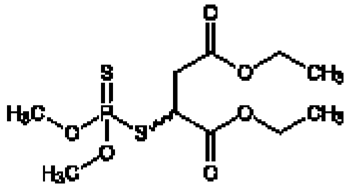
**Miljøministeriet**
Miljøstyrelsen

# Fastsættelse af kvalitetskriterier for vandmiljøet

# malathion

## CAS nr. 121-75-5



| | | |
|---|---|---|
| Vandkvalitetskriterium | $VKK_{ferskvand}$ | 0,003 µg/l |
| Vandkvalitetskriterium | $VKK_{saltvand}$ | 0,0006µg/l |
| Korttidsvandkvalitetskriterium | $KVKK_{ferskvand}$ | 0,4 µg/l |
| Korttidsvandkvalitetskriterium | $KVKK_{saltvand}$ | 0,4 µg/l |
| Sedimentkvalitetskriterium | $SKK_{ferskvan}$ | 0,04 µg/kg tørvægt (5% OC) |
| Sedimentkvalitetskriterium | $SKK_{ferskvan}$ | 0,8 µg/kg tørvægt x $f_{oc}$ |
| Sedimentkvalitetskriterium | $SKK_{saltvand}$ | 0,007 µg/kg tørvægt (5% OC) |
| Sedimentkvalitetskriterium | $SKK_{saltvand}$ | 0,14 µg/kg tørvægt x $f_{oc}$ |
| Biota-kvalitetskriterium, sekundær forgiftning | $BKK_{sek.forgiftn.}$ | 0,27 mg/kg musling (bløddele), vådvægt |
| Biota-kvalitetskriterium, human konsum | HKK | 3,7 mg/kg fiskeriprodukter, vådvægt |

**Januar 2023**

*Databladet er i april 2024 opdateret i forhold til at tydeliggøre ved hvilket organisk kulstof (OC) indhold sedimentkvalitetskriterierne er bestemt ved.*

# Indholdsfortegnelse

# Forord

Et kvalitetskriterium i vandmiljøet er det højeste koncentrationsniveau, ved hvilket der skønnes, ikke at forekomme uacceptable negative effekter på vandøkosystemer.

Miljøstyrelsen (MST) udarbejder kvalitetskriterier for kemikalier i vandsøjlen, i sediment, i dyr og planter (biota) og for human konsum.

Miljøstyrelsen bruger kvalitetskriterierne som det faglige grundlag til at kunne fastsætte miljøkvalitetskrav, hvorved der forstås den endelige koncentration af et bestemt forurenende stof i vand, sediment eller biota, som ikke må overskrides af hensyn til beskyttelsen af miljøet og menneskers sundhed.

Metodikken, der anvendes til udarbejdelse af miljøkvalitetskrav er harmoniseret i EU og baserer sig på vandrammedirektivet (EU, 2000), EU's vejledning til fastsættelse af kvalitetskriterier i vandmiljøet (EU, 2018a) og Miljøstyrelsens vejledning til fastsættelse af vandkvalitetskriterier (Miljøstyrelsen, 2004). Metodikken er endvidere i overensstemmelse med EU's vejledning til risikovurdering under REACH forordningen (EU, 2008).

Den sidste litteratursøgning er foretaget oktober 2022.

# English Summary and Conclusions

Derivation of environmental quality standards (EQS) for the aquatic environment is following the EU Guidance Document No. 27. Technical Guidance Document (TGD) for Deriving Environmental Quality Standards (EU, 2018).

Primary reference sources were FMC 2019, and US EPA's database ECOTOX. Data from FMC 2019 were not further checked for reliability as that dataset already has been through such a process.

Especially concerning sediment toxicity, searches have also been made in the following databases: Agris, Biological Abstracts, GeoScience World, PubMed and Google Scholar.

Statistically, differences between sensitivities of freshwater and marine organisms were insignificant, in the case of chronic as well as acute aquatic toxicity. The marine and freshwater datasets may thus be pooled.

**AA-EQS for water**
For **chronic studies**, all other references were, as far as possible, procured and the reliability assessed (CRED), and only studies with reliability indexes 1 or 2 were accepted.

In ECOTOX the chronic studies were first sorted according to duration of study (should be "long term"). Further, studies where concentrations were not measured were not taken on board unless flow through or renewal was employed. If a formulation or a low purity of the substance was employed, then the study was also not accepted unless concentrations had been measured.
Only types of effects that can be related to effects on populations were accepted.

The combined chronic dataset includes 23 species representing 9 major taxonomic groups, and a species sensitivity distribution analysis (SSD) can be performed.

The resulting chronic $HC_{5\ \text{freshwater + saltwater}}$ = 0.0141 µg/l (90% CI: 0.00063-0.126).
Lognormality is accepted at all significance levels listed in ETx. The standard deviation (s) of $\log_{10}$ transformed data is 2.04.

The standard deviation is high. Further, the lowest $EC_{10}$ or NOEC is much lower than the $HC_5$ (0.0008 µg/l), and a number of species that are most sensitive in the acute dataset are not represented in the chronic dataset. Therefore, the assessment factor (AF) is not reduced from the default of 5.

Only one species that, according to EU 2018a, can be regarded as representing a specific marine group is included in the chronic dataset. Therefore, an extra AF of 5 is applied for estimation of the marine QS.
**$\text{AA-EQS}_{\text{freshwater}}$ = 0.014 µg/l / 5 = 0.0028 µg/l ≈ 0.003 µg/l**
**$\text{AA-EQS}_{\text{saltwater}}$ = 0.0028 µg/l / 5 = 0.00056 µg/l ≈ 0.0006 µg/l**

## MAC-EQS for water

For **acute studies** the dataset in ECOTOX is huge (1795). The sorting criteria were the same as for chronic studies except that up to two days test without measurements of the substance were accepted because we are dealing with acute (short-term) effects, and the half-life of malathion probably is around 2 days. This means that for many species where the standard is a 4-day test, 2-day tests have been accepted, giving a bias towards greater values. On the other hand, where multiple values occurred for the same species, in ECOTOX, the lowest value was chosen. When multiple values were available from other sources the geometric mean was used – given the studies were performed under the same general conditions and with the same endpoints.

After the first sorting the acute database was reduced to 311 values. Following this, the studies of the lowest and largest values were retrieved and subject to CRED assessment, in all 47 studies covering 58 values.

The combined acute dataset encompasses 272 species representing 16 major taxonomic groups, including groups that are expected to contain some of the most sensitive species i.e., insects and crustaceans. An SSD analysis is thus relevant.

The acute $HC_5$ = 0.88 µg/l, with s = 1.47.

However, the distribution of data is clearly two-peaked, and therefore an SSD based only on data from the lower group was performed. The resulting $HC_5$ was 1.2 µg/l, and the dataset included data for 159 species and 7 major taxonomic groups. Crustacea and insects were richly represented with a variety of classes and orders, respectively.

Given the large number of species and major taxonomic groups, including the most sensitive the default AF of 10 is reduced to 3.

There are multiple specific marine species in the dataset, so the $MAC_{freshwater} = MAC_{saltwater}$.

**$MAC\text{-}EQS_{freshwater}$ = 1.2 µg/l / 3 = 0.4 µg/l**
**$MAC\text{-}EQS_{saltwater}$ = 1.2 µg/l / 3 = 0.4 µg/l**

## QS for sediment

No reliable tests with organisms in sediment were found and the EqP method was employed.

An EU standard sediment with 5% organic carbon (OC) and a $K_{OC}$ value of 216 l/kg (geometric mean) is used. The partition coefficient between solid and water in sediment, $Kp_{sed}$ is determined based on the following equation:

$Kp_{sed} = F_{OCsed} \times K_{OC} = 0.05 \times 216$ l/kg = 10.8 l/kg

The partition coefficient between sediment and water $K_{sed\text{-}water}$ can be determined based on the equation below and by using the default values from EU 2018a:

$K_{sed\text{-}water} = Fair_{sed} \times K_{air\text{-}water} + Fwater_{sed} + Fsolid_{sed} \times (Kp_{sed} / 1000) \times RHO_{solid} =$
$K_{sed\text{-}water} = 0 + 0.8 + 0.2 \times (10.8 / 1000) \times 2500 = 6.2\ m^3m^{-3}$

The QS for sediment can be determined based on the following equations, and by applying AA-$EQS_{freshwater}$ of 0.003 µg/l and AA-$EQS_{saltwater}$ of 0.0006 µg/l:

$QS_{sediment,\ freshwater} = (K_{sed\text{-}water} / RHOsed) \times QS_{water} \times 1000 = (6.2 / 1300) \times 0.003 \times 1000 = 0.014\ \mu g/kg_{wet\ weight}$

$QS_{sediment,\ saltwater} = (K_{sed\text{-}water} / RHOsed) \times QS_{water} \times 1000 = (6.2 / 1300) \times 0.0006 \times 1000 = 0.0027\ \mu g/kg_{wet\ weight}$

The $QS_{sediment}$ in wet weight can be converted to dry weight by applying the conversion factor of 2.6 (EU 2018a):

$QS_{sediment,\ freshwater} = 0.014\ \mu g/kg_{wet\ weight} \times 2.6 = 0.04\ \mu g/kg_{dry\ weight}$

$QS_{sediment,\ saltwater} = 0.0027\ \mu g/kg_{wet\ weight} \times 2.6 = 0.007\ \mu g/kg_{dry\ weight}$

**$QS_{sediment,\ freshwater}$ = 0.04 µg/kg dry weight (5% OC)**
**= 0.8 µg/kg dry weight x $f_{oc}$**
**$QS_{sediment,\ saltwater}$ = 0.007 µg/kg dry weight (5% OC)**
**= 0.14 µg/kg dry weight x $f_{oc}$**

## QS for secondary poisoning

Data on birds and mammal were taken primarily from FMC 2019 and ECOTOX. As malathion is most likely bio-diluted the $QS_{biota\text{-}secondary\ poisoning}$ was calculated for bivalves. All NOEC values for birds and mammal described in Bilag A are energy normalized by appling method B from EU 2018a, assuming that the animals food items contain an energy concent of 15.1 kJ/$g_{dry\ weight}$ and a moisture fraction of 8% (table 8 in EU 2018a). Afterwards, all NOEC values were energy normalized to concentrations in mussels, assuming that mussels contain an energy content of 19 kJ/$g_{dry\ weight}$ and a moisture fraction of 92% (table 7 in EU 2018a) (se Bilag B).

The lowest NOEC presented in Bilag B is 2.7 mg/kg mussels (wet weight) and an AF of 10 is applied.

**$QS_{sec.\ pois.}$ = 2.7 mg/kg mussels / 10 = 0.27 mg/kg mussels wet weight**

## QS for human health

The $QS_{biota\text{-}human\ health}$ was based on an ADI of 0.03 mg/kg bw per day and determined from the following equation:

$QS_{human\ health} = 0.2 \times ADI / 0.00163 = 0.2 \times 30 / 0.00163 = 3681$ µg/kg fishery products ≈

**$QS_{human\ health}$ = 3.7 mg/kg wet weight Fish, Fishery products**

**$QS_{water}$ based on $QS_{sec. pois.}$ and $QS_{human\ health}$**

The corresponding concentration in water was calculated based on the lowest value for $QS_{water, sec.pois.}$ = 0.27 mg/kg and a BCF of 100 l/kg:

**$QS_{water, biota}$ = 0.27 mg/kg / 100 l/kg = 0.0027 mg/l ≈ 2.7 µg/l**

The QS is above the AA-EQS for both fresh- and saltwater, and the derived AA-EQS is considered to protect against secondary poisoning and human health.

In conclusion, the following EQS for the aquatic environment have been derived for malathion:

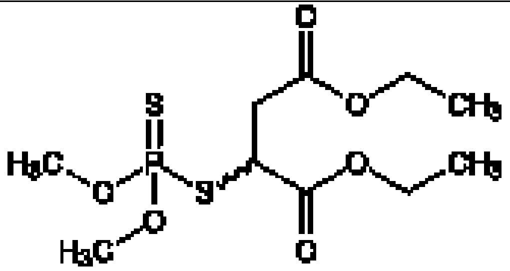
**$AA\text{-}EQS_{freshwater}$ = 0.003 µg/l**
**$AA\text{-}EQS_{saltwater}$ = 0.0006 µg/l**
**$MAC\text{-}EQS_{freshwater}$ = 0.4 µg/l**
**$MAC\text{-}EQS_{saltwater}$ = 0.4 µg/l**
**$QS_{sediment, freshwater}$ = 0.04 µg/kg dry weight (5% OC)**
**= 0.8 µg/kg dry weight x $f_{oc}$**
**$QS_{sediment, saltwater}$ = 0.007 µg/kg dry weight (5% OC)**
**= 0.14 µg/kg dry weight x $f_{oc}$**
**$QS_{sec. pois.}$ = 0.27 mg/kg mussels wet weight**
**$QS_{human\ health}$ = 3.7 mg/kg wet weight Fish, Fishery products**
**$QS_{water, biota}$ = 2.7 µg/l**

# 1 Indledning

Identiteten af malathion fremgår af tabel 1.1.

Malathion er et acetylcholinesterasehæmmende insekti- og acaricid. Stoffet er godkendt til visse brug i EU.

Tabel 1.1. Identitet af malathion

| | |
|---|---|
| IUPAC navn | diethyl 2-dimethoxyphosphinothioylsulfanylbutanedioate |
| Strukturformel |  |
| CAS nr. | 121-75-5 |
| EINECS nr. | 204-497-7 |
| Kemisk formel | $C_{10}H_{19}O_6PS_2$ |
| SMILES | CCOC(=O)CC(C(=O)OCC)SP(=S)(OC)OC |
| Harmoniseret klassificering | Acute Tox. 4; H302 (Farlig ved indtagelse)<br>Skin Sens. 1; H317 (Kan forårsage allergisk hudreaktion)<br>Aquatic Acute 1; H400 (Meget giftigt for vandlevende organismer)<br>Aquatic Chronic 1; H410 (Meget giftigt med langvarige virkninger for vandlevende organismer) |
| Selvklassificering | |

# 2 Fysisk kemiske egenskaber

De fysisk kemiske egenskaber for malathion fremgår af tabel 2.1.

Tabel 2.1. Fysisk kemiske egenskaber for malathion

| **Parameter** | **Værdi** | **Reference** |
|---|---|---|
| Molekylevægt, $M_w$ ($g{\cdot}mol^{-1}$) | 330,4 | EFSA 2009 |
| Smeltepunkt, $T_m$ (ºC) | < -20 | EFSA 2009 |
| Kogepunkt, $T_b$ (ºC) | Desintegrerer ved 174 grader | EFSA 2009 |
| Damptryk, $P_v$ (Pa) | $4{,}5*10^{-4}$ | EFSA 2009 |
| Henry's konstant, H (Pa $m^3$ $mol^{-1}$)[a] | $1*10^{-3}$ | EFSA 2009 |
| Vandopløselighed, $S_w$ ($g{\cdot}L^{-1}$) | 0,148[a]<br>0,143-0,145[b] | EFSA 2009, FMC 2019: 1994; 076 FYF<br>PubChem |
| Dissociationskonstant, $pK_a$ | Dissocierer ej | EFSA 2009 |
| Octanol/vand fordelingskoefficient, log $K_{ow}$ | 2,75<br>2,36-2,86 | EFSA 2009, FMC 2019<br>PubChem |
| Sediment/vand fordelingskoefficient, normaliseret til organisk karbon, $K_{oc}$ ($L{\cdot}kg^{-1}$). $K_{oc}$ for jord er brugt | 151-308 | EFSA 2009 |

[a] Ved 25˚C

[b] Ved 20˚C

# 3 Skæbne i miljøet

## 3.1 Nedbrydelighed

Omdannelse af moderstoffet i jord (primær nedbrydelighed) har en halveringstid på $DT_{50}$ mellem 0,08 dag og 1,87 dag (FMC (2019), Document M-CA Section 7).

