliphatic alcohol [-OH]	1.0041	3.0124
Frag	1	Tertiary amine	-0.8396	-0.8396
Frag	6	-CH2- [linear]	0.4295	2.5770
MolWt	*	Molecular Weight Parameter		-4.3070
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.9511

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

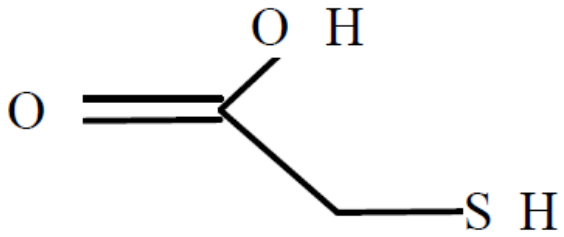
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Aliphatic alcohol [-OH]	0.1328	0.3983
Frag	1	Tertiary amine	-1.0749	-1.0749
Frag	6	-CH2- [linear]	0.0260	0.1559
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.3155

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Thioglycolic acid




```
SMILES : O=C(O)CS
CHEM   :
MOL FOR: C2 H4 O2 S1
MOL WT : 92.11
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Days-Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days
   Biowin5 (MITI Linear Model Prediction)     :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Biodegrades Fast
   Ready Biodegradability Prediction:  YES

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.0727 |  0.0727
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.0439
 Const|  *  |  Equation Constant                        |         |  0.7475
============+===========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)    |         |  0.7764
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.6431 |  0.6431
 MolWt|  *  |  Molecular Weight Parameter               |         | -1.3080
============+===========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)  |         |  0.9124
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.3646 |  0.3646
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.2036
 Const|  *  |  Equation Constant                        |         |  3.1992
============+===========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg) |         |  3.3602
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.3856 |  0.3856
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.1329
 Const|  *  |  Equation Constant                        |         |  3.8477
============+===========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg) |         |  4.1004
============+===========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	0.1812	0.1812
Frag	1	-CH2- [linear]	0.0494	0.0494
MolWt	*	Molecular Weight Parameter		-0.2740
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.6687

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	1.1346	1.1346
Frag	1	-CH2- [linear]	0.4295	0.4295
MolWt	*	Molecular Weight Parameter		-2.6592
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.8070

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

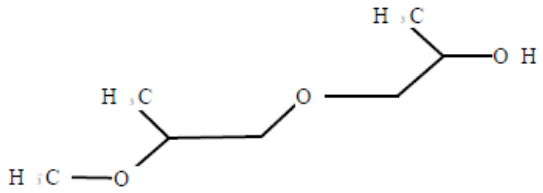
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	0.1868	0.1868
Frag	1	-CH2- [linear]	0.0260	0.0260
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		1.0488

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

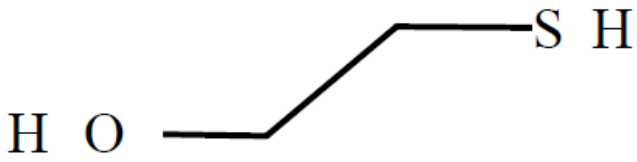
Dipropylene glycol methyl ether



```
SMILES : COC(C)COCC(C)O
CHEM   :
MOL FOR: C7 H16 O3
MOL WT : 148.20
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Does Not Biodegrade Fast
   Biowin2 (Non-Linear Model Prediction):  Does Not Biodegrade Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)     :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1587 |  0.1587
 Frag |  2  |  Aliphatic ether  [C-O-C]               | -0.3474 | -0.6947
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.0706
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.1410
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  1.1178 |  1.1178
 Frag |  2  |  Aliphatic ether  [C-O-C]               | -3.4294 | -6.8588
 MolWt|  *  |  Molecular Weight Parameter             |         | -2.1045
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.0079
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1600 |  0.1600
 Frag |  2  |  Aliphatic ether  [C-O-C]               | -0.0087 | -0.0173
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.3275
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  3.0143
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1294 |  0.1294
 Frag |  2  |  Aliphatic ether  [C-O-C]               | -0.0097 | -0.0195
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2138
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|         |  3.7439
============+=========================================+=========+=========
```

```
 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1611 |  0.1611
 Frag |  2  |  Aliphatic ether  [C-O-C]               |  0.0015 |  0.0029
 Frag |  3  |  Methyl  [-CH3]                         |  0.0004 |  0.0012
 Frag |  2  |  -CH2-  [linear]                        |  0.0494 |  0.0988
 Frag |  2  |  -CH-  [linear]                         | -0.0507 | -0.1013
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.4409
 Const|  *  |  Equation Constant                      |         |  0.7121
============+=========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)|         |  0.4340
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  1.0041 |  1.0041
 Frag |  2  |  Aliphatic ether  [C-O-C]               | -0.1071 | -0.2143
 Frag |  3  |  Methyl  [-CH3]                         |  0.0194 |  0.0583
 Frag |  2  |  -CH2-  [linear]                        |  0.4295 |  0.8590
 Frag |  2  |  -CH-  [linear]                         | -0.0998 | -0.1995
 MolWt|  *  |  Molecular Weight Parameter             |         | -4.2785
============+=========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|      |  0.4390
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1328 |  0.1328
 Frag |  2  |  Aliphatic ether  [C-O-C]               | -0.2573 | -0.5145
 Frag |  3  |  Methyl  [-CH3]                         | -0.0796 | -0.2387
 Frag |  2  |  -CH2-  [linear]                        |  0.0260 |  0.0520
 Frag |  2  |  -CH-  [linear]                         | -0.1659 | -0.3317
 Const|  *  |  Equation Constant                      |         |  0.8361
============+=========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)|         | -0.0641
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
 Criteria for the YES or NO prediction:  If the Biowin3 (ultimate survey
 model) result is "weeks" or faster (i.e. "days", "days to weeks", or
 "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
 the prediction is YES (readily biodegradable).  If this condition is not
 satisfied, the prediction is NO (not readily biodegradable).  This method
 is based on application of Bayesian analysis to ready biodegradation data
 (see Help).  Biowin5 and 6 also predict ready biodegradability, but for
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.
```

Mercaptoethanol




```
SMILES : OCCS
CHEM   :
MOL FOR: C2 H6 O1 S1
MOL WT : 78.13
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days
   Biowin5 (MITI Linear Model Prediction)     :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Biodegrades Fast
   Ready Biodegradability Prediction:  YES

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                 |  0.1587 |  0.1587
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.0372
 Const|  *  |  Equation Constant                        |         |  0.7475
============+===========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)    |         |  0.8691
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                 |  1.1178 |  1.1178
 MolWt|  *  |  Molecular Weight Parameter               |         | -1.1094
============+===========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)  |         |  0.9533
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                 |  0.1600 |  0.1600
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.1727
 Const|  *  |  Equation Constant                        |         |  3.1992
============+===========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg) |         |  3.1865
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic alcohol  [-OH]                 |  0.1294 |  0.1294
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.1127
 Const|  *  |  Equation Constant                        |         |  3.8477
============+===========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg) |         |  3.8645
============+===========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1611	0.1611
Frag	2	-CH2- [linear]	0.0494	0.0988
MolWt	*	Molecular Weight Parameter		-0.2324
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.7397

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	1.0041	1.0041
Frag	2	-CH2- [linear]	0.4295	0.8590
MolWt	*	Molecular Weight Parameter		-2.2555
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.8941

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

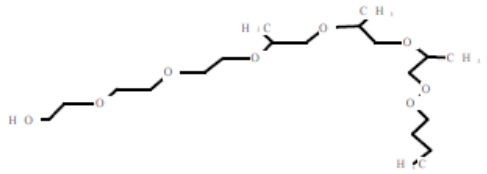
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1328	0.1328
Frag	2	-CH2- [linear]	0.0260	0.0520
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		1.0208

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Polyoxyalkylene glycol



```
SMILES : OCCOCCOCCOC(C)COC(C)COC(C)COOCCCC
CHEM   :
MOL FOR: C19 H40 O8
MOL WT : 396.53
--------------------------- BIOWIN v4.10 Results ---------------------------

   Biowin1 (Linear Model Prediction)     :  Does Not Biodegrade Fast
   Biowin2 (Non-Linear Model Prediction):  Does Not Biodegrade Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks-Months
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)     :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.1084 |  0.1084
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1587 |  0.1587
 Frag |  5  |  Aliphatic ether  [C-O-C]               | -0.3474 | -1.7368
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1888
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         | -0.9109
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  1.8437 |  1.8437
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  1.1178 |  1.1178
 Frag |  5  |  Aliphatic ether  [C-O-C]               | -3.4294 |-17.1470
 MolWt|  *  |  Molecular Weight Parameter             |         | -5.6307
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.0000
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2983 |  0.2983
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1600 |  0.1600
 Frag |  5  |  Aliphatic ether  [C-O-C]               | -0.0087 | -0.0434
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.8763
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  2.7379
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2691 |  0.2691
 Frag |  1  |  Aliphatic alcohol  [-OH]               |  0.1294 |  0.1294
 Frag |  5  |  Aliphatic ether  [C-O-C]               | -0.0097 | -0.0487
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.5721
```

Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.6255

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	0.1611	0.1611
Frag	5	Aliphatic ether [C-O-C]	0.0015	0.0074
Frag	4	Methyl [-CH3]	0.0004	0.0016
Frag	12	-CH2- [linear]	0.0494	0.5930
Frag	3	-CH- [linear]	-0.0507	-0.1520
MolWt	*	Molecular Weight Parameter		-1.1797
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.1436

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic alcohol [-OH]	1.0041	1.0041
Frag	5	Aliphatic ether [C-O-C]	-0.1071	-0.5357
Frag	4	Methyl [-CH3]	0.0194	0.0777
Frag	12	-CH2- [linear]	0.4295	5.1539
Frag	3	-CH- [linear]	-0.0998	-0.2993
MolWt	*	Molecular Weight Parameter		-11.4472
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0287

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

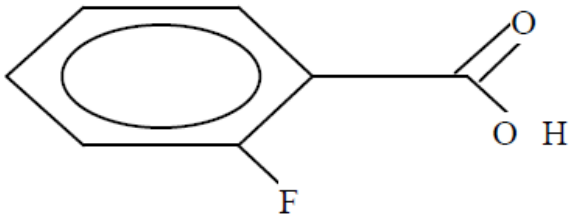
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	-0.3177	-0.3177
Frag	1	Aliphatic alcohol [-OH]	0.1328	0.1328
Frag	5	Aliphatic ether [C-O-C]	-0.2573	-1.2863
Frag	4	Methyl [-CH3]	-0.0796	-0.3183
Frag	12	-CH2- [linear]	0.0260	0.3119
Frag	3	-CH- [linear]	-0.1659	-0.4976
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-1.1391