Ifølge Dortland (1980) var halveringstiden i vand omkring 2 dage, hvilket er i overensstemmelse med forsøg indleveret til pesticidgodkendelsen (Dobson & Petts (2019) i FMC, 2019), der fandt en halveringstid på 2,24 dage.

De vigtigste omdannelsesprodukter af malathion i vand er malathion mono-carboxylsyre (MMCA) og malathion di-carboxylsyre (MDCA). Deres giftighed overfor *Lepomis macrochirus* og *Daphnia magna* er flere tusinde gange mindre end malathions, så de bidrager efter alt at dømme kun meget lidt til den samlede giftighed, selvom de er i vandet længere end malathion. (FMC 2019: Document MCA, section 7 og 8).

I studier med både vand og sediment ser halveringstiden for malathion i vandet ud til at være mindre end et døgn, mens MMCA har en halveringstid på 1,4 – 2,9 døgn og MDCA har en halveringstid på 5,5 døgn (Knoch 2001 og Cooke 2019).

## 3.2 Bioakkumulering

Som det fremgår af tabel 2.1, varierer de angivne log $K_{ow}$ mellem 2,36 og 2,86.

Upubliseret (1994, dokument 076 FYF, refereret i FMC, 2019) angiver at, BCF for hel fisk er 95, og at kinetisk[1] BCF er 103. Forsøget er udført med *Lepomis macrochirus.* Forsøget er også citeret, og altså vurderet og accepteret, i EFSA 2009.

Den danske QSAR database (Danish (Q)SAR Database (dtu.dk))(se datablad i bilag C) forudsiger en BCF mellem 16,8 – 25,4 og en BAF mellem 24,4 – 26,4, afhængig af den valgte model.
De målte værdier har større vægt end QSAR, men resultaterne fra QSAR peger ikke på, at BCF og BAF skulle være større end de målte værdier.

I rotter omsættes malathion hurtigt. Stoffet udskilles således med over 90% på 24 timer.

Det er derfor usandsynligt, at malathion opkoncentreres i fødekæden, man vil snarere forvente det modsatte.

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[1] Kinetisk BCF = koncentrationen i fisk / udskillelsesrate i fisk.

Martinez-Tabche et al. 2002 angiver en BCF i en snegl (*Stagnicola sp.*) på 45 l/kg. Det angives dog, at det er koncentrationen i dyrene divideret med koncentrationen i sedimentet. Det er derfor usikkert, hvor sammenligneligt det er med BCF i fisk, og énheden l/kg er i øvrigt tvivlsom.

Man kan dog sige, at der ikke umiddelbart er noget, der tyder på en større BCF i snegle end i fisk, og efter 3 dage var malathion stort set ude af dyrene.

### 3.3 Naturlig forekomst

Der er ingen naturlig forekomst af malathion.

# 4 Toksicitetsdata

## 4.1 Toksicitet over for vandlevende organismer

De akutte og kroniske datasæt ses i bilag A. De værdier, der er brugt i SSD (Species Sensitivity Distribution) analyserne er i bilaget mærket med fed skrift.

Som udgangspunkt er data taget fra FMC (2019) og US EPAs database ECOTOX. Der er meget store datamængder i ECOTOX databasen, specielt vedrørende akut toksicitet.

Den første sortering af kroniske data fra ECOTOX er sket udfra oplysninger givet om varighed af test, effekttyper (endpoints), om der er analytisk bekræftelse af testkoncentrationerne og om der er anvendt en formulering eller aktivstoffet. Generelt er studier af for kort varighed i forhold til standardtest udeladt, og effekttyper, der vanskeligt kan relateres til effekter på populationer, er heller ikke medtaget. Studier, hvor der anvendes en formulering, og koncentrationerne af stoffet ikke er analytisk målt, er også udeladt. Studier med kun en eller to testkoncentrationer, udover kontrollen, er ikke medtaget. Studier er dog blevet accepteret, hvor stoffet ikke er målt, men aktivstof har været anvendt, og testopløsningerne er blevet fornyede gennem forsøget.

Så vidt muligt er alle referencerne til de kroniske test, som ikke er med i FMC (2019), skaffet og kvalitetsvurderet efter CRED (Moermond et al, 2016). Kun studier med et troværdighedsindeks (RI) på 1 eller 2 er medtaget i beregningerne af vandkvalitetskriterierne.

Studier accepteret i FMC (2019) er accepteret uden yderligere CRED-vurdering.

Der er meget store mængder akutte data i ECOTOX (1795). Udvælgelsen af akutte data er sket efter de samme principper som for de kroniske data. Dog er manglende målinger accepteret i op til 2 dage, da halveringstiden skønnes at være højst 2 dage og da der er tale om akutte virkninger. For at få så mange af arterne repræsenteret i datasættet er mange 2-dages test blevet accepteret, hvor standardtestens varighed f.eks. er 4 dage. Til gengæld er den laveste af værdierne for hver art blevet valgt. Efter første grovsortering var der 311 værdier. For de laveste og de højeste værdier i ECOTOX er referencerne, så vidt muligt, fremskaffet og CRED vurderede, 47 i alt, dækkende 58 af effektkoncentrationerne. De øvrige effektkoncentrationer er ikke troværdighedsvurderede.

Hvor der er flere værdier for den samme art fra andre kilder end ECOTOX er alle værdierne medtaget, forudsat de ser ud til at være foretaget under de samme betingelser og vedrører samme typer effekter. I det endelige datasæt er det geometriske gennemsnit så anvendt.

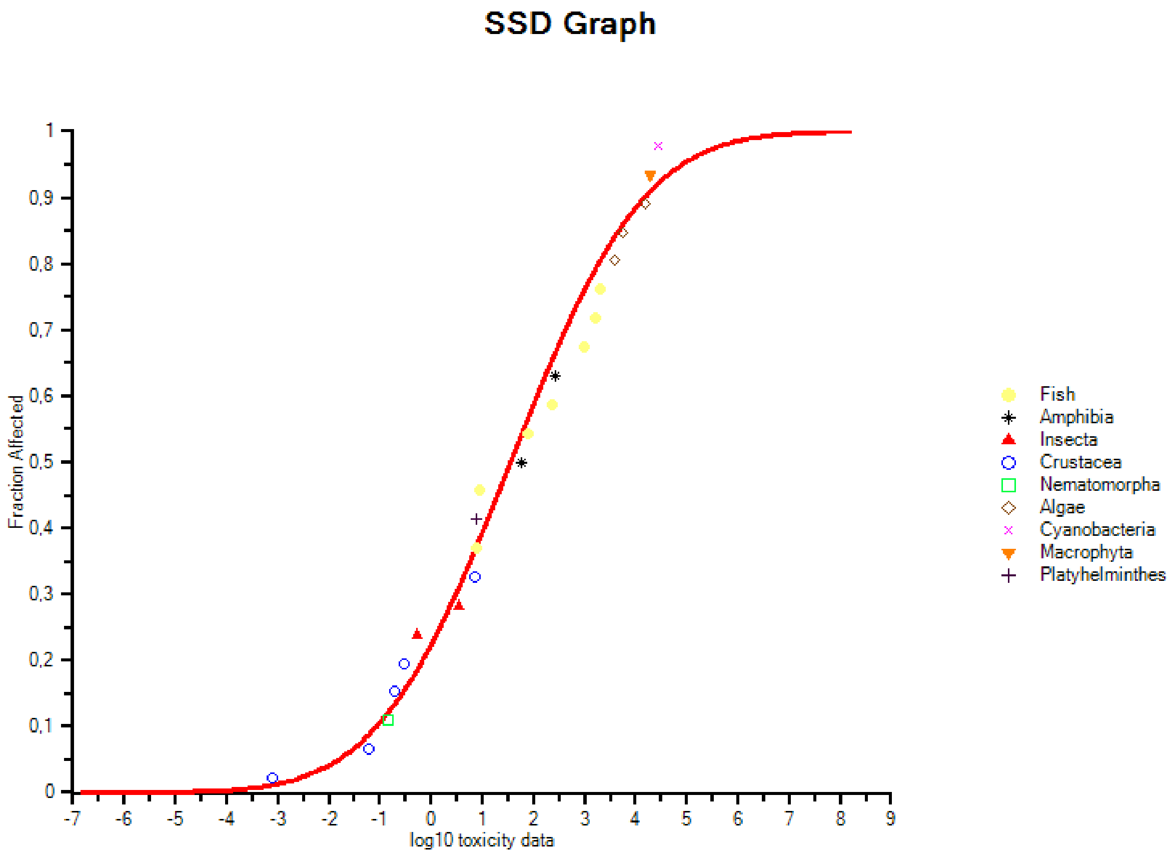
Der er, statistisk set, ikke signifikant forskel mellem den akutte giftighed overfor ferskvandsorganismer og saltvandsorganismer (t-test, P = 0,076; N1 = 55, N2 = 271). Det skal her bemærkes, at det er et meget stort datamateriale, og at selv ganske små forskelle vil resultere i statistisk signifikans.

Der er heller ikke statistisk signifikant forskel mellem kronisk giftighed overfor fersk- og saltvandsorganismer (t-test, P = 0,613; N1 = 4, N2 = 21).

For både akut og kronisk toksicitet gælder det derfor at datasættene for fersk- og saltvand kan lægges sammen.

Kronisk toksicitet:

Det kroniske datasæt indeholder værdier for 23 arter repræsenterende 9 overordnede systematiske grupper, og en artsfølsomhedsanalyse (SSD) kan derfor udføres. Data er analyseret med programmet ETx2, der kan hentes på RIVMs hjemmeside (ETX | Risico's van stoffen (rivm.nl)). Værdierne, der indgår i SSD-analysen er markeret med fed i bilag A.



$HC_{5\text{-kronisk, fersk+salt}}$ = 0,0141 µg/l, 90% CI = 0,00063 µg/l – 0,126 µg/l. Standardafvigelsen af de $\log_{10}$ transformerede data = 2,04. Alle tre ”goodness of fit” test i ETx accepterer hypothesen om log-normalfordeling på alle de listede signifikansniveauer.

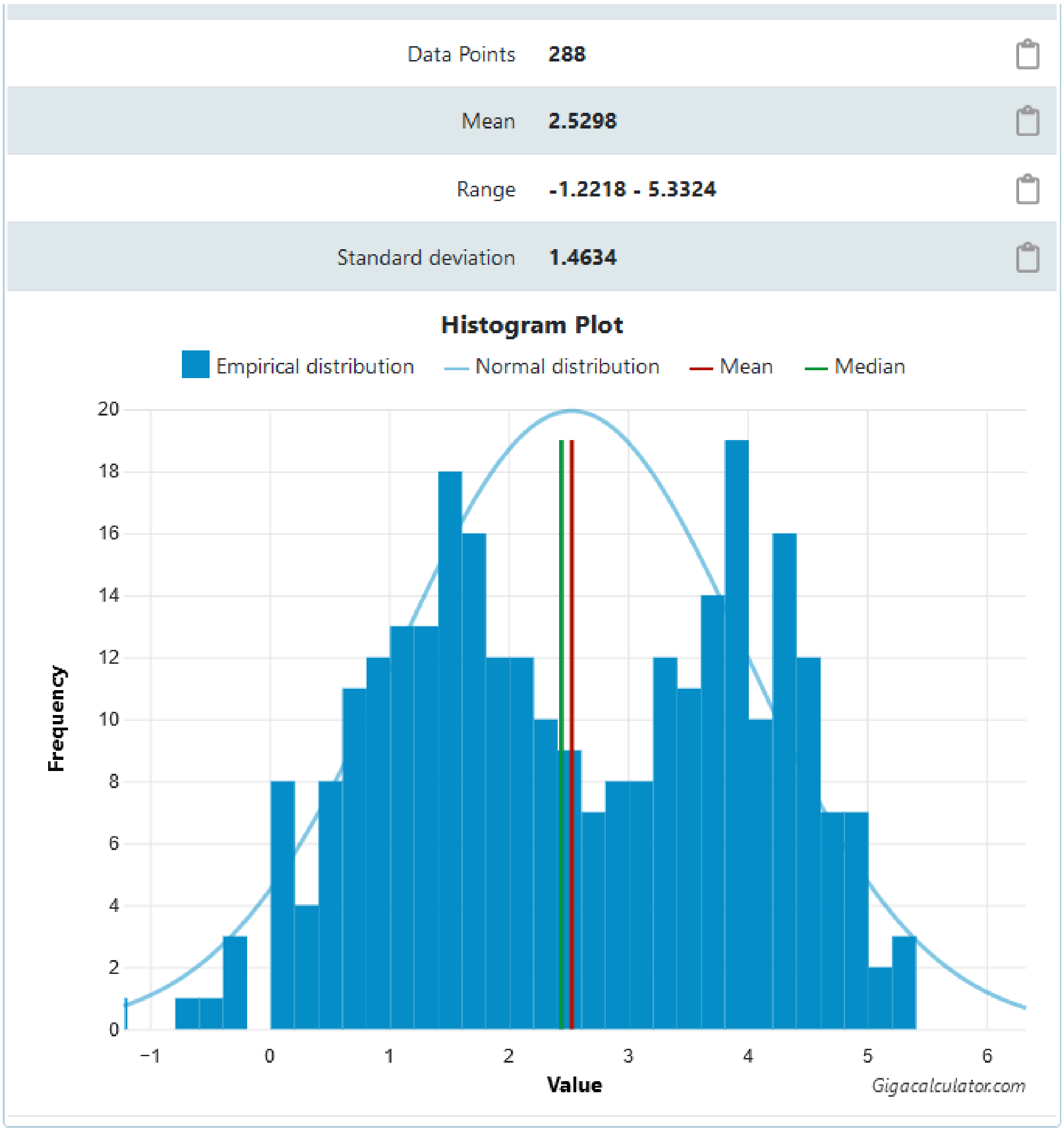
Akut toksicitet:

Det akutte datasæt indeholder $EC_{50}$ værdier for 272 arter repræsenterende 16 systematiske hovedgrupper og en SSD kan derfor bruges. Værdierne, der indgår i SSD-analysen er markeret med fed i bilag A.
$HC_5$ for det samlede materiale er 0,88 µg/l med en standardafvigelse (SD) for de $\log_{10}$ transformerede værdier på 1,47.

Data fordeler sig meget klart i to grupper (se figur nedenfor) og data er klart ikke normaltfordelte. Der udføres derfor en SSD analyse med data repræsenterende den nedre halvdel af fordelingen.

$HC_5$ for den nedre halvdel af fordelingen er 1,2 µg/l med nedre og øvre 90% konfidensgrænser på 0,8 µg/l – 1,8 µg/l samt en SD på 0,80 (N = 159). Alle tre ”goodness of fit” programmer i ETx accepterer lognormalfordeling på alle signifikansniveauerne.

Dette datasæt omfatter 159 arter repræsenterende syv overordnede systematiske grupper (hjuldyr, muslinger, snegle, krebsdyr, insekter, fisk og padder). De grupper, som må forventes at indeholde de mest følsomme arter, krebsdyr og insekter er rigt repræsenterede. Der er således 53 arter krebsdyr og 70 arter insekter. Krebsdyene og insekterne kan underopdeles i meget forskellige grupper med hensyn til generel økologi og f.eks. fødesøgningsstrategier. Krebsdyrene omfatter: Branchiopoda (bladfødder), Amphipoda, Decapoda, Ostracoda (muslingekrebs) og Isopoda. Insekterne omfatter: Tæger, døgnfluer, guldsmede, slørvinger, vårfluer tovinger og biller.



| | |
|---|---|
| Data Points | **288** |
| Mean | **2.5298** |
| Range | **-1.2218 - 5.3324** |
| Standard deviation | **1.4634** |

## 4.2 Toksicitet over for sedimentlevende organismer

Der foreligger $EC_{50}$-værdier fra test i vand uden sediment med en række organismer, som normalt lever i eller på sediment. Disse er bl.a.:

Visse Chironomus arter med $EC_{50}$ < 1 µg/l
Visse Gammarus arter med $EC_{50}$ < 1 "
Hyalella sp. Med $EC_{50}$ = 0,06 "

Der er således en klar indikation på stor giftighed overfor sedimentlevende organismer.

Der er ikke fundet brugbare data for sediment ved søgning i FMC 2019, ECOTOX databasen, Agris, Biological Abstracts, GeoScience World, PubMed og Google Scholar.

Der er dog én reference, som giver en $LC_{50}$ værdi (Martínez-Tabche 2001) for *Limnodrilus hoffmeisteri* (en oligochaet) på 0,269 mg/kg sediment (2,25% OC). En $LC_{50}$ er ikke relevant og studiets opfyldelse af validitestkriterierne kan ikke vurderes på grund af manglende oplysninger.

### 4.3 Toksicitet over for pattedyr og fugle

Giftigheden overfor fugle og pattedyr er angivet i bilag A.

Data er hentet fra FMC (2019) og ECOTOX databasen.

Malathion betragtes ikke som biomagnificerende, og det kritiske fødeemne for vilde fugle og pattedyr er derfor invertebrater som f.eks. muslinger.
Da stoffet ikke er specielt hydrofobt (vandopløselighed er 143 mg/l), og da lipidkoncentrationen i muslinger er lav (omkr. 1%, EU 2018b) beregnes koncentrationen i muslinger som mg/kg tørvægt.

NOEC i muslinger for de enkelte arter er givet i bilag B. Hvor der er flere NOEC-værdier for en art er det geometriske gennemsnit brugt.

Laveste NOEC i muslinger er 2,7 $mg/kg_{vådvægt}$ musling (bløddele), som anvendes i udledningen af biotakvalitetskriteriet for sekundær forgiftning.

### 4.4 Toksicitet over for mennesker

For menneskers sundhed er malathion klassificeret med H302 (giftigt, hvis slugt) og H317 (hudsensibiliserende) (Annex VI til CLP, ATP17: https://echa.europa.eu/documents/10162/17218/annex_vi_clp_table_atp17_en.xlsx/4dcec79c-f277-ed68-5e1b-d435900dbe34?t=1638888918944&download=true.).

ADI (Acceptable Daily Intake) = 0,03 mg/kg lgv/d (EFSA 2009). Værdien er baseret på langtids studier med rotter.

Jævnfør EU (2018b) er ADI 0,03 mg/kg lgv/d svarende til 30 µg/kg lgv d

# 5 Andre effekter

Der er ikke fundet oplysninger om andre typer af effekter.

# 6 Udledning af vandkvalitetskriterium

Kvalitetskriterierne er fastsat i overensstemmelse med EU's Guidance Document no. 27: Technical Guidance for Deriving Environmental Quality Standards (EU, 2018a).

For beregning af VKK er retningslinjerne for fastsættelse af usikkerhedsfaktorer (UF), der skal anvendes på $HC_5$-værdier fra SSD analyser begrænset til, at faktoren skal være mellem 5-1, samt at der er en række aspekter, som man skal tages højde for (f.eks. antal arter, varians m.m., EU 2018a, side 45 afsnit 3.3.1.2). Udgangspunktet er en UF = 5, når betingelserne for at udføre en SSD analyse lige akkurat er opfyldt. Med flere og bedre data kan UF reduceres. Ved beregning af KVKK er udgangspunktet en UF = 10.

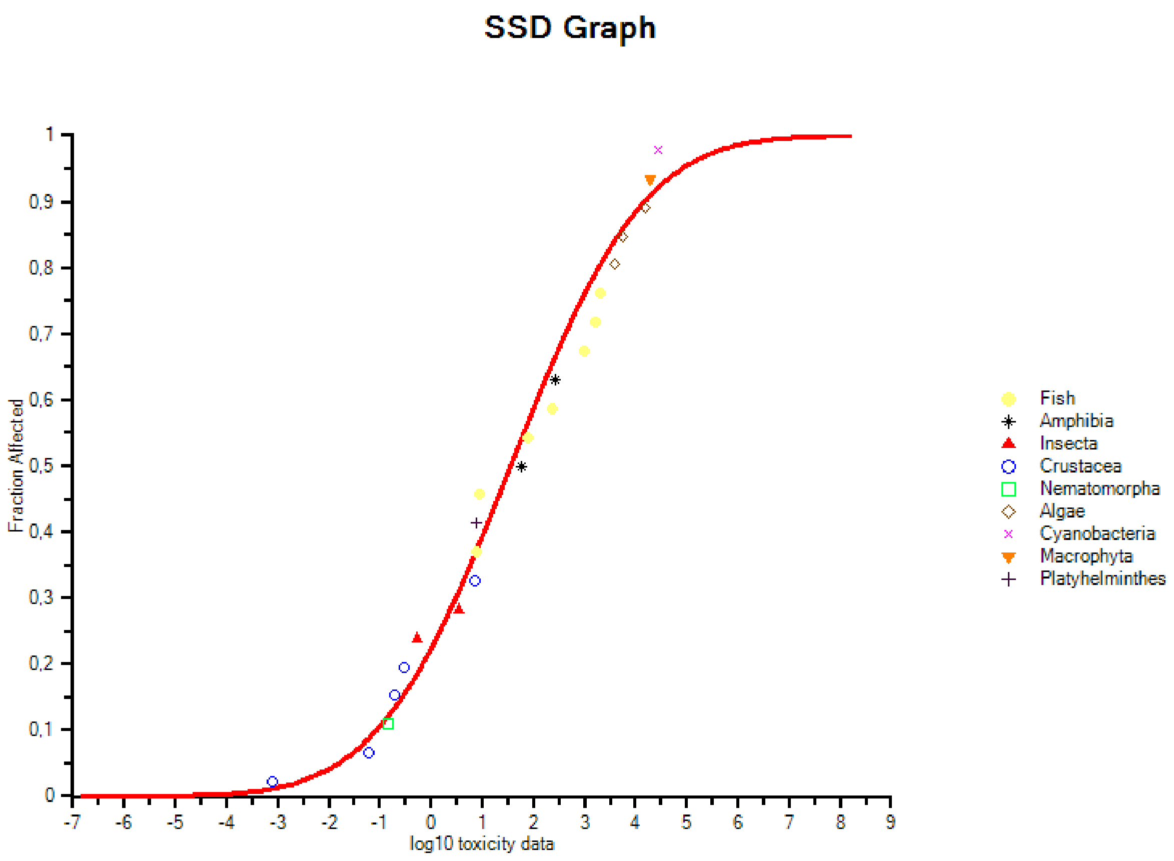
UF værdierne 5-1 blev fastlagt i 2001 førend man var helt på det rene med hvilken grad af effekt NOEC svarede til og hvilken effektstørrelse $EC_x$ skulle repræsentere. Da det i dag er klart, at NOEC i gennemsnit svarer til omkr. 10% effekt og, at man foretrækker at bruge $EC_{10}$ giver det ikke længere mening at anvende en UF = 1.

I en årrække har Miljøstyrelsen anvendt følgende "tommelfingerregel" i nedenstående tabel ved valg af UF på $HC_5$ (VKK):

| **Antal arter** | | **Antal overordnede systematiske grupper** | **Usikkerheds-faktor** |
|---|---|---|---|
| **10-14** | og | **8-9** | **5** |
| **15-20** | **eller** | **10-11** | **4** |
| **21-30** | **eller** | **12-14** | **3** |
| **≥31** | **eller** | **≥15** | **2** |

## 6.1 Vandkvalitetskriterium (VKK)

$HC_5$ = 0,014 µg/l og standardafvigelsen af de $\log_{10}$ transformerede værdier er 2,04. Anderson-Darling, Kolmogorov-Smirnov og Kramer von Mises tests for normalfordeling accepterer lognormalfordelingen på alle signifikansniveauerne.



Der er 23 arter og 9 overordnede systematiske grupper, og som udgangspunkt vælges en usikkerhedsfaktor (UF) på 3.

Variansen er dog stor (SD = 2,04) og i det akutte datasæt er der tretten arter, der er mere følsomme end Ceriodaphnia, som er den mest følsomme kroniske art. Tolv af disse tretten arter er ikke repræsenteret i det kroniske datasæt. Af de nævnte tolv arter er 10 krebsdyr eller insekter, grupper som må forventes at være blandt de mest følsomme.

Derfor ville man nok vælge en UF på 4.

VKK$_{\text{ferskvand}}$ ville derfor blive 0,014 µg/l / 4 = 0,0035 µg/l

Det bemærkes dog, at denne værdi er større end EC$_{10}$ for den mest følsomme af de testede arter, 0,0008 µg/l for *Ceriodaphnia dubia*, samt at det akutte datasæt indeholder tretten arter, der er mere følsomme end *C. dubia*, og tolv af disse arter er ikke repræsenteret i det kroniske datasæt.

Det vælges derfor ikke at sænke UF men beholde UF på 5. Dette resulterer i en værdi på:

**VKK$_{\text{ferskvand}}$** = 0,014 µg/l / 5 = **0,0028 µg/l ≈ 0,003 µg/l**

Denne værdi er stadig 3,75 gange større end $EC_{10}$ for *Ceriodaphnia dubia*, men tyve gange mindre end værdien for *Daphnia magna*, som er den næstmest følsomme i det kroniske datasæt.

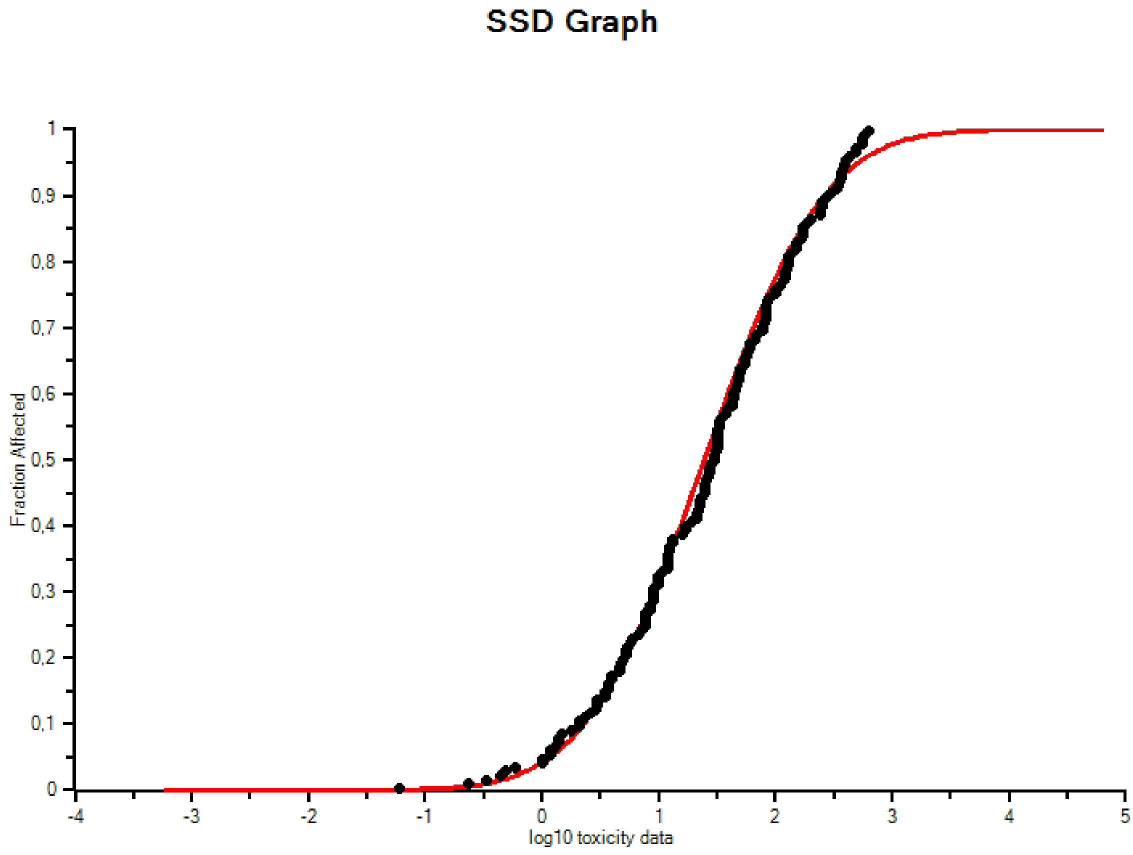
I det kroniske datasæt for saltvand er der kun én speciel repræsentant for det marine miljø, krabben *Cancer magister*. Der skal derfor anvendes en ekstra usikkerhedsfaktor på 5 ved beregning af VKK for det marine miljø.

**$VKK_{saltvand}$** = 0,0028 µg/l / 5 = **0,00056 µg/l ≈ 0,0006 µg/l**

### 6.2 Korttidsvandkvalitetskriterium (KVKK)

Da fordelingen af $EC_{50}$ værdier er to-toppet anvendes $HC_5$ for den nedre gruppe i fordelingen.

$HC_{5\text{-akut}}$ =1,2 for den nedre del af fordelingen, og SD af de $\log_{10}$ transformerede tal = 0,80. En lognormal fordeling er accepteret i alle tilfælde.



I det akutte marine datasæt er der adskillige arter, der, jævnfør EU vejledningen (EU 2018a), kan regnes for specielle repræsentanter for saltvand inden for de taksonomiske grupper hjuldyr, muslinger og pighuder. Der skal derfor ikke føjes en ekstra usikkerhedsfaktor til beregning af KVKK for saltvand. KVKK for saltvand bliver lig KVKK for ferskvand.

$LC_{50}$ datasættet er meget omfattende (272 arter, 15 overordnede grupper) og omfatter mange arter, som må forventes at være blandt de mest følsomme, nemlig insekter og krebsdyr. Der er således 53 arter krebsdyr og 70 arter insekter, og materialet omfatter 6 klasser af krebsdyr og 7 insektordener. Ovennævnte $HC_5$ er for den "nederste" gruppering af $EC_{50}$ værdierne. Denne gruppering omfatter 159 arter repræsenterende 7 overordnede sytstematiske grupper. Krebsdyrene og insekterne kan underopdeles i økologisk meget forskellige grupper, og betingelserne for at udføre en SSD analyse er klart til stede.
Som udgangspunkt skal man, ifølge EU vejledningen (EU 2018a), anvende en UF på 10. Men, med det meget omfattende datamateriale og omfattende repræsentation af særligt følsomme grupper, foreslås det at anvende en UF på 3, også selvom variansen er stor.

**$KVKK_{ferskvand}$ = $KVKK_{saltvand}$** = 1,2 µg/l / 3 = **0,4 µg/l**

Der er 4 arter, som har en lavere $EC_{50}$ end denne værdi: *Hyalella azteca* (0,06 µg/l), *Jordanella floridae* (0,24 µg/l), *Gammarus pulex* (0,33 µg/l) og *G. fasciatus* (0,48 µg/l). Dette kunne være et argument for, at anvende en større UF, men dels er datamængden særdeles omfattende, dels udgør disse arter kun 1,5% af alle de testede arter og 2,5% af den "nedre gruppe". Endvidere lægges der større vægt på kroniske effekter, som relaterer til vedvarende udledninger.

### 6.3 Kvalitetskriterium for sediment (SKK)

Den store akutte giftighed (test i vand) over for en række organismer, der normalt lever i/på sediment er en klar indikation på, at et SKK kan være relevant, og et kvalitetskriterie for sediment bør udarbejdes.

EqP-metoden (EU 2018a) anvendes, da der ikke er troværdige tilgængelige kronisk effektdata fra sedimentstudier.