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

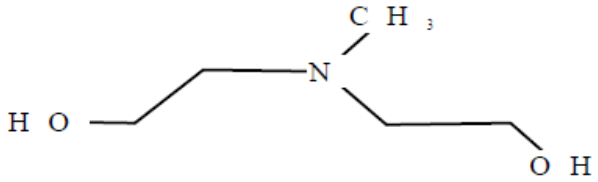
2-Fluorobenzoic acid




```
SMILES : O=C(O)c(c(F)ccc1)c1
CHEM   :
MOL FOR: C7 H5 F1 O2
MOL WT : 140.11
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Does Not Biodegrade Fast
   Biowin2 (Non-Linear Model Prediction):  Does Not Biodegrade Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks-Months
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)     :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Biodegrades Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic acid    [-C(=O)-OH]           |  0.1769 |  0.1769
 Frag |  1  |  Aromatic fluoride    [-F]              | -0.8100 | -0.8100
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.0667
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.0477
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic acid    [-C(=O)-OH]           |  2.4224 |  2.4224
 Frag |  1  |  Aromatic fluoride    [-F]              |-10.5318 |-10.5318
 MolWt|  *  |  Molecular Weight Parameter             |         | -1.9896
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.0008
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic acid    [-C(=O)-OH]           |  0.0879 |  0.0879
 Frag |  1  |  Aromatic fluoride    [-F]              | -0.4069 | -0.4069
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.3096
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|        |  2.5705
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic acid    [-C(=O)-OH]           |  0.0077 |  0.0077
 Frag |  1  |  Aromatic fluoride    [-F]              |  0.0135 |  0.0135
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2022
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|        |  3.6668
============+=========================================+=========+=========
```

```
 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic acid   [-C(=O)-OH]            |  0.3770 |  0.3770
 Frag |  1  |  Fluorine  [-F]                         |  0.0174 |  0.0174
 Frag |  4  |  Aromatic-H                             |  0.0082 |  0.0329
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.4168
 Const|  *  |  Equation Constant                      |         |  0.7121
============+=========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |         |  0.7225
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic acid   [-C(=O)-OH]            |  2.4449 |  2.4449
 Frag |  1  |  Fluorine  [-F]                         | -3.9878 | -3.9878
 Frag |  4  |  Aromatic-H                             |  0.1201 |  0.4806
 MolWt|  *  |  Molecular Weight Parameter             |         | -4.0449
============+=========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.0703
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic acid   [-C(=O)-OH]            |  0.2656 |  0.2656
 Frag |  1  |  Aromatic fluoride   [-F]               |  0.0000 |  0.0000
 Frag |  1  |  Fluorine  [-F]                         |  0.0000 |  0.0000
 Frag |  4  |  Aromatic-H                             | -0.0954 | -0.3817
 Const|  *  |  Equation Constant                      |         |  0.8361
============+=========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)   |         |  0.7199
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
 Criteria for the YES or NO prediction:  If the Biowin3 (ultimate survey
 model) result is "weeks" or faster (i.e. "days", "days to weeks", or
 "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
 the prediction is YES (readily biodegradable).  If this condition is not
 satisfied, the prediction is NO (not readily biodegradable).  This method
 is based on application of Bayesian analysis to ready biodegradation data
 (see Help).  Biowin5 and 6 also predict ready biodegradability, but for
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.
```

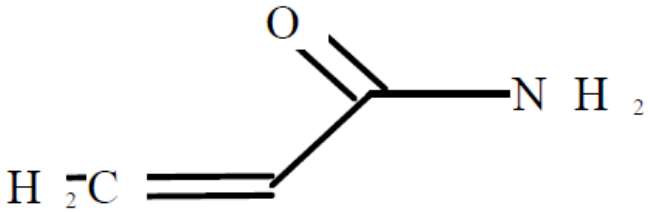
N-methyldiethanolamine




```
SMILES : OCCN(CCO)C
CHEM   :
MOL FOR: C5 H13 N1 O2
MOL WT : 119.16
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)     :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  YES

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Aliphatic alcohol  [-OH]               |  0.1587 |  0.3175
 Frag |  1  |  Tertiary amine                         | -0.2053 | -0.2053
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.0567
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.8030
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Aliphatic alcohol  [-OH]               |  1.1178 |  2.2356
 Frag |  1  |  Tertiary amine                         | -2.2229 | -2.2229
 MolWt|  *  |  Molecular Weight Parameter             |         | -1.6921
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.7907
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Aliphatic alcohol  [-OH]               |  0.1600 |  0.3199
 Frag |  1  |  Tertiary amine                         | -0.2548 | -0.2548
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2633
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  3.0010
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Aliphatic alcohol  [-OH]               |  0.1294 |  0.2589
 Frag |  1  |  Tertiary amine                         | -0.2880 | -0.2880
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1719
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|         |  3.6467
============+=========================================+=========+=========
```

```
 Result Classification:   5.00 -> hours      4.00 -> days     3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months     1.00 -> longer

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  2  |  Aliphatic alcohol  [-OH]                 |  0.1611 |  0.3223
 Frag |  1  |  Tertiary amine                           | -0.0848 | -0.0848
 Frag |  1  |  Methyl  [-CH3]                           |  0.0004 |  0.0004
 Frag |  4  |  -CH2-  [linear]                          |  0.0494 |  0.1977
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.3545
 Const|  *  |  Equation Constant                        |         |  0.7121
============+===========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability) |         |  0.7931
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  2  |  Aliphatic alcohol  [-OH]                 |  1.0041 |  2.0083
 Frag |  1  |  Tertiary amine                           | -0.8396 | -0.8396
 Frag |  1  |  Methyl  [-CH3]                           |  0.0194 |  0.0194
 Frag |  4  |  -CH2-  [linear]                          |  0.4295 |  1.7180
 MolWt|  *  |  Molecular Weight Parameter               |         | -3.4401
============+===========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.8799
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  2  |  Aliphatic alcohol  [-OH]                 |  0.1328 |  0.2655
 Frag |  1  |  Tertiary amine                           | -1.0749 | -1.0749
 Frag |  1  |  Methyl  [-CH3]                           | -0.0796 | -0.0796
 Frag |  4  |  -CH2-  [linear]                          |  0.0260 |  0.1040
 Const|  *  |  Equation Constant                        |         |  0.8361
============+===========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)  |         |  0.0511
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
 Criteria for the YES or NO prediction:  If the Biowin3 (ultimate survey
 model) result is "weeks" or faster (i.e. "days", "days to weeks", or
 "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
 the prediction is YES (readily biodegradable).  If this condition is not
 satisfied, the prediction is NO (not readily biodegradable).  This method
 is based on application of Bayesian analysis to ready biodegradation data
 (see Help).  Biowin5 and 6 also predict ready biodegradability, but for
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.
```

Acrylamide, monomer




```
SMILES : C=CC(=O)N
CHEM   :
MOL FOR: C3 H5 N1 O1
MOL WT : 71.08
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)    :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days
   Biowin5 (MITI Linear Model Prediction)    :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  YES

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  0.2102 |  0.2102
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.0338
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.9239
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  2.6913 |  2.6913
 MolWt|  *  |  Molecular Weight Parameter             |         | -1.0093
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.9909
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Amide   [-C(=O)-N  or -C(=S)-N]        | -0.0542 | -0.0542
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1571
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|        |  2.9879
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  0.2054 |  0.2054
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1026
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|        |  3.9506
============+=========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Amide [-C(=O)-N or -C(=S)-N]	0.1266	0.1266
Frag	3	-C=CH [alkenyl hydrogen]	0.0062	0.0186
MolWt	*	Molecular Weight Parameter		-0.2115
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.6459

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Amide [-C(=O)-N or -C(=S)-N]	0.8859	0.8859
Frag	3	-C=CH [alkenyl hydrogen]	0.0285	0.0855
MolWt	*	Molecular Weight Parameter		-2.0520
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.8092

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

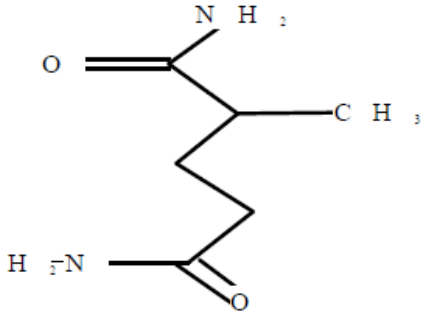
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Amide [-C(=O)-N or -C(=S)-N]	-0.5679	-0.5679
Frag	3	-C=CH [alkenyl hydrogen]	-0.0735	-0.2206
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.0476

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Acrylamide, dimer



```
SMILES : O=C(N)C(C)CCC(=O)(N)
CHEM   :
MOL FOR: C6 H12 N2 O2
MOL WT : 144.17
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)    :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days
   Biowin5 (MITI Linear Model Prediction)    :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  YES

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  0.2102 |  0.4203
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.0686
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  1.0992
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  2.6913 |  5.3826
 MolWt|  *  |  Molecular Weight Parameter             |         | -2.0473
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.9982
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Amide   [-C(=O)-N  or -C(=S)-N]        | -0.0542 | -0.1084
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.3186
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|        |  2.7721
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  0.2054 |  0.4109
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2080
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|        |  4.0506
============+=========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Amide [-C(=O)-N or -C(=S)-N]	0.1266	0.2533
Frag	1	Methyl [-CH3]	0.0004	0.0004
Frag	2	-CH2- [linear]	0.0494	0.0988
Frag	1	-CH- [linear]	-0.0507	-0.0507
MolWt	*	Molecular Weight Parameter		-0.4289
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.5850

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Amide [-C(=O)-N or -C(=S)-N]	0.8859	1.7717
Frag	1	Methyl [-CH3]	0.0194	0.0194
Frag	2	-CH2- [linear]	0.4295	0.8590
Frag	1	-CH- [linear]	-0.0998	-0.0998
MolWt	*	Molecular Weight Parameter		-4.1621
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.7138