Der anvendes et EU standard sediment med et organisk kulstof (OC)-indhold på 0,05 (5%) og en $K_{oc}$-værdi. Det geometriske gennemsnit af $K_{oc}$ værdierne angivet i tabel 2.1 er 216 l/kg.

Fordelingskoefficienten mellem fast stof og vand i sediment, $Kp_{sed}$ bestemmes ved følgende formel:

$Kp_{sed} = F_{OCsed} \times K_{OC} = 0{,}05 \times 216$ l/kg = 10,8 l/kg

Fordelingskoefficienten mellem sediment og vand, $K_{sed\text{-}vand}$ kan hernæst bestemmes ved følgende formel, med de nedenfor angivne "default" værdier fra EU vejledningen (EU 2018a):

$K_{sed\text{-}vand} = Fluft_{sed} \times K_{luft\text{-}vand} + Fvand_{sed} + Ffast_{sed} \times (Kp_{sed} / 1000) \times RHO_{fast}$

"Default" værdier fra EU vejledningen:

| | |
|---|---|
| $Fluft_{sed} \times K_{luft\text{-}vand}$: | 0 |
| $Fvand_{sed}$: | 0,8 $m^3m^{-3}$ |
| $Ffast_{sed}$: | 0,2 |
| $RHO_{fast}$: | 2500 $kg*m^{-3}$ |
| RHOsed: | 1300 $kg*m^{-3}$ |

$K_{sed\text{-}vand} = 6{,}2\ m^3m^{-3}$

SKK for ferskvand og saltvand kan bestemmes ved anvendelse af nedenstående formler, hvor VKK på 0,003 µg/l og 0,0006 µg/l for hhv. ferskvand og saltvand anvendes:

$SKK_{vådvægt,\ ferskvand} = (K_{sed\text{-}vand} / RHOsed) \times VKK_{ferskvand} \times 1000 = (6{,}2 / 1300) \times 0{,}003 \times 1000 = 0{,}014\ \mu g/kg_{vådvægt}$

Faktor til konvertering til tørvægt: $RHOsed / Ffast_{sed} \times RHO_{fast} = 2{,}6$

**$SKK_{tørvægt,\ ferskvand}$** $= SKK_{vådvægt} \times 2{,}6 = 0{,}014\ \mu g/kg_{vådvægt} \times 2{,}6 =$ **$0{,}04\ \mu g/kg_{tørvægt}$ (5% OC)**

**$SKK_{tørvægt,\ ferskvand}$** $= 0{,}04 / 0{,}05\ \mu g/kg =$ **$0{,}80\ \mu g/kg_{tørvægt} \times foc$**

$SKK_{vådvægt,\ saltvand} = (K_{sed\text{-}vand} / RHOsed) \times VKK_{saltvand} \times 1000 = (6{,}2 / 1300) \times 0{,}0006 \times 1000 = 0{,}0027\ \mu g/kg_{vådvægt}$

**$SKK_{tørvægt,\ saltvand}$** $= 0{,}0027 \times 2{,}6 =$ **$0{,}0069\ \mu g/kg_{tørvægt} \approx 0{,}007\ \mu g/kg_{tørvægt}$ (5% OC)**

**$SKK_{tørvægt,\ saltvand}$** $= 0{,}0069 / 0{,}05 =$ **$0{,}14\ \mu g/kg_{tørvægt} \times f_{OC}$**

### 6.4 Kvalitetskriterium for biota, sekundær forgiftning ($BKK_{sek.forgiftn.}$)

Da BCF er målt til omkring 100 bør der udarbejdes BKK for sekundær forgiftning (fødekæde effekt) (EU 2018a).

I rotter elimineres malathion med mere end 90% på 24 timer og alt i alt tyder det på TMF (trophic magnification factor) og BMF (bio-magnification factor) værdier er mindre end 1, og $BKK_{sek.forgiftn}$ bør sættes for muslinger snarere end fisk.

NOEC-værdierne angivet i bilag A er alle energinormaliserede (mg/kJ), idet det antages at dyrenes foder har et energiindhold på 15,1 $kJ/g_{tørvægt}$ og et vandindhold på 8% (tabel 8 i EU-vejledningen, EU 2018a). Det er EU vejledningens metode B i afsnit 4.4.5, der er benyttet ved beregningerne da effektværdierne er koncentrationer i føden.

NOEC-værdierne er derefter omregnet til koncentrationer i muslinger, idet det antages at muslinger har et energiindhold på 19 $kJ/g_{tørvægt}$ og et vandindhold på 92% jævnfør afsnit 4.4.6 i EU vejledningen (EU 2018a). Værdierne er præsenteret i bilag B.

I bilag A er alle NOAEL (mg/kg lgv/ d) værdier blevet omregnet til NOEC-værdier med en omregningsfaktor givet i tabel 21 i EU vejledningen, og $LC_{50}$-værdien for fasan er omregnet til NOEC ved at dividere med 100 (tabel 9 i EU 2018a).

Laveste NOEC er 2,7 mg/kg musling (vådvægt, bløddele) (se bilag B) og der anvendes en usikkerhedsfaktor på 10.

**BKK** = 2,7 mg/kg musling / 10 = **0,27 mg/kg musling**

### 6.5 Kvalitetskriterium for human konsum af vandlevende organismer (HKK)

BCF er omkring 100, og sammenholdt med klassificeringen Acute Tox. 4 bør der udarbejdes kvalitetskriterium for menneskers sundhed, human konsum (HKK).

Der er ikke fundet danske eller EU grænseværdier for malathion i fiskeriprodukter, og grænseværdien beregnes derfor med følgende formel (EU 2018a), ved anvendelse af ADI på 30 µg/kg lgv/ d (EFSA 20009):

HKK = 0,2 x ADI / 0,00163 = 0,2 x 30 / 0,00163 = 3681 µg/kg fiskeriprodukt ≈

**HKK = 3,7 mg/kg fiskeriprodukt**

### 6.6 Vandkvalitetskriterium baseret på $BKK_{sek.forgiftn.}$ og HKK

Jævnfør EU vejledningen (EU, 2018a) skal der laves en tilbageregning fra biotakvalitetskriterierne ($BKK_{sek.forgiftn.}$ og HKK) til en vandkoncentration, for at se om vandkvalitetskriteriet fastsat for direkte effekter, også beskytter for sekundær forgiftning gennem fødekæden, samt beskytter mod forgiftning ved human konsum.

Der haves ingen BAF værdier, men for stoffer, der ikke opkoncentreres i fødekæden, svarer BAF stort set til BCF.

BCF ≈100 l/kg

$VKK_{vand,\ biota}$ = BKK / BCF

Laveste BKK eller HKK er BKK = 0,27 mg/kg

**$VKK_{vand,\ biota}$** = 0,27 mg/kg / 100 l/kg = 0,0027 mg/l = **2,7 µg/l**

Denne værdi er højere end VKK for vand, og bliver derfor ikke udslagsgivende.

# 7 Konklusion

Følgende kvalitetskriterier for vandmiljøet er udregnet for malathion:

Vandkvalitetskriterium

| | |
|---|---|
| $\text{VKK}_{\text{ferskvand}}$ | 0,003 µg/l |
| $\text{VKK}_{\text{saltvand}}$ | 0,0006 µg/l |

Korttidsvandkvalitetskriterium

| | |
|---|---|
| $\text{KVKK}_{\text{ferskvand}}$ | 0,4 µg/l |
| $\text{KVKK}_{\text{saltvand}}$ | 0,4 µg/l |

Sedimentkvalitetskriterium

| | |
|---|---|
| $\text{SKK}_{\text{ferskvand}}$ | 0,04 µg/$\text{kg}_{\text{tørvægt}}$ sediment (5% OC)<br>0,8 µg/$\text{kg}_{\text{tørvægt}}$ x $f_{oc}$ |
| $\text{SKK}_{\text{saltvand}}$ | 0,007 µg/$\text{kg}_{\text{tørvægt}}$ sediment (5% OC)<br>0,14 µg/$\text{kg}_{\text{tørvægt}}$ x $f_{oc}$ |

Biotakvalitetskriterium, sekundær forgiftning

| | |
|---|---|
| $\text{BKK}_{\text{sek.forgiftn.}}$ | 0,27 mg/kg musling vådvægt |

Biotakvalitetskriterium, human konsum

| | |
|---|---|
| HKK | 3,7 mg/kg fiskeriprodukter, vådvægt |

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# Bilag A

## Giftighed over for vandorganismer ($EC_x$, $LC_x$, NOEC, osv.)

### Ferskvandsorganismer

Akut giftighed

*Freshwater, acute toxicity*

Akutte data for malathion, $EC_{50}$ og $LC_{50}$. For alger og cyanobakterier bruges normalt vækstraten, dvs. $E_rC_{50}$, hvis den er tilgængelig. Alle referencer fra FMC (2019) betragtes som troværdige med et troværdighedsindeks på RI1 eller RI2. Da disse studier ofte bare angives som "acceptable" er der i tabellen ikke angivet en RI-værdi udfor FMC-studier.

Acute toxicity data for malathion, $EC_{50}$ and $LC_{50}$. For algae and cyanobacteria the $EC_{50}$ is normally for growth rate, i.e. $E_rC_{50}$ is employed if available. All references from FMC 2019 are regarded as reliable with a reliability index of RI1 or RI2

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| **Cyanobacteria** | *Anabaena flos-aquae* | 41425 | 3 | y | 96 | | FMC 2019: Dobbins et al. 2012, 1262 FYF | |
| **Alger ( Algae)**<br>**Chlorophyta** | *Raphidocelis subcapitata* | 131218 | 3 | y | 96,4 | | FMC 2019: Jenkins 1993, 071 FYF,<br>FMC 2019: Dobbins 2012, 1246 FYF<br>Yeh & Chen 2006 | Geometrisk gennemsnit af de tre studier. Yeh & Chen studiet havde den laveste værdi (2040 µg/l). Værdien er fra ECOTOX og er ikke blevet evalueret. Endvidere var koncentrationerne ikke målt og renheden af stoffet ikke angivet.<br>Konsekvensen af brugen af nominelle koncentrationer og af at have en lavere renhed vil være, at man overvurderer koncentrationen, dvs. får en større $EC_{50}$ end den skulle være.<br>Da dette studie giver den laveste værdi, vil det være betænkeligt at udelade det. |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| | *Scenedesmus obtusiusculus* | 55380 | 6 | n | 60 | | Piri & Ordog 1999 | |
| **Bacillariophyseae** | *Navicula pelliculosa* | 23669 | 3 | y | 96 | | FMC 2019: Dobbins et al 2012, 1245 FYF, | |
| **Højere planter (Macrophyta)** | *Lemna gibba* | 81150 | 7 | y | 96 | | FMC 2019: Dobbins et al 2012, 1264 FYF, | |
| **Protozoa** | *Spirostomum ambiguum* | 39100 | 1 | n | | | Nalecz-Jawecki et al 2002 | |
| **Protozoa** | *Tetrahymena pyriformis* | 32000 | 0,375 | n | 90 | | Bogaerts et al 2001 | Eksponential vækstfase (log) |
| **Fladorme (Platyhelminthes) Trematoda** | *Schistosoma mansoni* | 69360 | 0,167 | n | 91 | | Tchounwou et al 1992 | |
| **Fladorme (Platyhlminthes) Turbellaria** | *Dugesia dorotocephala* | 6000 | 7 | n | | | Villar et al 1993 | |
| | *Girardia tigrina* | 4400 | 4 | n | 54,4 | | Villar et al 1994 | |
| **Hjuldyr (Rotifera)** | *Brachionus calyciflorus* | 33720 | 1 | n | 95 | | Fernandez-Casalderry et al 1992 | Cyst |
| | *Brachionus rubens* | 35300 | 1 | n | | | Snell et Persoone 1989 | Neonat |
| | *Lecane papuana* | 42840 | 2 | n | 97,1 | | Garza-Leon et al 2017 | Neonate |
| | ***Philodina acuticornis*** | **165,176** | 3 | n | | | Nogrady et Keshmirian 1986 | Voksne |
| **Rundorme (Nematoda)** | *Romanomermis culicivorax* | 6780 | 1 | n | | | Winner et al 1978 | |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| **Bløddyr (Mollusca) Bivalvia** | *Anodonta anatina* | 2030 | 2 | n | 95 | 2 | Varanka 1986 | Larve |
| | *Anodonta cygnea* | 10210 | 2 | n | 95 | 2 | Varanka 1986 | Larve |
| | *Elliptio icterina* | 32000 | 4 | n | 96 | 2 | Keller et Ruessler 1997 | Juvenile |
| | ***Indonaia caerulea*** | **12** | 4 | n | 95 | | Mane et al 1984 | |
| | ***Lamellidens corrianus*** | **118,55** | 4 | n | | | Mane et Muley 1987 | Voksne |
| | ***Lamellidens marginalis*** | **55,63** | 4 | n | | | Mane et Muley 1987 | Voksne |
| | *Lampsilis siliquoidea* | 7000 | 2 | n | 96 | 2 | Keller et Ruessler 1997 | Voksne |
| | *Lampsilis straminea ssp. claibornensis* | 24000 | 4 | n | 96 | 2 | Keller et Ruessler 1997 | Juvenile |
| | *Lampsilis subangulata* | 28000 | 4 | n | 96 | 2 | Keller et Ruessler 1997 | Juvenile. Blev faktisk malt, men var tæt på nominelle |
| | *Lampsilis teres* | 28000 | 0,167 | n | 96 | 2 | Keller et Ruessler 1997 | Glochidia. Blev faktisk malt, men var tæt på nominelle |
| | *Megalonaias nervosa* | 22000 | 1 | n | 96 | 2 | Keller et Ruessler 1997 | Voksne |
| | *Utterbackia imbecillis* | 215000 | 4 | n | 96 | 2 | Keller et Ruessler 1997 | Juvenile. Blev faktisk malt, men var tæt på nominelle |
| | *Villosa lienosa* | 54000 | 1 | n | 96 | 2 | Keller et Ruessler 1997 | Voksne |
| | *Villosa villosa* | 117000 | 1 | n | 96 | 2 | Keller et Ruessler 1997 | Voksne |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| **Bløddyr (Mollusca)**<br>**Gastropoda** | *Bellamya bengalensis* | 17500 | 4 | n | | | Vankhede et Dhande 1991 | |
| | *Biomphalaria havanensis* | 94780 | 1 | n | 91 | 2 | Tchounwou et al 1991 | Æg |
| | *Helisoma duryi* | 1760 | 1 | n | | | Bakry et al 2011 | Voksne |
| | *Helisoma trivolvis* | 187650 | 1 | n | 91,5 | 2 | Tchounwou et al 1991 | Æg (fostre) |
| | ***Lymnaea acuminata*** | **16,9** | 2 | n | 50 | | Chaudhari et al 1988 | |
| | *Lymnaea stagnalis* | 7400 | 2 | n | 40 | | Frumin et 1992 | Voksne |
| | *Pila globosa* | 10000 | 2 | n | 50 | | Ahamad et al 1978 | |
| | *Planorbella trivolvis* | 187650 | 1 | n | 91 | 2 | Tchounwou et al 1991 | Æg |
| | *Planorbis corneus* | 62000 | 2 | n | 40 | | Frumin et 1992 | Voksne |
| | *Pomacea canaliculata* | 18680 | 2 | n | | | Tejada et al 1994 | |
| | ***Thiara lineata*** | **31,1** | 2 | n | 50 | | Chaudhari et al 1988 | |
| | ***Thiara scabra*** | **37,4** | 2 | n | 50 | | Chaudhari et al 1988 | |
| | *Viviparus bengalensis* | 1510 | 4 | n | | | Lomte et Alam 1985 | |
| **Ledorme (Annelida)**<br>**Oligochaeta** | *Lumbriculus variegatus* | 20500 | 4 | n | | | Bailey et Liu 1980 | |