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

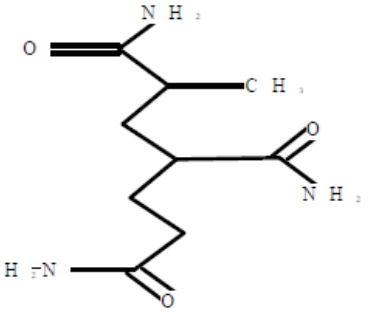
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Amide [-C(=O)-N or -C(=S)-N]	-0.5679	-1.1358
Frag	1	Methyl [-CH3]	-0.0796	-0.0796
Frag	2	-CH2- [linear]	0.0260	0.0520
Frag	1	-CH- [linear]	-0.1659	-0.1659
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.4931

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Acrylamide, trimer



```
SMILES : O=C(N)C(C)CC(C(=O)(N))CCC(=O)(N)
CHEM   :
MOL FOR: C9 H17 N3 O3
MOL WT : 215.25
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)    :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks-Months
   Biowin4 (Primary  Biodegradation Timeframe):  Days
   Biowin5 (MITI Linear Model Prediction)    :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  0.2102 |  0.6305
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1025
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  1.2755
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  2.6913 |  8.0739
 MolWt|  *  |  Molecular Weight Parameter             |         | -3.0566
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.9997
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Amide   [-C(=O)-N  or -C(=S)-N]        | -0.0542 | -0.1626
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.4757
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  2.5609
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  0.2054 |  0.6163
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.3106
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|         |  4.1535
============+=========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Amide [-C(=O)-N or -C(=S)-N]	0.1266	0.3799
Frag	1	Methyl [-CH3]	0.0004	0.0004
Frag	3	-CH2- [linear]	0.0494	0.1482
Frag	2	-CH- [linear]	-0.0507	-0.1013
MolWt	*	Molecular Weight Parameter		-0.6404
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.4990

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Amide [-C(=O)-N or -C(=S)-N]	0.8859	2.6576
Frag	1	Methyl [-CH3]	0.0194	0.0194
Frag	3	-CH2- [linear]	0.4295	1.2885
Frag	2	-CH- [linear]	-0.0998	-0.1995
MolWt	*	Molecular Weight Parameter		-6.2141
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.5194

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

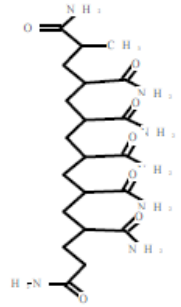
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Amide [-C(=O)-N or -C(=S)-N]	-0.5679	-1.7036
Frag	1	Methyl [-CH3]	-0.0796	-0.0796
Frag	3	-CH2- [linear]	0.0260	0.0780
Frag	2	-CH- [linear]	-0.1659	-0.3317
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-1.2008

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Acrylamide, heptamer



```
SMILES : O=C(N)C(C)CC(C(=O)(N))CC(C(=O)(N))CC(C(=O)(N))CC(C(=O)(N))CC(C(=O)(N)
         )CCC(=O)(N)
CHEM   :
MOL FOR: C21 H37 N7 O7
MOL WT : 499.57
-------------------------- BIOWIN v4.10 Results ---------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Recalcitrant
   Biowin4 (Primary  Biodegradation Timeframe):  Hours-Days
   Biowin5 (MITI Linear Model Prediction)     :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  7  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  0.2102 |  1.4711
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2378
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  1.9808
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  7  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  2.6913 | 18.8391
 MolWt|  *  |  Molecular Weight Parameter             |         | -7.0939
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  1.0000
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  7  |  Amide   [-C(=O)-N  or -C(=S)-N]        | -0.0542 | -0.3795
 MolWt|  *  |  Molecular Weight Parameter             |         | -1.1040
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|        |  1.7157
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  7  |  Amide   [-C(=O)-N  or -C(=S)-N]        |  0.2054 |  1.4380
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.7208
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|        |  4.5650
============+=========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	7	Amide [-C(=O)-N or -C(=S)-N]	0.1266	0.8864
Frag	1	Methyl [-CH3]	0.0004	0.0004
Frag	7	-CH2- [linear]	0.0494	0.3459
Frag	6	-CH- [linear]	-0.0507	-0.3040
MolWt	*	Molecular Weight Parameter		-1.4862
Const	*	Equation Constant		0.7121
RESULT	Biowin5 (MITI Linear Biodeg Probability)			0.1546

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	7	Amide [-C(=O)-N or -C(=S)-N]	0.8859	6.2011
Frag	1	Methyl [-CH3]	0.0194	0.0194
Frag	7	-CH2- [linear]	0.4295	3.0065
Frag	6	-CH- [linear]	-0.0998	-0.5986
MolWt	*	Molecular Weight Parameter		-14.4220
RESULT	Biowin6 (MITI Non-Linear Biodeg Probability)			0.0367

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	7	Amide [-C(=O)-N or -C(=S)-N]	-0.5679	-3.9751
Frag	1	Methyl [-CH3]	-0.0796	-0.0796
Frag	7	-CH2- [linear]	0.0260	0.1819
Frag	6	-CH- [linear]	-0.1659	-0.9951
Const	*	Equation Constant		0.8361
RESULT	Biowin7 (Anaerobic Linear Biodeg Prob)			-4.0318

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Polyacrylamide (decamer)

```
SMILES : O=C(N)C(C)CC(C(=O)(N))CC(C(=O)(N))CC(C(=O)(N))CC(C(=O)(N)
         )CC(C(=O)(N))CC(C(=O)(N))CC(C(=O)(N))CCC(=O)(N)
CHEM   :
MOL FOR: C30 H52 N10 O10
MOL WT : 712.81
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Recalcitrant
   Biowin4 (Primary  Biodegradation Timeframe):  Hours
   Biowin5 (MITI Linear Model Prediction)     :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO

------+-----+---------------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag | 10  |  Amide    [-C(=O)-N  or -C(=S)-N]           |  0.2102 |  2.1015
 MolWt|  *  |  Molecular Weight Parameter                 |         | -0.3394
 Const|  *  |  Equation Constant                          |         |  0.7475
============+=============================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)      |         |  2.5097
============+=============================================+=========+=========

------+-----+---------------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag | 10  |  Amide    [-C(=O)-N  or -C(=S)-N]           |  2.6913 | 26.9130
 MolWt|  *  |  Molecular Weight Parameter                 |         |-10.1219
============+=============================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)    |         |  1.0000
============+=============================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+---------------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag | 10  |  Amide    [-C(=O)-N  or -C(=S)-N]           | -0.0542 | -0.5421
 MolWt|  *  |  Molecular Weight Parameter                 |         | -1.5752
 Const|  *  |  Equation Constant                          |         |  3.1992
============+=============================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)   |         |  1.0819
============+=============================================+=========+=========

------+-----+---------------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION          |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag | 10  |  Amide    [-C(=O)-N  or -C(=S)-N]           |  0.2054 |  2.0543
 MolWt|  *  |  Molecular Weight Parameter                 |         | -1.0284
 Const|  *  |  Equation Constant                          |         |  3.8477
============+=============================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)   |         |  4.8736
============+=============================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days     3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	10	Amide [-C(=O)-N or -C(=S)-N]	0.1266	1.2663
Frag	1	Methyl [-CH3]	0.0004	0.0004
Frag	10	-CH2- [linear]	0.0494	0.4942
Frag	9	-CH- [linear]	-0.0507	-0.4560
MolWt	*	Molecular Weight Parameter		-2.1206
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.1037

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	10	Amide [-C(=O)-N or -C(=S)-N]	0.8859	8.8587
Frag	1	Methyl [-CH3]	0.0194	0.0194
Frag	10	-CH2- [linear]	0.4295	4.2949
Frag	9	-CH- [linear]	-0.0998	-0.8979
MolWt	*	Molecular Weight Parameter		-20.5779
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0031

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

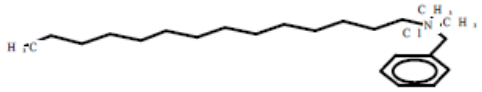
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	10	Amide [-C(=O)-N or -C(=S)-N]	-0.5679	-5.6788
Frag	1	Methyl [-CH3]	-0.0796	-0.0796
Frag	10	-CH2- [linear]	0.0260	0.2599
Frag	9	-CH- [linear]	-0.1659	-1.4927
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-6.1550

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

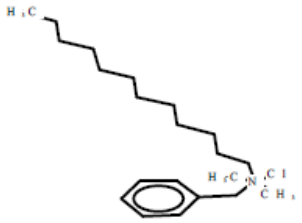
Alkyl(C12-C16)dimethylbenzylammonium chloride



```
SMILES : c1ccccc1CN(CL)(CCCCCCCCCCCCCC)(C)(C)
CHEM   :
MOL FOR: C23 H42 CL1 N1
MOL WT : 368.05
--------------------------- BIOWIN v4.10 Results ---------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks-Months
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)     :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.1084 |  0.1084
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  0.1281 |  0.1281
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1752
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.8088
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  1.8437 |  1.8437
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  1.7991 |  1.7991
 MolWt|  *  |  Molecular Weight Parameter             |         | -5.2263
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.8061
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2983 |  0.2983
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  0.0220 |  0.0220
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.8133
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  2.7062
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2691 |  0.2691
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  0.0049 |  0.0049
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.5310
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|         |  3.5907
============+=========================================+=========+=========
```

```
 Result Classification:   5.00 -> hours      4.00 -> days     3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months     1.00 -> longer

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic-CH2                           | -0.0557 | -0.0557
 Frag |  5  |  Aromatic-H                             |  0.0082 |  0.0411
 Frag |  3  |  Methyl  [-CH3]                         |  0.0004 |  0.0012
 Frag | 13  |  -CH2-  [linear]                        |  0.0494 |  0.6424
 Frag |  1  |  Quaternary amine                       | -0.0093 | -0.0093
 MolWt|  *  |  Molecular Weight Parameter             |         | -1.0950
 Const|  *  |  Equation Constant                      |         |  0.7121
============+=========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)|         |  0.2370
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Aromatic-CH2                           | -0.1246 | -0.1246
 Frag |  5  |  Aromatic-H                             |  0.1201 |  0.6007
 Frag |  3  |  Methyl  [-CH3]                         |  0.0194 |  0.0583
 Frag | 13  |  -CH2-  [linear]                        |  0.4295 |  5.5834
 Frag |  1  |  Quaternary amine                       |  0.2550 |  0.2550
 MolWt|  *  |  Molecular Weight Parameter             |         |-10.6252
============+=========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.1510
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    | -0.3177 | -0.3177
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  0.2182 |  0.2182
 Frag |  1  |  Aromatic-CH2                           | -0.0073 | -0.0073
 Frag |  5  |  Aromatic-H                             | -0.0954 | -0.4772
 Frag |  3  |  Methyl  [-CH3]                         | -0.0796 | -0.2387
 Frag | 13  |  -CH2-  [linear]                        |  0.0260 |  0.3379
 Frag |  1  |  Quaternary amine                       | -0.4377 | -0.4377
 Const|  *  |  Equation Constant                      |         |  0.8361
============+=========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)|         | -0.0865
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
 Criteria for the YES or NO prediction:  If the Biowin3 (ultimate survey
 model) result is "weeks" or faster (i.e. "days", "days to weeks", or
 "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
 the prediction is YES (readily biodegradable).  If this condition is not
 satisfied, the prediction is NO (not readily biodegradable).  This method
 is based on application of Bayesian analysis to ready biodegradation data
 (see Help).  Biowin5 and 6 also predict ready biodegradability, but for
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.
```

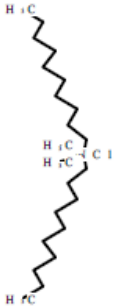
N-Benzyl-N,N-dimethyl-1-tridecanaminium chloride



```
SMILES : CN(CL)(Cclccccc1)(CCCCCCCCCCCC)C
CHEM   :
MOL FOR: C21 H38 CL1 N1
MOL WT : 340.00
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days-Weeks
   Biowin5 (MITI Linear Model Prediction)     :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.1084 |  0.1084
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  0.1281 |  0.1281
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1619
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.8222
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  1.8437 |  1.8437
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  1.7991 |  1.7991
 MolWt|  *  |  Molecular Weight Parameter             |         | -4.8280
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.8610
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2983 |  0.2983
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  0.0220 |  0.0220
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.7513
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|        |  2.7682
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2691 |  0.2691
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)     |  0.0049 |  0.0049
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.4905
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|        |  3.6312
============+=========================================+=========+=========
```

```
 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin5 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aromatic-CH2                             | -0.0557 | -0.0557
 Frag |  5  |  Aromatic-H                               |  0.0082 |  0.0411
 Frag |  3  |  Methyl  [-CH3]                           |  0.0004 |  0.0012
 Frag | 11  |  -CH2-  [linear]                          |  0.0494 |  0.5436
 Frag |  1  |  Quaternary amine                         | -0.0093 | -0.0093
 MolWt|  *  |  Molecular Weight Parameter               |         | -1.0115
 Const|  *  |  Equation Constant                        |         |  0.7121
============+===========================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability) |         |  0.2216
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aromatic-CH2                             | -0.1246 | -0.1246
 Frag |  5  |  Aromatic-H                               |  0.1201 |  0.6007
 Frag |  3  |  Methyl  [-CH3]                           |  0.0194 |  0.0583
 Frag | 11  |  -CH2-  [linear]                          |  0.4295 |  4.7244
 Frag |  1  |  Quaternary amine                         |  0.2550 |  0.2550
 MolWt|  *  |  Molecular Weight Parameter               |         | -9.8153
============+===========================================+=========+=========
   RESULT   |Biowin6 (MITI Non-Linear Biodeg Probability)|         |  0.1448
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable


------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Linear C4 terminal chain  [CCC-CH3]      | -0.3177 | -0.3177
 Frag |  1  |  Unsubstituted phenyl group (C6H5-)       |  0.2182 |  0.2182
 Frag |  1  |  Aromatic-CH2                             | -0.0073 | -0.0073
 Frag |  5  |  Aromatic-H                               | -0.0954 | -0.4772
 Frag |  3  |  Methyl  [-CH3]                           | -0.0796 | -0.2387
 Frag | 11  |  -CH2-  [linear]                          |  0.0260 |  0.2859
 Frag |  1  |  Quaternary amine                         | -0.4377 | -0.4377
 Const|  *  |  Equation Constant                        |         |  0.8361
============+===========================================+=========+=========
   RESULT   |   Biowin7 (Anaerobic Linear Biodeg Prob)  |         | -0.1385
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)
----------------------------------------------
 Criteria for the YES or NO prediction:  If the Biowin3 (ultimate survey
 model) result is "weeks" or faster (i.e. "days", "days to weeks", or
 "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then
 the prediction is YES (readily biodegradable).  If this condition is not
 satisfied, the prediction is NO (not readily biodegradable).  This method
 is based on application of Bayesian analysis to ready biodegradation data
 (see Help).  Biowin5 and 6 also predict ready biodegradability, but for
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.
```

N-Decyl-N,N-dimethyl-1-decanaminium chloride



```
SMILES : N(CL)(C)(C)(CCCCCCCCCC)CCCCCCCCCC
CHEM   :
MOL FOR: C22 H48 CL1 N1
MOL WT : 362.09
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days
   Biowin5 (MITI Linear Model Prediction)     :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  YES

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Linear C4 terminal chain  [CCC-CH3]    |  0.1084 |  0.2169
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.1724
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         |  0.7920
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Linear C4 terminal chain  [CCC-CH3]    |  1.8437 |  3.6874
 MolWt|  *  |  Molecular Weight Parameter             |         | -5.1416
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.8256
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2983 |  0.5967
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.8002
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|        |  2.9957
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  2  |  Linear C4 terminal chain  [CCC-CH3]    |  0.2691 |  0.5381
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.5224
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|        |  3.8635
============+=========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	4	Methyl [-CH3]	0.0004	0.0016
Frag	18	-CH2- [linear]	0.0494	0.8895
Frag	1	Quaternary amine	-0.0093	-0.0093
MolWt	*	Molecular Weight Parameter		-1.0772
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.5168

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	4	Methyl [-CH3]	0.0194	0.0777
Frag	18	-CH2- [linear]	0.4295	7.7309
Frag	1	Quaternary amine	0.2550	0.2550
MolWt	*	Molecular Weight Parameter		-10.4530
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.5340

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

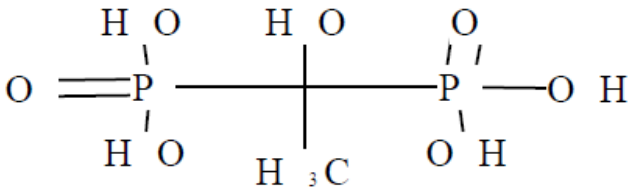
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	-0.3177	-0.6355
Frag	4	Methyl [-CH3]	-0.0796	-0.3183
Frag	18	-CH2- [linear]	0.0260	0.4678
Frag	1	Quaternary amine	-0.4377	-0.4377
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.0875

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

HEDP



SMILES : O=P(O)(O)C(O)(P(=O)(O)O)C
CHEM :
MOL FOR: C2 H8 O7 P2
MOL WT : 206.03

---------- BIOWIN v4.10 Results ----------

Biowin1 (Linear Model Prediction) : Does Not Biodegrade Fast
Biowin2 (Non-Linear Model Prediction): Does Not Biodegrade Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months
Biowin4 (Primary Biodegradation Timeframe): Days-Weeks
Biowin5 (MITI Linear Model Prediction) : Not Readily Degradable
Biowin6 (MITI Non-Linear Model Prediction): Not Readily Degradable
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
Ready Biodegradability Prediction: NO

TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1839	-0.1839
MolWt	*	Molecular Weight Parameter		-0.0981
Const	*	Equation Constant		0.7475
RESULT		Biowin1 (Linear Biodeg Probability)		0.4655

TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-1.7232	-1.7232
MolWt	*	Molecular Weight Parameter		-2.9256
RESULT		Biowin2 (Non-Linear Biodeg Probability)		0.1624

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2121	-0.2121
MolWt	*	Molecular Weight Parameter		-0.4553
Const	*	Equation Constant		3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)		2.5318

TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.1534	-0.1534
MolWt	*	Molecular Weight Parameter		-0.2973
Const	*	Equation Constant		3.8477
RESULT		Biowin4 (Survey Model - Primary Biodeg)		3.3970

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	0.0676	0.0676
Frag	1	Methyl [-CH3]	0.0004	0.0004
MolWt	*	Molecular Weight Parameter		-0.6129
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.1672

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	0.3990	0.3990
Frag	1	Methyl [-CH3]	0.0194	0.0194
MolWt	*	Molecular Weight Parameter		-5.9478
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0473

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

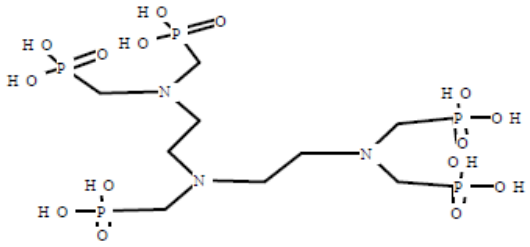
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.3342	-0.3342
Frag	1	Methyl [-CH3]	-0.0796	-0.0796
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.4223

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

DTPMP



```
SMILES : OP(O)(=O)CN(CCN(CP(O)(O)=O)CP(O)(O)=O)CCN(CP(O)(O)=O)CP(O)(O)=O
CHEM   : cas 15827-60-8
MOL FOR: C9 H28 N3 O15 P5
MOL WT : 573.20
--------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)    :  Does Not Biodegrade Fast
   Biowin2 (Non-Linear Model Prediction):  Does Not Biodegrade Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Recalcitrant
   Biowin4 (Primary  Biodegradation Timeframe):  Months
   Biowin5 (MITI Linear Model Prediction)    :  Not Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Not Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Does Not Biodegrade Fast
   Ready Biodegradability Prediction:  NO

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Tertiary amine                         | -0.2053 | -0.6158
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.2729
 Const|  *  |  Equation Constant                      |         |  0.7475
============+=========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)  |         | -0.1411
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Tertiary amine                         | -2.2229 | -6.6687
 MolWt|  *  |  Molecular Weight Parameter             |         | -8.1395
============+=========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)|         |  0.0000
============+=========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Tertiary amine                         | -0.2548 | -0.7644
 MolWt|  *  |  Molecular Weight Parameter             |         | -1.2667
 Const|  *  |  Equation Constant                      |         |  3.1992
============+=========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg)|         |  1.1681
============+=========================================+=========+=========

------+-----+-----------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+-----------------------------------------+---------+---------
 Frag |  3  |  Tertiary amine                         | -0.2880 | -0.8640
 MolWt|  *  |  Molecular Weight Parameter             |         | -0.8270
 Const|  *  |  Equation Constant                      |         |  3.8477
============+=========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg)|         |  2.1567
============+=========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Tertiary amine	-0.0848	-0.2545
Frag	9	-CH2- [linear]	0.0494	0.4447
MolWt	*	Molecular Weight Parameter		-1.7053
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		-0.8029

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Tertiary amine	-0.8396	-2.5189
Frag	9	-CH2- [linear]	0.4295	3.8654
MolWt	*	Molecular Weight Parameter		-16.5477
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.0000

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

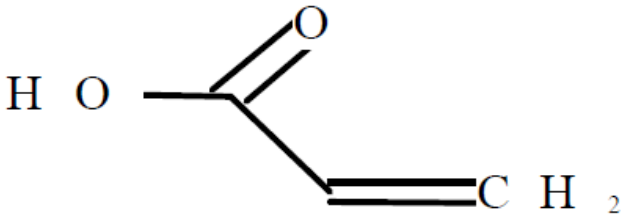
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	Tertiary amine	-1.0749	-3.2246
Frag	9	-CH2- [linear]	0.0260	0.2339
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-2.1546

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Acrylate