| Overordnet systematiske gruppe | Art | EC$_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Tubifex sp.* | 43100 | 2 | n | 40 | | Frumin et al 1992 | Voksne |
| | *Tubificidae* | 20700 | 2 | n | 99,6 | | Whitten et Goodnight 1966 | |
| **Ledorme (Annelida)**<br>**Hirudinea** | *Erpobdella octoculata* | 27000 | 4 | n | | | Yang et Zhang 1989 | |
| | *Glossiphonia sp.* | 13000 | 4 | n | | | Yang et Zhang 1989 | |
| **Krebsdyr (Crustacea)**<br>**Amphipoda** | ***Gammarus fasciatus*** | **0,48** | 5 | n | | 2 | Sanders 1972 | ”Flow-through” |
| | ***Gammarus lacustris*** | **1,8** | 2 | n | | | US EPA 1992 | II tre andre studier med RI3 og RI4 lå værdierne på1,6, 1,8 og 3,8µg/l,altså meget tæt på den her viste værdi på 1,8. Så selvom studierne ikke er troværdige understøtter de samlet set værdien på 1,8 µg/l |
| | ***Gammarus pseudolimnaeus*** | **2,1** | 4 | y | 96,8 | | FMC 2019: Brougher et al 2014, 1417 FYF | |
| | ***Gammarus pulex*** | **0,33** | 4 | y | 97,8 | 2 | Ashauer et al 2011 | Voksne |
| | ***Hyalella sp.*** | **0,06** | 4 | y | 99,1 | | Cothran et al 2009 | |
| **Krebsdyr (Crustacea)**<br>**Branchiopoda** | ***Alona guttata*** | **5,26** | 2 | n | 97,1 | | Garza-Leon et al 2017 | Neonate |
| | ***Ceriodaphnia dubia*** | **2,12** | 2 | n | | | Ankley et al 1991 | |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Daphnia magna* | 0,27 | 1 | n | | 2 | Gaaboub et al 1975 | Neonate |
| | *Daphnia magna* | 0,72 | 2 | y | 96,9 | | FMC 2019: Gries et Purghart 2201, 310 FYF | |
| | *Daphnia magna* | 0,75 | 2 | y | 96,8 | | FMC 2019: Juckeland 2019, 4136 ETX-FYF | Lavt isomalathion content |
| | *Daphnia magna* | 0,8 | 2 | y | 96 | | FMC 2019: Juckeland 2019, 4136 ETX-FYF | Højt isomalathion i indhold.<br>QSAR forudsigelser (danske QSAR database, https://qsardb.food.dtu.dk/db/index.html) estimerer en lavere giftighed af isomalathion overfor vandlevende organismer end for malathion. |
| | *Daphnia magna* | 2,1 | 2 | y | 99,4 | | FMC 2019: Mattock 20021, 369 FYF | |
| | *Daphnia magna* | 11,32 | 2 | n | 95 | | FMC 2019: Zhang et al 2011 | Racemisk blanding |
| | *Daphnia magna* | 6,94 | 2 | n | 95 | | FMC 2019: Zhang et al 2011 | R-malathion |
| | *Daphnia magna* | 11,62 | 2 | n | 95 | | FMC 2019: Zhang et al 2011 | S-malathion |
| | *Daphnia magna* | 0,36 | 2 | n | 50 | | FMC 2019:Toumi et al 2015 | Strain S1 |
| | *Daphnia magna* | 0,44 | 2 | n | 50 | | FMC 2019:Toumi et al 2015 | Strain S2 |
| | *Daphnia magna* | 0,46 | 2 | n | 50 | | FMC 2019:Toumi et al 2015 | Strain S3 |
| | ***Daphnia magna*** | **1,3** | | | | | | Geometrisk gennemsnit af *D. magna* værdierne ovenfor. |
| | *Daphnia similis* | 1710 | 2 | y | 1113 g/l | | FMC 2019: Perina et al 1995, 248 FYF | |
| | ***Moina macrocopa*** | **58** | 0,125 | n | | | Nishiuchi et Hashimoto 1969 | Voksne |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | ***Simocephalus vetulus*** | **2,9** | 2 | y | | | Olvera-Hernandez et al 2004 | Neonate |
| **Krebsdyr (Crustacea) Branchiopoda Anostraca** | *Branchinecta sandiegonensis* | 24450 | 1 | n | | | Ripley et al 2002 | |
| | *Streptocephalus proboscideus* | 64418, 45 | 1 | n | | | Calleja et al 1994 | |
| | *Streptocephalus rubricaudatus* | 73700 | 1 | n | | 2(3) | Crisinel et al 1994 | Larver. |
| | *Streptocephalus sudanicus* | 67750 | 2 | n | | 2 | Lahr et al 2001 | Voksne |
| | *Streptocephalus texanus* | 54600 | 1 | n | | RI2(3) | Crisinel et al 1994 | Larver. |
| | ***Thamnocephalus platyurus*** | **25,05** | 1 | n | | | Ripley et al 2002 | Larver |
| **Krebsdyr (Crustacea) Copepoda** | *Cyclops viridis* | 1300 | 2 | n | | | Konar et Ghosh 1981 | |
| **Krebsdyr (Crustacea) Decapoda** | ***Barytelphusa cunicularis*** | **380** | 4 | n | | | Rao et Nagabhushanam 1987 | |
| | ***Macrobrachium lamarrei*** | **130** | 4 | n | 50 | | Nagabhushanam et al 1983 | Intermolt |
| | *Macrobrachium lar* | 851 | 2 | n | | | Bajet et al 2012 | |
| | ***Macrobrachium rosenbergii*** | **9** | 4 | n | | | Natarajan et al 1992 | Post-larve |
| | ***Orconectes nais*** | **290** | 1 | n | 95 | | Mayer et Ellersieck 1986 | Larver |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Oziotelphusa senex ssp. senex* | 6000 | 4 | n | 50 | | Victor 1989 | Voksne |
| | ***Palaemonetes kadiakensis*** | **12** | 4 | n | 95 | | Mayer et Ellersieck 1986 | Voksne |
| | ***Palaemonetes pugio*** | **9,06** | 4 | n | ”Technical grade” | 2 | Key et al 1998 | Koncentrationerne var omkring 85% of nominelle |
| | ***Palaemonetes pugio*** | **7,7** | 4 | n | | | Key et Fulton 2006 | Nyklækkede eller nyligt klækkede |
| | *Procambarus clarkii* | 21000 | 4 | y | 96,8 | | FMC 2019: Brougher et al 2014, 1481 FYF | |
| **Krebsdyr (Crustacea) Isopoda** | *Asellus aquaticus* | 32100 | 2 | n | 40 | | Frumin et 1992 | Voksne |
| | *Caecidotea brevicauda* | 6000 | 1 | n | 95 | | Mayer et Ellersieck 1986 | Voksne |
| **Krebsdyr (Crustacea) Ostracoda** | ***Cypridopsis vidua*** | **47** | 2 | n | 95 | | Mayer et Ellersieck 1986 | Voksne |
| **Insekter (Insecta) Hemiptera** | ***Anisops sardeus*** | **42,2** | 2 | n | | 2 | Lahr et al 2001 | Voksne |
| | ***Notonecta undulata*** | **110** | 2 | n | 94 | | Federle et Collins 1976 | Voksne |
| **Insekter (Insecta) Ephemeroptera** | ***Centroptilum triangulifer*** | **23** | 2 | y | 96,8 | | FMC 2019: Brougher et al 2014, 1442 FYF | |
| | ***Cloeon sp.*** | **5,5** | 1 | n | | | Cano et al 1999 | Larver |
| | ***Drunella grandis*** | **100** | 4 | n | | | Gaufin et al 1965 | Nymfer |
| | *Hexagenia sp.* | 631 | 1 | n | 95 | | Carlson 1966 | Naiad |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| **Insekter (Insecta) Odonata** | ***Lestes congener*** | **27** | 1 | n | 95 | | Mayer et Ellersieck 1986 | Larver |
| | *Orthetrum albistylum ssp. speciosum* | 730 | 2 | n | | | Nishiuchi et al Asano 1978 | |
| **Insekter (Insecta) Plecoptera** | ***Claassenia sabulosa*** | **13** | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | ***Hesperoperla pacifica = Acroneuria p.*** | **7,7** | 5 | n | 95 | 2 | Jensen et Gaufin 1964a | niads, flow-through |
| | ***Isoperla sp.*** | **4,6** | 1 | n | 95 | | Mayer et Ellersieck 1986 | Naiad |
| | ***Pteronarcella badia*** | **10** | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | ***Pteronarcys californica*** | **10** | 4 | n | 95 | | Mayer et Ellersieck 1986 | |
| **Insekter (Insecta) Trichoptera** | ***Arctopsyche grandis*** | **32** | 4 | n | | | Gaufin et al 1965 | Larver |
| | ***Hydropsyche californica*** | **22,5** | 4 | n | | | Gaufin et al 1965 | Larver |
| | ***Hydropsyche sp.*** | **12,3** | 1 | n | 95 | | Carlson 1966 | Larver |
| | ***Limnephilus sp.*** | **6,8** | 1 | n | 95 | | Mayer et Ellersieck 1986 | Larver |
| **Insekter (Insecta) Diptera** | ***Aedes aegypti*** | **5,3** | 1 | n | 96 | 2 | Failloux et al 1994 | Larvere |
| | ***Aedes albopictus*** | **50** | 1 | n | 99,2 | | Polnlawat et al 2005 | Larver |
| | ***Aedes atropalpus*** | **172** | 1 | n | 91 | | Cilek et al 1995 | |
| | ***Aedes cantans*** | **48,8** | 1 | n | | | Rettich 1977 | Larver |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | ***Aedes communis*** | **38,2** | 1 | n | | | Rettich 1977 | Larver |
| | ***Aedes excrucians*** | **30,3** | 1 | n | | | Rettich 1977 | Larver |
| | ***Aedes hendersoni*** | **66** | 1 | n | 91 | | Cilek et al 1995 | Larver |
| | ***Aedes nigromaculis*** | **68** | 1 | n | | | Mulla et al 1964 | Larver |
| | ***Aedes polynesiensis*** | **3,5** | 1 | n | 96 | 2 | Failloux et al 1994 | Larvere |
| | ***Aedes punctor*** | **44,1** | 1 | n | | | Rettich 1977 | Larver |
| | ***Aedes quadrimaculatus*** | **1** | 2 | n | | 2 | Milam et al 2000 | Larvere |
| | ***Aedes taeniorhynchus*** | **25,88** | 1 | n | | | Montada et al 1994 | Larver |
| | ***Aedes triseriatus*** | **43** | 1 | n | 91 | | Cilek et al 1995 | |
| | ***Aedes trivittatus*** | **32,2** | 1 | n | 95 | | Rubio-Moran et al 1981 | Larver |
| | ***Aedes vexans*** | **26,1** | 1 | n | | | Rettich 1977 | Larver |
| | ***Anopheles albimanus*** | **120** | 1 | n | 5 | | Kawada et al 1993 | Larver |
| | ***Anopheles coustani*** | **200** | | n | | | Hamed et al 1983 | Larver |
| | ***Anopheles gambiae*** | **190** | 1 | n | 5 | | Kawada et al 1993 | Larver |
| | ***Anopheles pseudopunctipennis*** | **2,27** | 1 | n | | | Ocampo et al 2000 | Larver |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | ***Anopheles quadrimaculatus*** | **1** | 2 | n | | 2 | Milam et al 2000 | |
| | ***Anopheles stephensi*** | **4** | 1 | n | | | Chitra et Pillai 1984 | Larver |
| | *Atherix variegata* | 1450 | 1 | n | 95 | | Mayer et Ellersieck 1986 | Instar |
| | ***Chironomus crassicaudatus*** | **56** | 1 | n | | | Ali 1981 | Larver |
| | ***Chironomus decorus*** | **32** | 1 | n | | | Ali 1981 | Larver |
| | ***Chironomus plumosus*** | **8,4** | 4 | n | | | Vedamanikam 2009 | Larver |
| | ***Chironomus riparius*** | **0,44** | 1 | n | 97 | 2 | Hoffman et Fisher 1994 | Larver |
| | ***Chironomus tentans*** | **3,5** | 2 | y | 96,8 | | FMC 2019: Brougher et al 2014, 1443 FYF | |
| | ***Chironomus tepperi*** | **8,4** | 1 | n | | | Stevens 1992 | Larver |
| | ***Chironomus utahensis*** | **3** | 1 | n | | 2(3) | Ali et Mulla 1977 | Instar . |
| | ***Cricotopus sp.*** | **25** | 1 | n | | 2(3) | Ali et Mulla 1977 | Instar. Not reported as a formulation |
| | ***Culex antennatus*** | **250** | | n | | | Hamed et al 1983 | Larver |
| | ***Culex fatigans*** | **16** | 1 | n | | | Das et Rajagopalan 1979 | Larver |
| | ***Culex fuscocephala*** | **44,426** | 1 | n | | | Vijayan et al 1993 | Larver |
| | ***Culex nigripalpus*** | **21,7** | 1 | n | | | Boike et al 1989 | Larver |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | ***Culex pipiens*** | **1,5** | 1 | n | | 2 | Gaaboub et al 1975 | 4th instar |
| | ***Culex pipiens*** | **1,6** | 2 | n | 95 | 2 | Zahran et Abdelgaleil 2011 | Fourth instar |
| | | | | | | | | |
| | ***Culex quinquefasciatus*** | **6,7** | 1 | n | 96 | 2 | Failloux et al 1994 | Larvere |
| | ***Culex quinquefasciatus*** | **3,5** | 1 | n | 95 | 2 | Aguilera et al 1995 | Larver |
| | | | | | | | | |
| | ***Culex sitiens*** | **4,6** | 1 | n | | | Komalamisra et al 2006 | Larver |
| | ***Culex tarsalis*** | **10** | 1 | n | | | Ziegler et al 1987 | Larver |
| | ***Culex tritaeniorhynchus*** | **21** | 1 | n | | | Shim& Self 1973 | Larver |
| | ***Culiseta annulata*** | **24,5** | 1 | n | | | Rettich 1977 | Larver |
| | ***Culiseta longiareolata*** | **17** | 1 | n | | | Cano et al 1999 | Larver |
| | ***Dicrotendipes californicus*** | **80** | 1 | n | | | Ali et Mulla 1980 | Larver |
| | ***Glyptotendipes paripes*** | **4** | 1 | n | | | Ali 1981 | Larver |
| | ***Goeldichironomus holoprasinus*** | **28** | 1 | n | | | Ali 1981 | Larver |
| | ***Procladius sp.*** | **5** | 1 | n | | 2(3) | Ali et Mulla 1977 | Larver. I ECOTOX angivet at en formulering er brugt, men dette er |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | ikke angivet i artiklen |
| | ***Simulium vittatum*** | **54,2** | 2 | y | 98 | | Overmyer et al 2003 | Larver |
| | ***Tanytarsus sp.*** | **32** | 1 | n | | | Ali 1981 | Larver |
| | ***Toxorhynchites splendens*** | **49,8** | 2 | n | | | Tietze et al 1993 | Larver |
| **Insekter (Insecta) Coleoptera** | ***Eretes sticticus*** | **430** | 2 | n | | | Jeyasingam et al 1978 | |
| | *Peltodytes sp.* | 1500 | 2 | n | 94 | | Federle et Collins 1976 | Voksne |
| **Fish** | *Alburnus alburnus* | 3780 | 4 | n | 95 | | Guylas et Csanyi 1984 | |
| | *Ameiurus melas* | 18500 | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Anabas testudineus* | 11800 | 4 | n | 95 | | Chandran et al 1991 | |
| | *Anguilla japonica* | 4100 | 2 | n | | | Yokoyama et al 1988 | |
| | *Aplocheilus lineatus* | 975 | 2 | n | | | Jacob et al 1982 | |
| | *Barbonymus gonionotus* | 6520 | 2 | n | 57 | | Hoque 2000 | |
| | *Barbus barbus ssp. plebejus* | 6600 | 1 | n | | | Scirocchi et D'Erme 1980 | |
| | *Barbus dorsalis* | 3700 | 4 | y | 50 | | Rao et al 1967 | |
| | ***Barbus ticto*** | **13** | 2 | n | 96,45 | | Bhatia 1971 | |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Barilius vagra* | 7390 | 4 | y | 57 | | Nishiuchi et al Asano 1978 | Voksne |
| | *Brachydanio rerio* | 266 | 4 | n | ? | | FMC 2019: Busquet et al 2014. | embryoner |
| | *Carassius auratus* | 3150 | 4 | y | | | Birge et al 1979 | Æg |
| | *Channa orientalis* | 16420 | 2 | n | 50 | | Verma et al 1984 | |
| | *Channa punctata* | 3890 | 4 | n | | | Haider et Inbaraj 1986 | Voksne |
| | *Cirrhinus mrigala* | 880 | 4 | n | | | Verma et al 1984 | Larver |
| | ***Clarias batrachus*** | **12** | 4 | n | | | Sinha et al 1991 | |
| | *Clarias gariepinus* | 8220 | 4 | n | 57 | | FMC 2019:Ahmad 2012 | |
| | *Colisa fasciata* | 5360 | 2 | n | 50 | | Verma et al 1984 | |
| | *Cyprinion watsoni* | 7930 | 1 | n | 57 | | Khattak et Hafeez 1996 | |
| | ***Cyprinus carpio*** | **85** | 4 | n | | | Verma et al 1981 | Larver |
| | ***Fundulus diaphanus*** | **240** | 4 | n | | | Rehwoldt et al 1977 | Unge fra samme år |
| | *Gambusia affinis* | 2900 | 4 | y | 96,8 | 1 or 2 | FMC 2019:Document 1426 FYF, 2014 | |
| | *Gambusia holbrooki* | 12780 | | n | | | Areekul,S. 1986 | |
| | *Garra gotyla ssp. gotyla* | 3500 | 4 | n | | | Thakur et Sahai 1994 | |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Gasterosteus aculeatus* | 21,7 | 4 | y | 96 | 1 or 2 | FMC 2019:Document 381 FYF, 2002 | |
| | *Gasterosteus aculeatus* | 46 | 4 | y | 96,8 | 1 or 2 | FMC 2019:Document 881 FYF, 2011 | |
| | ***Gasterosteus aculeatus*** | **31,6** | | | | | Geometrisk gennemsnit | |
| | *Gibelion catla* | 2350 | 3 | n | 50 | | Arora 1971 | |
| | *Gila elegans* | 15300 | 4 | y | 93 | | Beyers et al 1994 | Larver |
| | ***Heteropneustes fossilis*** | **11,798** | 4 | n | 50 | | Dutta et al 1992 | |
| | *Ictalurus furcatus* | 17000 | 4 | n | 98,1 | | Aker et al 2008 | ”Fingerling” stadie |
| | *Ictalurus punctatus* | 8900 | 2 | y | | | | |
| | ***Jordanella floridae*** | **0,235** | 9 | y | 95 | | Hermanutz 1978 | |
| | *Labeo fimbriatus* | 8500 | 2 | n | 50 | | Sreenivasan Swaminathan 1967 | |
| | ***Labeo rohita*** | **2** | 4 | n | 50 | | FMC 2019: Mishra et al 2012 | |
| | *Labeo rohita* | 4,5 | 4 | n | 50 | | Patil et David 2010 | ”Fingerling” stadie |
| | *Lepidocephalichthys thermalis* | 7750 | 2 | n | 50 | | Kumari et Nair 1978 | Juvenile |
| | ***Lepomis cyanellus*** | **130** | 4 | y | 96,8 | 1 or 2 | FMC 2019:Document 1408 FYF, 2014 | |
| | ***Lepomis gibbosus*** | **480** | 4 | n | | | Rehwoldt et al 1977 | Unge fra samme år |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Lepomis macrochirus* | 46 | 4 | y | 96,8 | 1 or 2 | FMC 2019:Document 879 FYF, 2011 | |
| | *Lepomis macrochirus* | 54 | 4 | y | 96,9 | 1 or 2 | FMC 2019:Document 314 FYF, 2001 | |
| | *Lepomis macrochirus* | 48 | 4 | n | 96,9 | | US EPA 1992 | |
| | ***Lepomis macrochirus*** | **49** | 4 | | | | Geometric mean of values above | |
| | ***Lepomis microlophus*** | **170** | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Leucaspius delineatus* | 7640 | 2 | n | | | Ardo 1974 | |
| | *Leuciscus cephalus* | 1807 | 4 | n | 20 | | Verep 2006 | |
| | *Melanotaenia fluviatilis* | 2090 | 4 | y | | | Reid et al 1995 | Voksne |
| | ***Micropterus salmoides*** | **368** | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Morone americana* | 1067 | 4 | n | | | Rehwoldt et al 1977 | Unge fra samme år |
| | ***Morone saxatilis*** | **12** | 4 | y | 94,2 | | Fujimura et al 1991 | Larver |
| | *Mystus tengara* | 8000 | 4 | n | 95 | | Chandran et al 1991 | |
| | *Mystus vittatus* | 2000 | 4 | n | 50 | | Verma et al 1984 | |
| | *Nemacheilus angorae* | 3023,7 | 4 | n | | | Gul et al 2007 | Voksne |
| | *Nothobranchius guentheri* | 2900 | 1 | y | | | Shedd et al 1999 | Små unger |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | ***Notopterus notopterus*** | **77** | 4 | n | | | Gupta et al 1994 | |
| | ***Oncorhynchus clarkii*** | **150** | 4 | n | 95 | | Post et Schroeder 1971 | |
| | *Oncorhynchus kisutch* | 720 | 4 | y | 96,8 | 1 or 2 | FMC 2019:Document 1445 FYF, 2014 | |
| | *Oncorhynchus kisutch* | 226 | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | ***Oncorhynchus kisutch*** | **403** | | | | | Geometrisk gennemsnit | |
| | *Oncorhynchus mykiss* | 39 | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Oncorhynchus mykiss* | 180 | 4 | y | 96,9 | 1 or 2 | FMC 2019:Document 306 FYF, 2001 | |
| | ***Oncorhynchus mykiss*** | **84** | | | | | Geometrisk gennemsnit | |
| | *Oncorhynchus tshawytscha* | 364 | 4 | y | 98,7 | | FMC 2019:Detrich et al 2014. 11˚C | Udført ved 11˚C. Foretrukne temperatur 0,7-8˚C |
| | *Oreochromis mossambicus* | 358,9 | 2 | n | 50 | | Sailatha et al 1981 | |
| | *Oreochromis niloticus* | 140 | 4 | n | 80 | | Liong et al 1988 | |
| | *Oryzias latipes* | 1500 | 4 | y | 96,8 | 1 or 2 | FMC 2019:Document 1407 FYF, 2014 | |
| | *Oryzias latipes* | 1800 | 2 | n | 95 | | Tsuda et al 1997 | |
| | *Pangasianodon hypophthalmus* | 7,76 | 4 | n | 50 | | FMC 2019: Shashikumar et al 2018 | Ved 30˚C. Ved 32˚ and 34˚ var LC50 henholdsvis 6,5 og 4,5 µg/l. |
| | *Pelophylax ridibundus* | 29000 | 4 | n | 25 | | Sayim 2008 | Haletudser |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Perca flavescens* | 482 | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Pimephales promelas* | 28000 | 4 | y | 96,8 | 1 or 2 | FMC 2019:Document 1380 FYF, 2013 | |
| | *Pimephales promelas* | 27000 | 4 | y | 99,1 | 1 or 2 | FMC 2019:Document 1381 FYF, 2013 | |
| | *Pimephales promelas* | 12400 | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Pimephales promelas* | 21085 | | | | | Geometric mean of values above | |
| | *Poecilia reticulata* | 880 | 4 | n | 100 | | Pickering et al 1962 | |
| | *Pseudorasbora parva* | 14500 | 4 | n | 98 | | Li et Fan 1996 | |
| | *Pseudosphromenus cupanus* | 4594 | 2 | n | | | Jacob et al 1982 | |
| | *Ptychocheilus lucius* | 9140 | 4 | y | 93 | | Beyers et al 1994 | Larver |
| | *Puntius sophore* | 1650 | 4 | n | 30 | | Khangarot et Ray 1988 | |
| | *Puntius stigma* | 9560 | 2 | n | | | Verma et al 1984 | |
| | *Rasbora daniconius* | 4000 | 4 | n | 95 | | Singh et al Sahai 1984 | |
| | *Rhodeus sericeus ssp. amarus* | 5060 | 4 | n | 95 | | Guylas et Csanyi 1984 | |
| | *Rutilus rutilus* | 12000 | 4 | n | | | Scirocchi et D'Erme 1980 | |
| | *Salmo salar* | 33 | 2 | n | | | Keenleyside 1958 | Unge |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Salmo trutta* | 128 | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Salvelinus fontinalis* | 120 | 4 | n | 95 | | Post et Schroeder 1971 | |
| | *Salvelinus namaycush* | 99 | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Sander vitreus* | 11 | 1 | n | 95 | | Mayer et Ellersieck 1986 | |
| | *Tilapia sp.* | 45,99 | 4 | n | | | Bajet et al 2012 | ”Fingerling” stadie |
| | *Tinca tinca* | 16200 | 3 | n | | | Scirocchi et D'Erme 1980 | |
| | *Trichogaster pectoralis* | 983,2 | 4 | n | 57 | | Mohsin et al 1984 | |
| | *Umbra pygmaea* | 240 | 4 | y | 99,5 | 2 | Bender et Westman 1976 | |
| | *Zacco platypus* | 9700 | 1 | n | | | Shim &Self 1973 | |
| **Amphibia** | *Bufo americanus* | 7968 | 4 | y | 50,6 | 2 | Relyea 2004 | Haletudser. Værdien skønnet udfra fig. 1 |
| | *Bufo woodhousei ssp. fowleri* | 1900 | 1 | n | 95 | | Mayer et Ellersieck 1986 | Haletudser |
| | *Euphlyctis cyanophlyctis* | 3523 | 4 | n | 50 | | Giri et 2012 | Haletudser |
| | *Hoplobatrachus tigerinus* | 170 | 6 | n | | | Abbasi et Soni 1991 | Haletudser |
| | *Hyla versicolor* | 8751 | 4 | y | 50,6 | 2 | Relyea 2004 | Haletudser, Værdien skønnet udfra fig. 1 |
| | *Lithobates palustris = Rana p.* | 16400 | 2 | y | "Pure" | 2 | Budischak et al 2009 | Haletudser. Geometrisk gennemsnit af nederste og øverste værdi i |