```
SMILES : OC(=O)C=C
CHEM   :
MOL FOR: C3 H4 O2
MOL WT : 72.06
-------------------------- BIOWIN v4.10 Results ----------------------------

   Biowin1 (Linear Model Prediction)     :  Biodegrades Fast
   Biowin2 (Non-Linear Model Prediction):  Biodegrades Fast
   Biowin3 (Ultimate Biodegradation Timeframe):  Days-Weeks
   Biowin4 (Primary  Biodegradation Timeframe):  Days
   Biowin5 (MITI Linear Model Prediction)     :  Readily Degradable
   Biowin6 (MITI Non-Linear Model Prediction):  Readily Degradable
   Biowin7 (Anaerobic Model Prediction):  Biodegrades Fast
   Ready Biodegradability Prediction:  YES

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin1 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.0727 |  0.0727
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.0343
 Const|  *  |  Equation Constant                        |         |  0.7475
============+===========================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)    |         |  0.7859
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.6431 |  0.6431
 MolWt|  *  |  Molecular Weight Parameter               |         | -1.0233
============+===========================================+=========+=========
   RESULT   |  Biowin2 (Non-Linear Biodeg Probability)  |         |  0.9327
============+===========================================+=========+=========

 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin3 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.3646 |  0.3646
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.1593
 Const|  *  |  Equation Constant                        |         |  3.1992
============+===========================================+=========+=========
   RESULT   |  Biowin3 (Survey Model - Ultimate Biodeg) |         |  3.4045
============+===========================================+=========+=========

------+-----+-------------------------------------------+---------+---------
 TYPE | NUM |       Biowin4 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+-------------------------------------------+---------+---------
 Frag |  1  |  Aliphatic acid   [-C(=O)-OH]             |  0.3856 |  0.3856
 MolWt|  *  |  Molecular Weight Parameter               |         | -0.1040
 Const|  *  |  Equation Constant                        |         |  3.8477
============+===========================================+=========+=========
   RESULT   |   Biowin4 (Survey Model - Primary Biodeg) |         |  4.1293
============+===========================================+=========+=========