| Overordnet systematiske gruppe | Art | $EC_{50}$ µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | spandet givet i artiklen |
| | *Pseudacris triseriata* | 560 | 1 | n | 95 | | Mayer et Ellersieck 1986 | Haletudser |
| | *Rana boylii* | 2137 | 4 | n | 99 | | Sparling et Fellers 2007 | Haletudser |
| | *Rana catesbeiana* | 5357 | 4 | y | 50,6 | 2 | Relyea 2004 | Haletudser, Værdien skønnet udfra fig. 1 |
| | *Rana clamitans = Lithobates c.* | 5323 | 4 | y | 50,6 | 2 | Relyea 2004 | Haletudser, Værdien skønnet udfra fig. 1 |
| | *Rana hexadactyla = Euphlyctis h.* | 0,59 | 4 | n | 50 | 2 | Khangarot et al 1985 | Haletudser |
| | *Rana limnocharis* | 2271 | 2 | n | 50 | | Pan,D.Y. et Liang 1993 | Haletudser |
| | *Rana pipiens = Lithobates p.* | 4842 | 4 | y | 50,6 | 2 | Relyea 2004 | Haletudser, Værdien skønnet udfra fig. 1 |
| | *Rana sylvaticus = Lithobates s,* | 5204 | 4 | y | 50,6 | 2 | Relyea 2004 | Haletudser, Værdien skønnet udfra fig. 1 |
| | *Rhinella arenarum* | 19200 | | n | | | Venturino et al 1992 | Larver |
| | *Xenopus laevis* | 790 | 4 | n | 90 | | Snawder et Chambers 1989 | Embryo |

**Ferskvandsorganismer**
Kronisk giftighed
*Freshwater, chronic toxicity*

| Overordnede systematiske grupper | Art | EC10 µg/l | NOEC µg/l | Valgte værdi | Varighed dage | Målt (Yes/no) | Effekt | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Cyano-bacteria** | *Anabaena flos-aquae* | 27900 | | **27900** | 3 | y | Vækstrate | 96 | RI2 | FMC 2019: Dobbins, Kendall, Porch 2012 | |
| **Alger (Algae) Chlorophyta** | *Raphidocelis subcapitata* | 4000 | | | 3 | y | Vækstrate | 96,4 | RI2 | FMC 2019: Jenkins 1993 | |
| | *Raphidocelis subcapitata* | 6500 | | | 3 | y | Vækstrate | 96 | RI2 | FMC 2019: Dobbins, Kendall and Porch 2012; | |
| | *Raphidocelis subcapitata* | | 1200 | | 2 | y | Tæthed af celler | 99 | RI2 | Yeh & Chen 2006 | |
| | *Raphidocelis subcapitata* | 8500 | | | 2 | n | Vækstrate | 95 | | Kusk et al 2018 | |
| | *Raphidocelis subcapitata* | | | **4035** | | | | | | Geometgrisk gennemsnit af værdierne ovenfor | |
| **Alger (Algae) Bacillariophyta** | *Navicula pelliculosa* | 15400 | | **15400** | 3 | y | Growth rate | 96 | RI2 | FMC 2019: Dobbins, Kendall, Porch 2012 | |
| **Macro-phyta** | *Lemna gibba* | 19900 | | **19900** | 7 | y | Growth rate | 96 | RI2 | FMC 2019: Dobbins, Kendall, Porch 2012 | |
| **Fladorme (Platyhelminthes) Trematoda** | *Echinoparyphium sp.* | 7,9 | | **7,9** | 6 h | y, initial | cercaria survival | "commercial grade" | RI2 | Hua et al. 2016 | EC10 blev estimeret udfra figur 1. Eksponering I 6 timer er rimelig da cerkarierne ikke ovelever i meget mere end 8 timer, hvis de ikke finder en vært. |

| Overordnede systematiske grupper | Art | EC10 µg/l | NOEC µg/l | Valgte værdi | Varighed dage | Målt (Yes/no) | Effekt | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Nema-tomorpha** | *Chordodes nobilii* | 0,15 |  | **0,15** | 2 | Initial | infection effectivity | #### | RI2 | Achiorno et al 2009 | De præparasitiske larver blev eksponeret for malathion i 48 timer og derefter sat sammen med Aedes aegyptii i 72 timer og infektionen observeret. Testmedier blev delvist udskiftet en gang I døgnet. |
| **Krebsdyr (Crustacea)**<br>**Branchiopoda** | *Ceriodaphnia dubia* | $8*10^{-04}$ | 0,001 | **8E-04** | 7 | y | number of offspring | 1103 g/L | 2 | FMC 2019: V.C. Franco Perina 1995 | EC$_{10}$ blev beregnet ved ekstrapolering mellem antallet af unger ved 0,00056 µg/l. Antallet af unger ved 0,00056 µg/l blev sat lig det geometriske gennemsnit af antallet I kontrollen, antallet ved 0,00032 µg/l og antallet ved 0,00056 µg/l, fordi det først er efter 0,00056 µg/l, at der sker et fald i antallet af unger. |
|  | *Daphnia magna* | 0,079 | 0,06 | 0,079 | 21 | y | juveniles/female reproductive days | 94 | 2 | FMC 2019: G. Blakemore, D. Burgess 1990 | Forfatterne beregnede en EC10 på 0,085 µg/l.<br>Men Analyse af sammenhængen |

| Overordnede systematiske grupper | Art | EC10 µg/l | NOEC µg/l | Valgte værdi | Varighed dage | Målt (Yes/no) | Effekt | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | | resulterede I en EC10 = 0,079 µg/l. Spearman rank korrelationen . var rs = -1,000 and product moment korrelation var r = -0,994, med P-værdier på henholdsvis [N = 6] 0,01 and 0,002 (tosidet) |
| | *Daphnia magna* | | 0,57 | 0,57 | 21 | y | Young produced | 99,8 | 2 | Ding et al 2019 | EC20 var 1,13 µg/l. Dette er ≈ LOEC. NOEC blev beregnet som 1,13/2. |
| | *Daphnia magna* | 0,0047 | | 0,0047 | 21 | n | Young produced | 50 | 2 | Toumi et al 2015 | |
| | *Daphnia magna* | | | **0,06** | | | | | | Geometric mean of values above | |
| **Krebsdyr (Crustacea)**<br>**Decapoda** | *Neocaridina denticulata* | | 7,2 | **7,2** | 28 | y | survival | 99,8 | 2 | Ding et al 2019 | $EC_{20}$ var 14,3 µg/l. Dette ≈ LOEC. NOEC blev beregnet ved 14,3/2. |
| **Insekter (Insecta)**<br>**Plecoptera** | *Acroneuria pacifica = Hesperoperla p.* | 0,54 | | **0,54** | 30 | n | naiads | 95 | 2 | Jensen & Gaufin 1964b | Beregnet fra data givet I figuren |
| | *Pteronarcys californica* | 3,5 | | **3,5** | 30 | n | naiads | 95 | 2 | Jensen & Gaufin 1964b | Beregnet fra data givet I figuren |
| **Fisk (Fish)** | *Brachydanio rerio* | 1994 | | **1994** | 5 | y | Hatching | 99 | 2 | Cook et al. 2005 | Koncentrationerne blev målt hver anden dag. EC10 for overlevelse var omkring 2000 µg/l. EC10 for øjediameter var lavere, men det er svært at relatere dette til effekt på populationer |

| Overordnede systematiske grupper | Art | EC10 µg/l | NOEC µg/l | Valgte værdi | Varighed dage | Målt (Yes/no) | Effekt | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | *Gila elegans* | | 990 | **990** | 32 | y | weight of Larvere | | RI2 | Beyers et al. 1994 | Forfatterne antager at der findes en tærskel værdi. Der er ikke givet nok data til kontrollere beregningerne og graden af effekt ved NOEC kan ikke vurderes. Koncentrationerne er blevet målt en gang om ugen, men det er ikke angivet om beregningerne er baseret på startkoncentrationen eller hvad. |
| | *Oncorhynchus mykiss* | 9,2 | 21 | **9,2** | 97 days, 60 days posthatch | y | survival | 94 | 2 | FMC 2019: "1989; 034 FYF" | FMC 2019 udtaler, at "goodness of fit" er lav, og at man derfor har valgt NOEC i stedet for LC10. Men korrelationen mellem koncentration og overlevelse er statistisk signifikant (rs = - 0,943, P = 0,02, tosidet og r = 0,982, P < 0,001, tosidert; N = 6). Endvidere er |

| Overordnede systematiske grupper | Art | EC10 µg/l | NOEC µg/l | Valgte værdi | Varighed dage | Målt (Yes/no) | Effekt | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | | usikkerhederne omkring NOEC snarere større, man har bare ikke mulighed for at se det. |
| | *Pimephales promelas* | | 80 | **80** | 21 | y | Weight | 96 | 2 | EFSA, 2019: "2011; 1058 FYF" | Svarer til ca. 9% effekt |
| | *Pseudorasboa parva* | | 237 | **237** | 28 | y | survival | 99,8 | 2 | Ding et al 2019 | EC20 var 473 µg/l. This ≈ LOEC. NOEC NOEC blev beregnet ved 473/2 |
| | *Ptychocheilus lucius* | | 1680 | **1680** | 32 | y | survival and weight of Larvere | | RI2 | Beyers et al. 1994 | Forfatterne antager at der findes en tærskel værdi. Der er ikke givet nok data til kontrollere beregningerne og graden af effekt ved NOEC kan ikke vurderes. Koncentrationerne er blevet målt en gang om ugen, men det er ikke angivet om beregningerne er baseret på startkoncentrationen eller hvad. |
| Padder (Amphibia) | *Rana catesbeiana* | 263 | | **263** | 28 | n | Tadpoles, days to first | 96 | RI2 | Fordham et al 2001 | Koncentrationerne i stamopløsningerne blev målt, og |

| Overordnede systematiske grupper | Art | EC10 µg/l | NOEC µg/l | Valgte værdi | Varighed dage | Målt (Yes/no) | Effekt | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | recorded loss of equilibrium | | | | testmedierne blev udskiftet dagligt. |
| | *Xenopus laevis* | | 59 | **59** | 14 | y | Wet weight | 96 | RI2 | FMC 2019: "2011; 1059 FYF" | Svarer til ca. 9,2% effekt |
| | *Xenopus laevis* | not applicc able | not applicc able | | 21 | | | | | FMC 2019: "2011; 1060 FYF" | Der blev ikke set en dosis-respons |
| | *Xenopus laevis* | 1294 | | | 7 | n | embryonal malformation | 99 | RI2 | Bonfanti et al. 2004 | Testmediet blev fornyet dagligt |

**Saltvandsorganismer**
Akut giftighed
*Saltwater, acute toxicity*

| Overordnet systematisk gruppe | Art | EC50 µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| **Algae** | *Skeletonema costatum* | 15110 | 3 | y | 96 | | FMC 2019: Dobbins et al 2012, 1263 FYF, | |
| **Rotifera** | *Brachionus plicatilis* | 67000 | 1 | y | 95 | | Guzzella et al 1997 | Neonate |
| **Bløddyr (Mollyusca) Bivalvia** | *Crassostrea virginica* | 2700 | 4 | y | 96,8 | | FMC 2019: Brougher 2014, 1418 FYF | |
| | ***Katelysia opima*** | **6** | 4 | n | 50 | | Akarte et al 1986 | |
| | *Mytilus edulis* | 13400 | 2 | y | 95 | | Liu et Lee 1975 | Æg |
| | *Mytilus galloprovincialis* | 6000 | 7 | n | | | Rao et Mane 1978 | |
| **Krebsdyr (Crustacea) Amphipoda** | ***Gammarus palustris*** | **5,85** | 3 | n | | | Leight,A.K., and R.F. Van Dolah 1999 | |
| **Krebsdyr (Crustacea) Anostraca** | *Artemia salina* | 37030 | 1 | n | | | Wilkins et Metcalfe 1993 | Larver |
| **Krebsdyr (Crustacea) Mysida** | *Americamysis bahia* | 4,8 | 4 | y | 96,8 | | FMC 2019: Brougher et al 2014, 1427 FYF | |
| | *Americamysis bahia* | 2,2 | 4 | y | 94 | | FMC 2019: Forbis 1990, 036 FYF | |
| | *Americamysis bahia* | 2,1 | 4 | y | 94 | | FMC 2019: Burgess 1989, 19 FYF | |

| Overordnet systematisk gruppe | Art | EC50 µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Americamysis bahia* | 1,96 | 4 | n | 94 | | US EPA 1992 | |
| | *Americamysis bahia* | 3 | 4 | y | 71,5 | 2 | Goodman et al 1988 | |
| | ***Americamysis bahia*** | **2,6** | | | | | Geometric mean of values abovel | |
| | ***Neomysis mercedis*** | **1,4** | 4 | y | 94,2 | 2 | Brandt et al. 1993 | neonate, geometrisk gennemsnit af 2,2; 1,5; 1,4 |
| | ***Neomysis mercedis*** | **1,4** | 4 | y | 94,2 | | Brandt et al 1993 | Neonate |
| **Krebsdyr (Crustacea) Copepoda** | ***Tigriopus brevicornis*** | **7,2** | 4 | n | | | Forget et al 1998 | Nauplii |
| **Krebsdyr (Crustacea) Decapoda** | ***Cancer magister*** | **1,2** | 4 | n | 95 | 2 | Caldwell 1977 | Zoea Larver. Testmedier fornyet dagligt |
| | ***Crangon septemspinosa*** | **33** | 4 | n | | | Eisler 1969 | |
| | ***Farfantepenaeus duorarum*** | **12,5** | 2 | y | | | Bahner et Nimmo 1975 | Unge voksne |
| | ***Homarus americanus*** | **3,7** | 2 | y | 98 | 2 | Zulkosky et al 2005 | Larver |
| | *Litopenaeus stylirostris* | 34197 | 2 | n | | | Reyes et al 2002 | Larver |
| | ***Litopenaeus vannamei*** | **21,46** | 4 | n | | 2 | Salame et al 1996 | Post-Larve |
| | *Metapenaeus monoceros* | 1120 | 4 | nnn | 95 | | Reddy et Rao 1992 | Intermolt |
| | ***Pagurus longicarpus*** | **83** | 4 | n | 95 | | Eisler 1969Reddy et Rao 1992Salame et al 1996 | Intermolt |

| Overordnet systematisk gruppe | Art | EC50 µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | ***Palaemon macrodactylus*** | **9** | 4 | n | 95 95 | | Schoettger 1970 | Intermolt |
| | *Palaemonetes pugio* | 7,7 | 4 | n | 95 | 2 | Key et al 19981969 | Nyklækkede |
| | *Palaemonetes vulgaris* | **82** | 4 | n | 95 | 2 | Eisler 1969Key et al 1998Schoettger 1970 | Nyklækkede |
| | *Palemonetes pugio* | 9,1 | 4 | y | "Technical grade" | 2 2 | Key 1995 | Nyklækkede |
| | ***Palemonetes pugio*** | **8,4** | | | | | Geometrisk gennemsnit | |
| | ***Penaeus monodon*** | **392** | 4 | n | | 2 | Rao et al 1988 | Intermolt |
| | ***Uca marionis*** | **60** | 1 | n | | 2 | Yeragi,S.G., and V.A. Koli | |
| **Insekter (Insecta)**<br>**Diptera** | *Culicoides sp.* | 87,9 | 1 | n | | | Kline et al 1985 | Larver |
| **Pighude (Echinodermata)** | *Echinometra mathaei* | 9790 | 4 | n | | | Verma et al 1982 | |
| **Fisk (Fish)** | ***Anguilla rostrata*** | **829** | 4 | n | | | Eisler 1970Verma et al 1982Kline et al 1985 | |
| **Fisk (Fish)** | ***Aphanius fasciatus*** | **348** | 2 | n | | | Boumaiza et al 1979 | |
| **Fisk (Fish)** | ***Barbus stigma*** | **19,5** | 4 | n | | | Khillare et al Wagh 1988 | |
| | *Cyprinodon variegatus* | 47,4 | 4 | y | 96,8 | 1 or 2 | FMC 2019:Document 1039 FYF, 2011 | |
| | *Cyprinodon variegatus* | 1354 | 4 | y | 96,8 | 1 or 21 | FMC 2019:Document 880 FYF, | |
| | *Cyprinodon variegatus* | 51 | 4 | y | | 2 | Hansen & Parrish 1977 | Juvenile |

| Overordnet systematisk gruppe | Art | EC50 µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | *Cyprinodon variegatus* | 40 | 4 | y | 94 | 1 or 2 | FMC 2019:Document 018 FYF, 1989 | |
| | ***Cyprinodon variegatus*** | **60** | | | | | | Geometrisk gennemsnit af værdierne ovenfor Juvenile |
| | ***Fundulus heteroclitus*** | **22,51** | 4 | ny | 50 | 1 or 2 | Scott et al 1987 | |
| | ***Fundulus majalis*** | **250** | 4 | nn | | | Eisler 1970 | |
| | ***Fundulus similis*** | **150** | 2 | n | 95 | | Hansen 1980 | |
| | *Gasterosteus aculeatus* | 76,9 | 4 | n | 57 | | Katz 1961 | |
| | *Leiostomus xanthurus* | 550 | 2 | n | | | Butler 1964 | Juvenile |
| | ***Menidia beryllina*** | **30** | 4 | n | | | Lewis 1993 | Juvenile |
| | ***Menidia menidia*** | **125** | 4 | n | | | Eisler 1970 | Juvenile |
| | ***Mugil cephalus*** | **330** | 2 | n | 95 | | Hansen 1980 | |
| | ***Mugil curema*** | **570** | 2 | n | | | Butler 1963 | Juvenile |
| | ***Oncorhynchus tshawytscha*** | **33,7** | 4 | n | 95 | | Schoettger 1970 | |
| | *Rivulus marmoratus* | 1100 | 4 | n | | | Lewis 1993 | |
| | *Sphoeroides maculatus* | 3250 | 4 | n | | | Eisler 1970 | |
| | | | | | | | | |

| Overordnet systematisk gruppe | Art | EC50 µg/l | Varighed dage | Målt yes/no | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|
| | ***Thalassoma bifasciatum*** | **27** | 4 | n | | | Eisler 1970 | |

**Saltvandsorganismer**
Kronisk giftighed
*Saltwater, chronic toxicity*

| Overordnede systematiske grupper | Art | EC10 µg/l | NOEC µg/l | Valgte værdi | Varighed dage | Målt (Yes/no) | Effekt | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Alger (Algae) Bacillariophyseae** | *Skeletonema costatum* | 5690 | | **5690** | 3 | y | Growth rate | 96 | 2 | FMC 2019: Dobbins, Kendall, Porch 2012 | |
| **Krebsdyr (Crustacea) Mysida** | *Americamysis bahia* | 0,295 | | **0,295** | 39 | y | juveniles/ day | 96 | RI2 | FMC 2019: M.B. Claude, T.Z. Kendall, S.P. Gallagher, H.O. Krueger 2012 | |
| **Krebsdyr (Crustacea) Decapoda** | *Cancer magister* | | 0,2 | **0,2** | 69 | n | zoea survival | 95 | 2 | Caldwell 1977 | Koncentrationerne blev ikke målt, men testmedier blev udskiftet tre gange om ugen. Der ser ud til at være en NOEC for forsinkelse af hamskifte i sidste zoea stadie på 0,02 µg/l, men det er ikke overbevisende |
| **Fisk (Fish)** | *Cyprinodon variegatus* | 7,9 | 8,2 | **7,9** | 28 days post hatch | y | survival | | 2 | FMC 2019: "2011; 1072 FYF" | FMC 2019 udtaler, at "goodness of fit" er lav, og at man derfor har valgt NOEC i stedet for LC10. Men korrelationen mellem koncentration og overlevelse er statistisk signifikant (rs = - 0,883, 0,02 < P <0,05, two-tailed and |

| Overordnede systematiske grupper | Art | EC10 µg/l | NOEC µg/l | Valgte værdi | Varighed dage | Målt (Yes/no) | Effekt | Renhed % | RI | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | | r = -0,965, P<0,001 ). Endvidere er usikkerhederne omkring NOEC snarere større, man har bare ikke mulighed for at se det. |
| | *Cyprinodon variegatus* | | | | 10 (?) weeks | y | survival | | 2 (==>4) | Hansen & Parrish 1977 | Oplysningerne om udførelsen af testene er mangelfulde, så det kan være lidt svært at vurdere forsøget (tenderer mod RI4). Da studiet ovenfor er betydeligt mere troværdigt bruges det. |