 Result Classification:   5.00 -> hours     4.00 -> days     3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months    1.00 -> longer
```

TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	0.1812	0.1812
Frag	3	-C=CH [alkenyl hydrogen]	0.0062	0.0186
MolWt	*	Molecular Weight Parameter		-0.2144
Const	*	Equation Constant		0.7121
RESULT		Biowin5 (MITI Linear Biodeg Probability)		0.6975

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	1.1346	1.1346
Frag	3	-C=CH [alkenyl hydrogen]	0.0285	0.0855
MolWt	*	Molecular Weight Parameter		-2.0804
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.8410

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Aliphatic acid [-C(=O)-OH]	0.1868	0.1868
Frag	3	-C=CH [alkenyl hydrogen]	-0.0735	-0.2206
Const	*	Equation Constant		0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		0.8023

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

3. EAWAG-BBD Pathway Prediction System

EAWAG-PPS Usage Tips

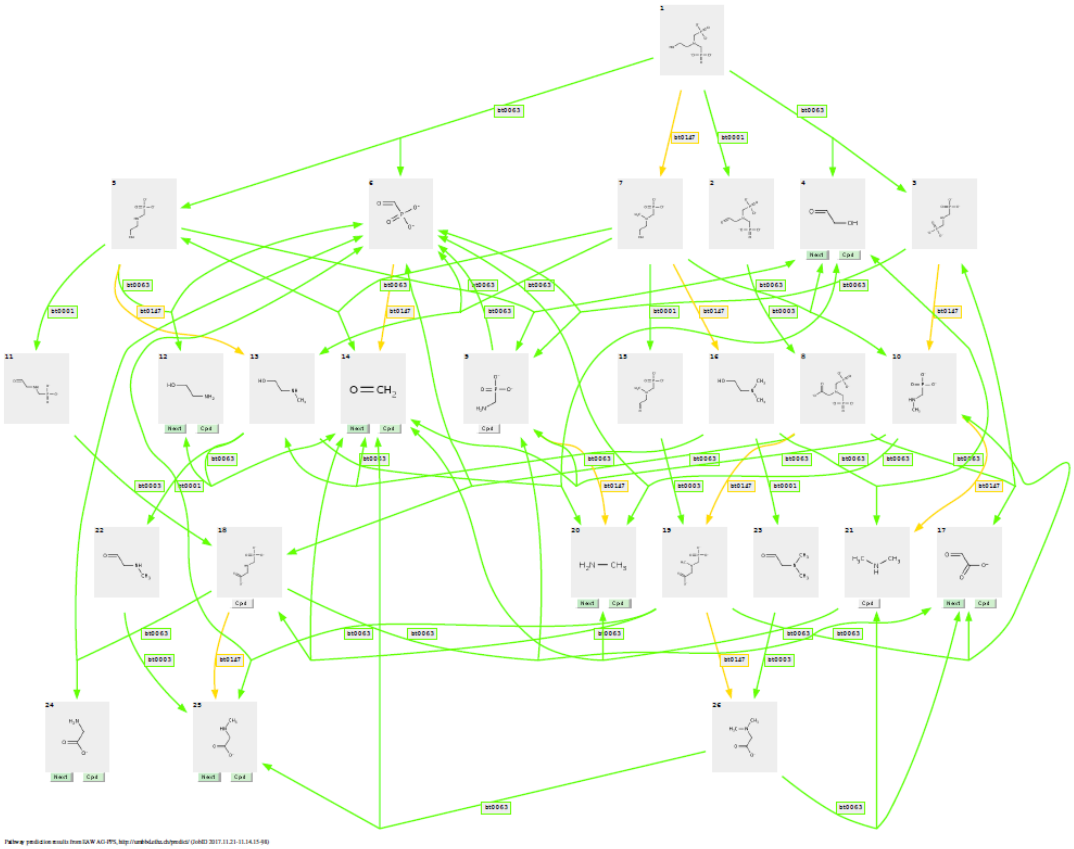
No.	ICON	Description
1	Cpd	Show UM-BBD compound page.
2	Cpd	Show a compound and its KEGG metabolism.
3	Next	Continue prediction using this branch.
4	Next	Next choice is aerobically unlikely.
5	Next	Prune unused branches and display.
6	bt0003	Show a rule page.
7	bt0005*	Show a super rule that covers multiple simple rules.
8		Aerobically very likely transformation.
9		Aerobically likely transformation.
10		Aerobically neutral transformation.
11		Aerobically unlikely transformation.
12		Aerobically very unlikely transformation.
13		CoA is not shown when present.
14		Readily degraded compounds should not be predicted.
15		Inorganic compounds should not be predicted.
16		High molecular weight compounds should not be predicted.
17		Mixtures should not be predicted.
18		Highly fluorinated compounds should not be predicted.
19		Does not predict the rate of transformations.
20		Does not predict phytochemical transformations.
21		Does not predict detoxification reactions.
22		Does not predict dimerizations.
23		Does not predict methylation of hydroxyl groups.
24		Does not predict acetylation of primary amines.
25		Does not predict formation of intramolecular rings.

For assessing the predicted degradation pathway, the following color scheme is used:

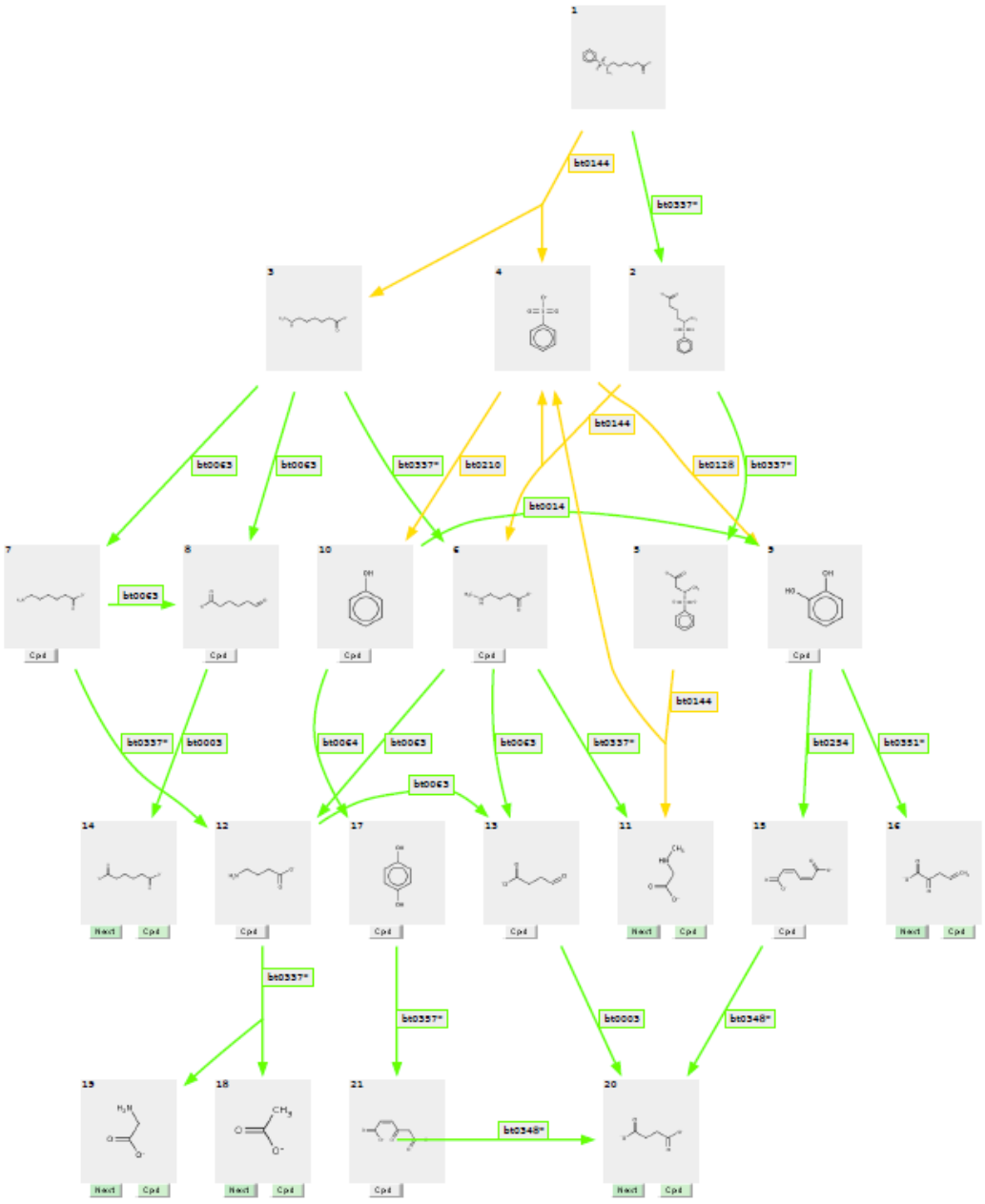
Aerobic Likelihood:

Very likely Likely Neutral

Alkyl amino phosphonic acid salt

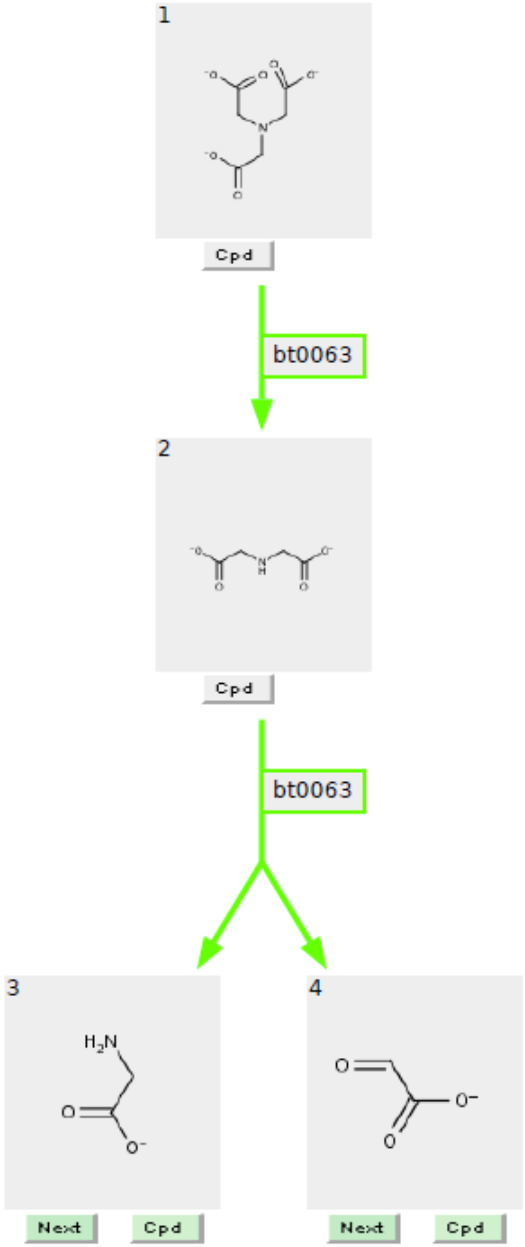


N-methylbenzenesulphonamido caproic acid



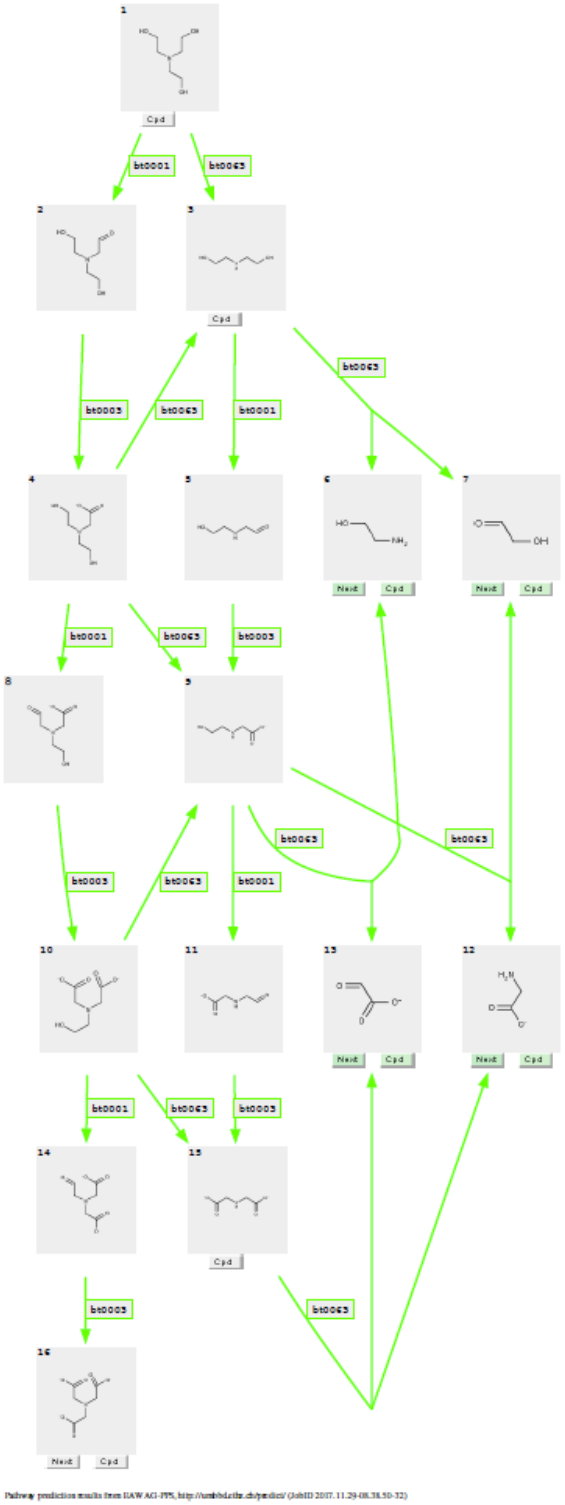
Pathway prediction results from EAWAG-PPS, http://umbbd.ethz.ch/predict/ (JobID 2017.11.21-11.29.22-68)

Nitriloacetic acid

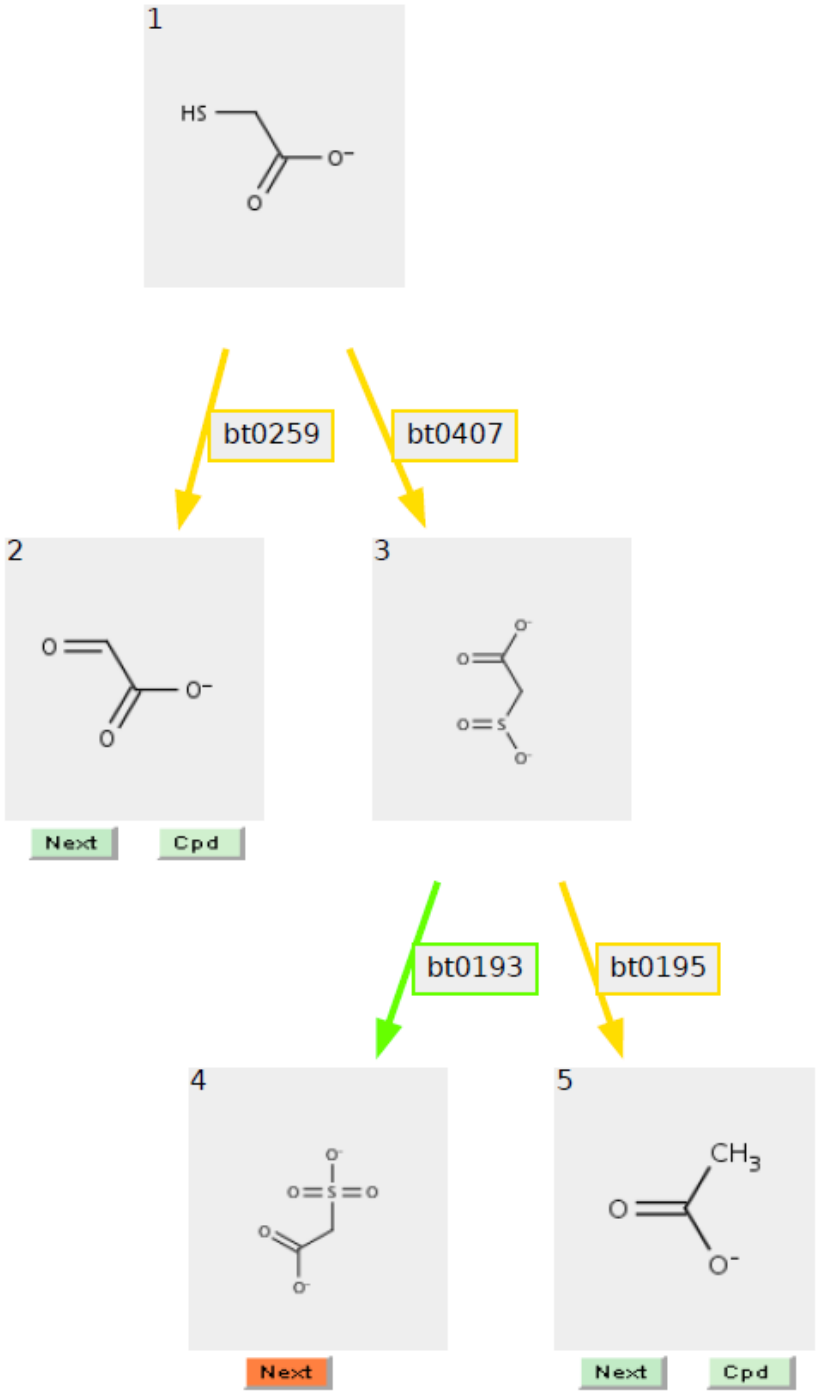


Pathway prediction results from EAWAG-PPS, http://umbbd.ethz.ch/predict/ (JobID 2017.11.21-12.14.47-15)

Triethanolamine

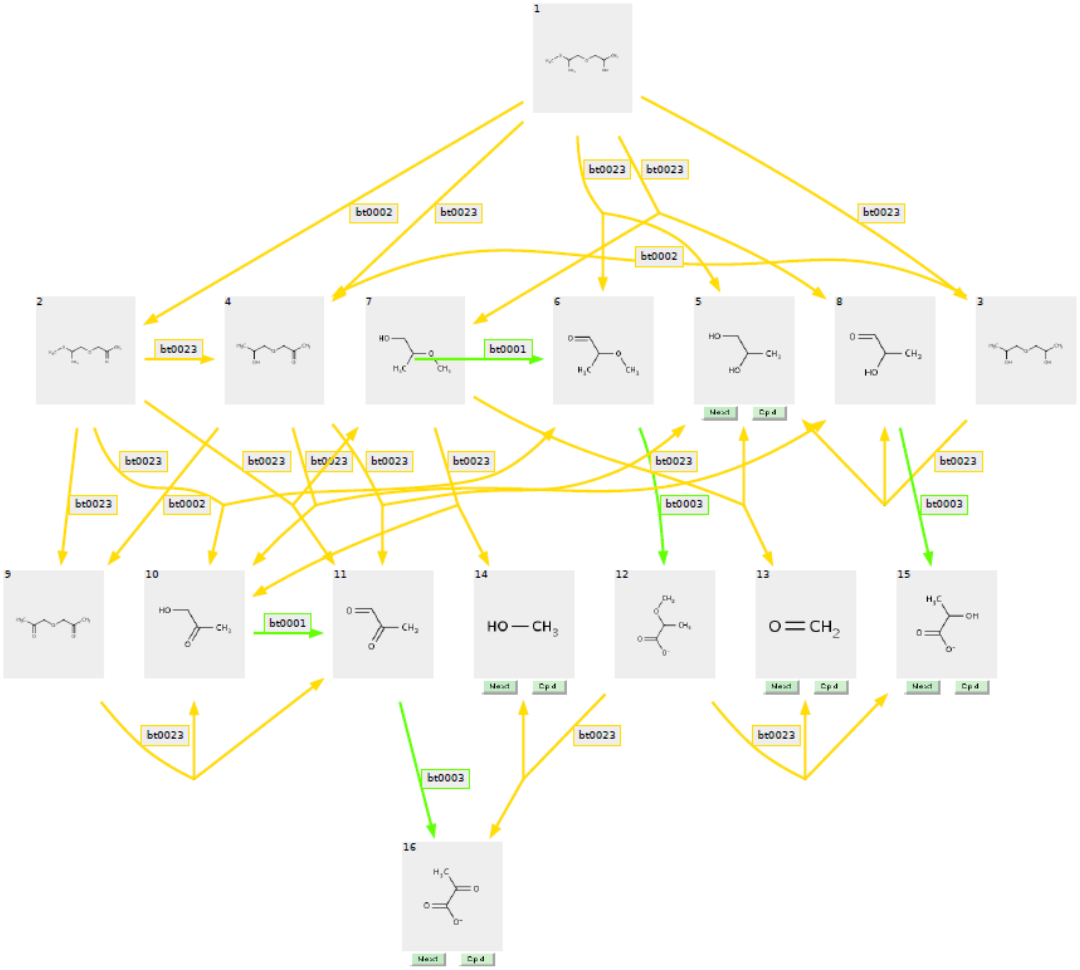


Thioglycolic acid



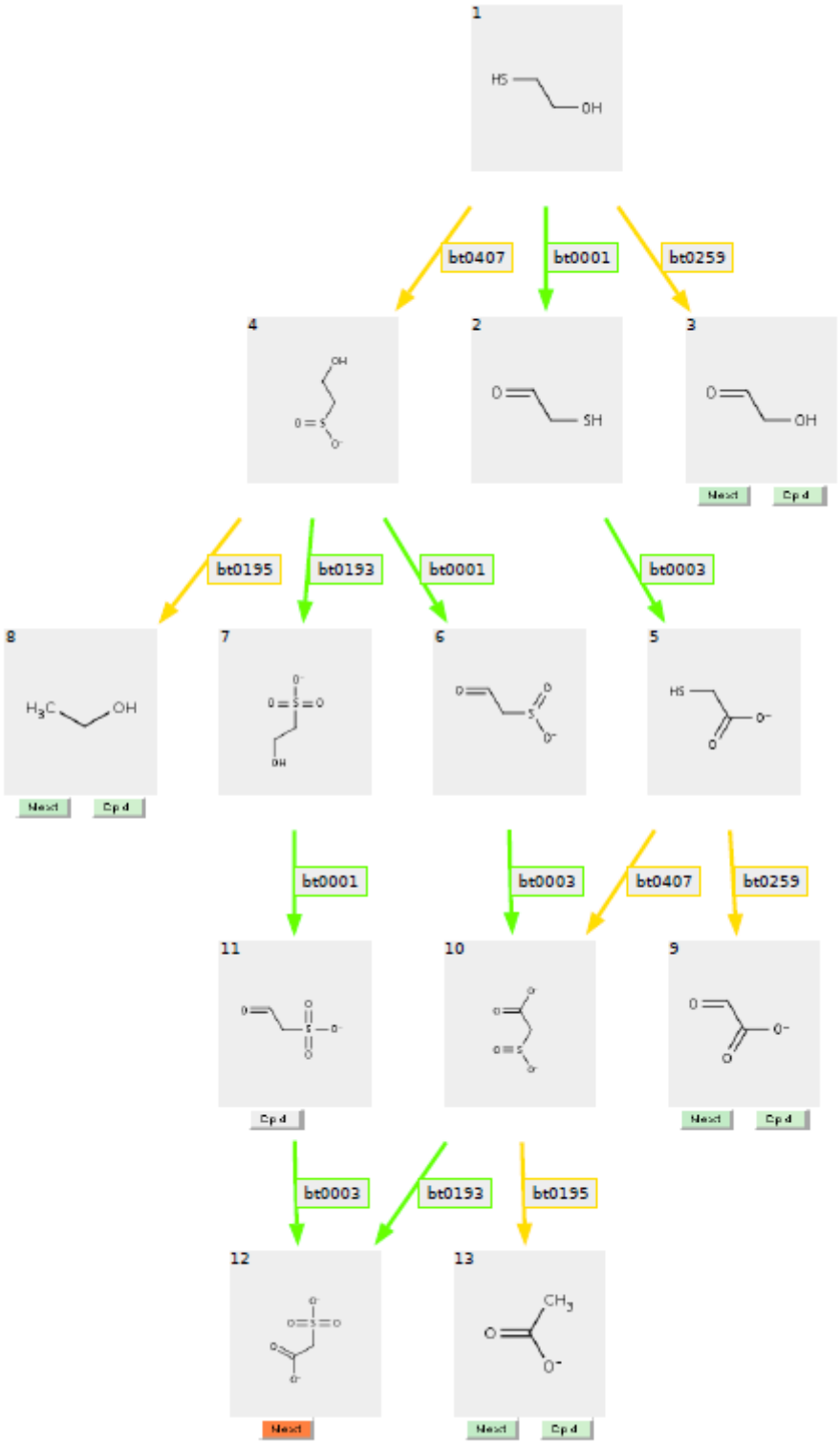
Pathway prediction results from EAWAG-PPS, http://umbbd.ethz.ch/predict/ (JobID 2017.11.29-08.48.43-75)

Dipropylene glycol methyl ether



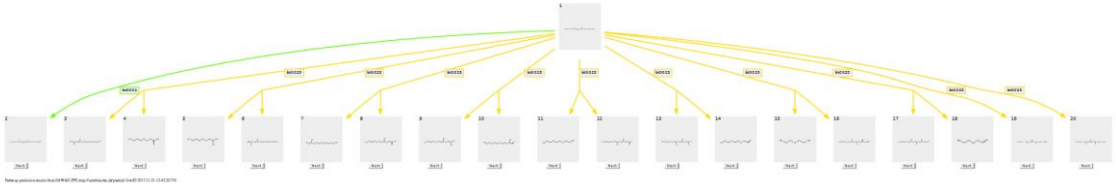
Pathway prediction results from EAWAG-PPS, http://umbbd.ethz.ch/predict/ (JobID 2017.11.21-12.31.09-72)

Mercaptoethanol

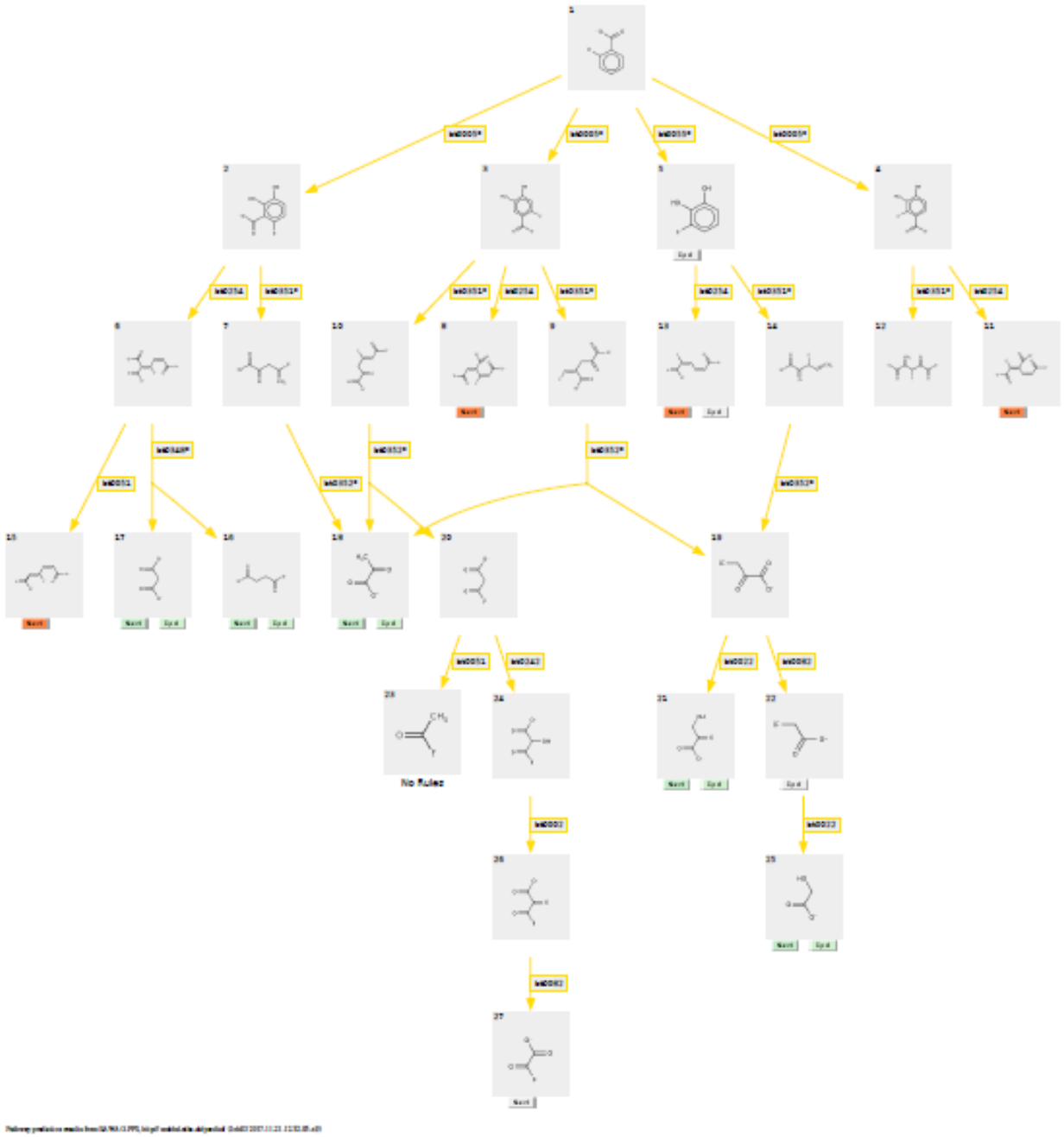


Pathway prediction results from EAWAG-PPS, http://umbbd.ethz.ch/predict/ (JobID 2017.11.21-12.48.08-52)

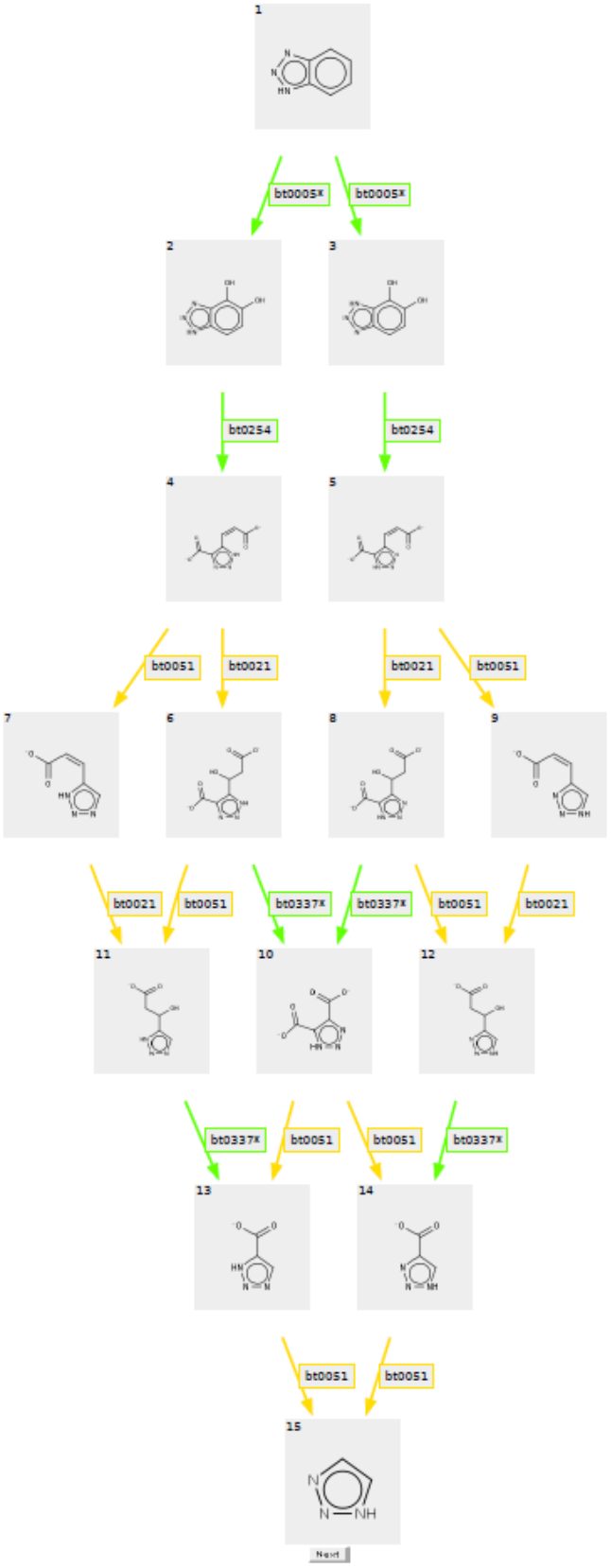
Polyoxyalkylene glycol



2-Fluorobenzoic acid

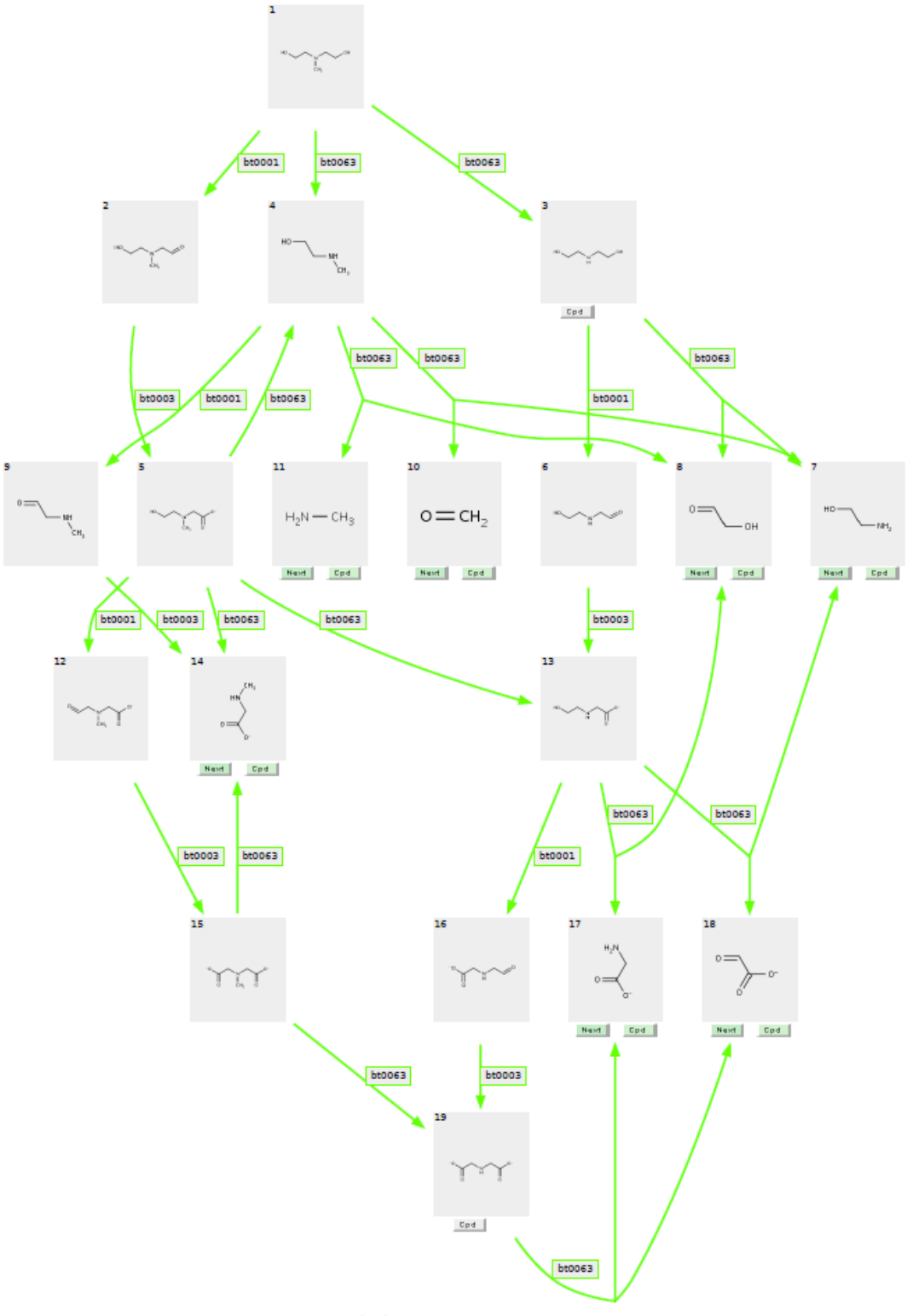


Benzotriazole



Pathway prediction results from EAWAG-PPS, http://umbbd.ethz.ch/predict/ (JobID 2017.11.29-09.18.20-28)

N-methyldiethanolamine



Pathway prediction results from EAWAG-PPS, http://umbbd.ethz.ch/predict/ (JobID 2017.11.21-12.58.12-56)

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The Norwegian Environment Agency is working for a clean and diverse environment. Our primary tasks are to reduce greenhouse gas emissions, manage Norwegian nature, and prevent pollution.

We are a government agency under the Ministry of Climate and Environment and have 700 employees at our two offices in Trondheim and Oslo and at the Norwegian Nature Inspectorate's more than sixty local offices.

We implement and give advice on the development of climate and environmental policy. We are professionally independent. This means that we act independently in the individual CASes that we decide and when we communicate knowledge and information or give advice.

Our principal functions include collating and communicating environmental information, exercising regulatory authority, supervising and guiding regional and local government level, giving professional and technical advice, and participating in international environmental activities.