**Fugle og pattedyr**
*Birds and mammals*

Det antages at både kaninerne, rotterne og fuglene i forsøgene er blevet fodret med kommercielt foder (”commercial fodder” i tabel 8 i vejledningen), da det er nemmere at få blandet stoffet i et sådant standardfoder. I rapporterne nævnes også standardfoder og ”basal ration”.
*It is assumed tha botht the mammals and the birds in the studies have been fed “commercial fodder”. This because it is more convenient to mix the substance into such a standard diet. The reports mention standard diets and “basal ration”.*

| Overordnet systematiske grupper | Art | Energi normaliseret EC10 eller NOEC, mg/kJ | Valgte værdi | EC10, mg/kg foder | NOEC, mg/kg foder | NOAEL, mg/kg lgv per dag | Dage | Renhed, % | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | | | |
| **Fugle (Aves)** | Colinus virginianus | 0,0079 | 110 | | 110 | 13,5 | 147 | 96,4 | FMC 2019: 103 FYF 1995 | 21 uger. Regressing ovaries etc. |
| | Anas platyrhynchos | 0,086 | 1200 | | 1200 | | 32 | 94 | FMC 2019: 069 FYF 1993 | Reproduktion |
| | Colinus virginianus | 0,022 | 300 | | 300 | | 147 | 94 | FMC 2019: 029 FYF | Reproduktion |

| Overordnet systematiske grupper | Art | Energi normaliseret EC10 eller NOEC, mg/kJ | Valgte værdi | EC10, mg/kg foder | NOEC, mg/kg foder | NOAEL, mg/kg lgv per dag | Dage | Renhed, % | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|
|  | Colinus virginianus | 0,016 | 218 | 218 |  |  | 28 | 94 | FMC 2019: 038 FYF 1989 | Overlevelse.<br>FMC 2019 hævder at Compliance with the OECD 206 validity criteria could not be verified" og at studiet derfor var ikke troværdigt. Men kontroldødelighed var mindre end 10% (1 fugl) og udover det var der ingen tegn på effekter i kontrollen. Der var endvidere en statistisk signifikant dosis-respons.<br>LC10 blev beregnet udfra data givet i rapporten |
| **Aves** | *Phasianus colchinus* | 0,0018 | 25,14 |  | 25,14 | 2514 ($LC_{50}$) |  |  |  |  |
|  | Species | Energy normalized $EC_{10}$ or NOEC, mg/kJ | Chosen value | $EC_{10}$, mg/kg feed | NOEC, mg/kg feed | NOAEL, mg/kg bw per day | Days | Purity, % | Reference | Comments |
| **Mammalia** | *Oryctolagus cuniculus* | 0,060 | 832,5 |  | 832,5 | 25 | 29 | 92,4 | FMC 2019: 008 FYF 1985 | Reproduction. NOEC calculated from NOAEL with factor 33,3 |

| Overordnet systematiske grupper | Art | Energi normaliseret EC10 eller NOEC, mg/kJ | Valgte værdi | EC10, mg/kg foder | NOEC, mg/kg foder | NOAEL, mg/kg lgv per dag | Dage | Renhed, % | Reference | Kommentarer |
|---|---|---|---|---|---|---|---|---|---|---|
|  | *Oryctolagus cuniculus* | 0,12 | 1665 |  | 1665 | 50 | 29 | 96 | FMC 2019: TOX-FYF 4597 2018 |  |
|  | *Rattus norvegicus* | 0,0014 | 20 |  | 20 | 1 |  |  | FMC 2019: 165 FYF 1996 | Reproduction. NOEC calculated from NOAEL with factor 20 |
|  | *Rattus norvegicus* | 0,0029 | 40 |  |  | EL10: 400 | 20 | 96 | FMC 2019: TOX-FYF4595 2018 | EC10 beregnet udfra data i rapporten og med en usikkerhedsfaktor på 10 for at tage højde for, at det er et korttidsforsøg |
|  | *Rattus norvegicus* | 0,0095 | 132 |  | 132 | 1700 | 20 | 96 | FMC 2019: TOX-FYF041 2018 | NOAEL og NOEC givet i rapporten. Standard ville være at dividere NOAEL med 10 for at skønne NOEC |
|  |  |  |  |  |  |  |  |  |  |  |

# Bilag B

NOEC værdier i muslinger.
Muslinger er valgt som kritiske fødekilde, da malathion ikke opkoncentreres gennem fødekæden. Jævnfør tabel 7 i EU vejledningen (EU 2018a) antages energiinholdet i muslinger at være 19 kJ/$g_{tørvægt}$ og vandindholdet 92% (0,92). Værdierne normaliseres ikke til lipidindholdet. Valgte værdier er mærket med fed skrift.
*NOEC values in mussels.*
*Mussels are chosen as critical diet because malathion does not biomagnify. The energy content of mussels is set at 19 kJ/$g_{dw}$ and the moisture content at 92%. Normalization to lipid content has not been employed as the lipid content of mussels is low and the substance isn't especially hydrophobic (water solubility is 143 mg/l).*

NOEC (mg/kg tørvægt) i muslinger =
energinormaliseret $NOEC_{lab\text{-}foder}$*energi i muslinger*(1-vandindhold i muslinger)

| Art/species | NOEC i muslinger/mussels mg/$kg_{dw}$ | | Studie i FMC 2019 |
|---|---:|---|---|
| *Colinus virginianus* | 12 | | 103 FYF |
| *Colinus virginianus* | 33 | | 029 FYF |
| *Colinus virginianus* | 24 | | 038 FYF |
| Geometrisk gennemsnit | **21** | | |
| *Anas platyrhynchos* | **131** | | 069 FYF |
| *Phasianus colchinus* | **2,7** | | 1249 FYF |
| *Oryctolagus cuniculus* | 91 | | 008 FYF |
| *Oryctolagus cuniculus* | 182 | | 4597 FYF |
| *Rattus norvegicus* | 2,2 | | 165 FYF |
| *Rattus norvegicus* | 44 | | 041 FYF |
| *Rattus norvegicus* | 14 | | 4595 FYF |
| Geometrisk gennemsnit | **11** | | |

# Bilag C

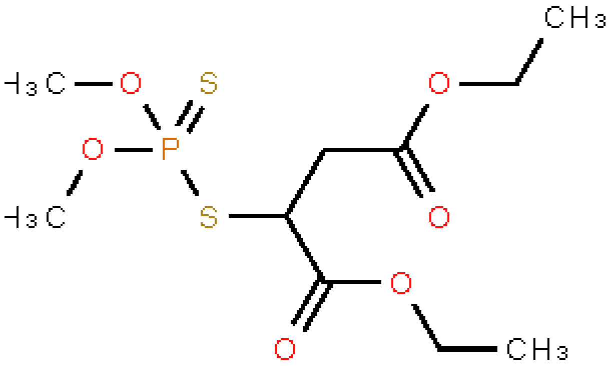
## Udtræk for malathion fra den danske QSAR database ([Danish (Q)SAR Database (dtu.dk)](#)).

Databasen udvikles og vedligeholdes af Danmarks Tekniske Universitet.

Danish (Q)SAR Database, http://qsar.food.dtu.dk Date: 09-11-2022

## (Q)SAR predicted profile

Structure (as used for QSAR prediction):



SMILES (used for QSAR prediction): C(=O)(C(CC(=O)OCC)SP(=S)(OC)OC)OCC

ID

| | | | |
|---|---|---|---|
| REACH EC Number (pre-registration, by 2013) | 204-497-7 | REACH EC Number (registration, by Dec. 2019) | |
| Registry Number | 121-75-5 | PubChem CID | |
| EU CLP Harmonized Classification* | Acute Tox. 4 *; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1 | DK-EPA / DTU QSAR-based CLP Advisory Classification | |
| REACH registration cumulated minimum annual tonnage | | US TSCA (Oct. 2021) | |
| Tox21 (2019) | Yes | ToxCast (Oct. 2021) | Yes |
| Molecular Formula | C10 H19 O6 P1 S2 | Molecular weight (g/mole) | 330.35 |
| Chemical Name | malathion | | |

*(Annex VI to CLP up to and including the 9th ATP, and including Nordic Council of Minister SPIN list for group entries)*

Melting point, Boiling point and Vapour pressure

| | | | |
|---|---|---|---|
| Melting Point (deg C) | -23.58 | Melting Point Experimental (deg C) | |
| Boiling Point (deg C) | 351.17 | Boiling Point Experimental (deg C) | 156-157 @ 0.7 mm Hg |
| Vapour Pressure (atm) | EPI.Estimated_VP_atm | Vapour Pressure Experimental (atm) | EPI.Exp_VP_atm |
| Vapour Pressure (mm Hg) | 0.000124 | Vapour Pressure Experimental (mm Hg) | 3.38E-06 |
| Vapour Pressure (Pa) | 0.01653 | Vapour pressure Subcooled Liquid (Pa) | |

*EPI MPBPVP models*

Henry's Law Constant

| | | | |
|---|---|---|---|
| HLC Bond Method (atm-m3/mole) | 8.392E-010 | HLC Group Method (atm-m3/mole) | |
| HLC Via VP/WSol (atm-m3/mole) | 6.871E-007 | HLC Via VP/WSol (Pa-m3/mole) | 0.06962 |
| Henrys Law Const. Exp db (Pa-m3/mole) | 0.000495 | Henrys Law Const. Exp db (atm- | 4.89E-009 |

*EPI HENRYWIN models*

Water Solubility

| | | | |
|---|---|---|---|
| Water solubility from Kow (mg/L) | 78.45 | Water solubility from Fragments (mg/L) | 427.53 |
| Water solubility Exp (mg/L) | 143 | Water solubility Exp Ref | BOWMAN,BT & SANS,WW (1983) |

*EPI WATERNT model*

Hydrolysis

| | | | |
|---|---|---|---|
| Hydrolysis Ka half-life pH 7 | | Hydrolysis Kb half-life pH 7 | 1324.762 |
| Hydrolysis Ka half-life pH 8 | | Hydrolysis Kb half-life pH 8 | 132.459 |

*EPI HYDROWIN model*

pKa

| | |
|---|---|
| pKa Acid | 999 |
| - Standard deviation (±) | 0 |
| pKa Base | -999 |
| - Standard deviation (±) | 0 |

*ACDLabs model*

*pKa estimate 999: no acidic moiety found. pKa estimate -999: no basic moiety found.*

Partition coefficients

| pH | 1 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|
| LogD | 2.41 | 2.41 | 2.41 | 2.41 | 2.41 | 2.41 | 2.41 |

| | | | |
|---|---|---|---|
| Minimum LogD in the pH interval 4-9 | 2.41 | Maximum LogD in the pH interval 4-9 | 2.41 |

*ACDLabs models*
*LogD: Log octanol-water partition coefficient, which for ionizable compounds varies with the pH-dependent amounts of neutral and ionized species*

| | | | |
|---|---|---|---|
| Log Koa | 9.059 | Log Kaw | -6.699 |

*EPI KOAWIN models*
*Koa: octanol-air partition coefficient. Kaw: air-water partition coefficient.*

| | | | |
|---|---|---|---|
| Log Kow | 2.29 | | |
| Log Kow Exp | 2.36 | Log Kow Exp Ref | HANSCH,C ET AL. (1995) |

*EPI WSKOW model*
*LogKow: log octanol-water partition coefficient*

| | | | |
|---|---|---|---|
| Kp (m3/ug) Mackay- | 0.00666 | Kp (m3/ug) Koa- | 0.000281 |
| Phi Junge-Pankow- | 0.194 | Phi Mackay-based | 0.347 |
| Phi Koa-based | 0.022 | | |

*EPI AEROWIN models*
*Kp: particle-gas partition coefficient. Phi: fraction of substance sorbed to atmospheric particulates*

| | | | |
|---|---|---|---|
| Koc from MCI (L/kg) | 31.27 | Log Koc from MCI | 1.4951 |
| Koc from Kow (L/kg) | 101.8 | Log Koc from Kow | 2.0076 |

*EPI KOCWIN models*
*Koc: soil adsorption coefficient of organic compounds. Kow: octanol-water partition coefficient. MCI: first order Molecular Connectivity Index*

Level III Fugacity Environmental Partitioning, emission to air, water and soil

| | Air | Water | Soil | Sediment |
|---|---|---|---|---|
| Mass Amount (%) | 0.0763 | 26 | 73.9 | 0.0814 |
| Half-Life (hr) | 3.32 | 360 | 720 | 3240 |
| Emissions (kg/hr) | 1000 | 1000 | 1000 | 0 |

*EPI Level III Fugacity Model*

| | |
|---|---|
| Persistence time (hr) | 610 |
| Persistence time (days) | 25.41667 |

*EPI Level III Fugacity Model*

Level III Fugacity Environmental Partitioning, emission only to water

| | Air | Water | Soil | Sediment |
|---|---|---|---|---|
| Mass Amount (%) | 6.95E-006 | 99.7 | 0.0026 | 0.312 |
| Half-Life (hr) | 3.32 | 360 | 720 | 3240 |
| Emissions (kg/hr) | 0 | 1000 | 0 | 0 |

*EPI Level III Fugacity Model*

| | |
|---|---|
| Persistence time (hr) | 343 |
| Persistence time (days) | 14.29167 |

*EPI Level III Fugacity Model*

Sewage Treatment Plant (STP) overall chemical mass balance using 10,000 hr

| | Total removal | Biodegradation | Sludge Adsorption | Volatilization |
|---|---|---|---|---|
| (%) | 2.76 | 0.1 | 2.66 | 0 |

*EPI STPWIN model*

Atmospheric oxidation (25 deg C)

| | OH | Ozone |
|---|---|---|
| Half-Life (d) | 0.1382 | 0 |
| Half-Life (hr) | 1.658 | |
| Overall Rate Const. (OH: E-12 cm3/molecule-sec and OZ: E-17 cm3/molecule-sec) | 77.4198 | |

*EPI AOPWIN models*

Biodegradation

| | |
|---|---|
| Biowin1 (linear model) Probability of Rapid | 1.2526 |
| Biowin2 (non-linear model) Probability of Rapid | 1 |
| Biowin3 Expert Survey Ultimate Biodegradation | 2.9033 |
| Biowin3 Expert Survey Ultimate Timeframe | weeks |
| Biowin4 Expert Survey Primary Biodegradation | 4.2944 |
| Biowin4 Exp. Survey Primary Timeframe | hours-days |
| Biowin5 (MITI linear model) Biodegradation | 0.6707 |
| Biowin6 (MITI non-linear model) Biodegradation | 0.5691 |
| Biowin7 (Anaerobic Linear) Biodegradation | 1.3006 |
| Petroleum Hydrocarbon Biodegradation Half-Life | |

*EPI BIOWIN models*

*SkinBiowin1 and Biowin2: ≥0.5: "Rapid" <0.5: "Slow"*
*Biowin3 and Biowin4: 5 ~ hours; 4 ~ days; 3 ~ weeks; 2 ~ months; 1 ~ years.*
*Biowin5 and Biowin6: ≥0.5: "Readily", <0.5: "Not readily".*

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| Not Ready Biodegradability (POS=Not Ready) | | INC_OUT | POS_IN | NEG_IN | INC_OUT |

*DTU-developed models*

Bioaccumulation

| | |
|---|---|
| BCF (L/kg wet-wt) | 16.75 |
| Log BCF (L/kg wet-wt) | 1.224 |
| Whole Body Primary Biotransformation Fisk, Fish Half-Life | 0.007579 |
| BCF Arnot-Gobas (upper trophic) Including Biotransformation | 24.39 |
| BCF Arnot-Gobas (upper trophic) Zero Biotransformation | 25.38 |
| BAF Arnot-Gobas (upper trophic) Including Biotransformation | 24.39 |
| BAF Arnot-Gobas (upper trophic) Zero Biotransformation | 26.4 |

*EPI BCFBAF models*
*BCF: Bioconcentration factor, BAF: Bioaccumulation factor*

Aquatic toxicity

| | Exp | Battery | Leadscope | SciQSAR |
|---|---|---|---|---|
| Fathead minnow 96h LC50 (mg/L) | 14.09205 | 5.942004 | 1.745494 | 10.13851 |
| Domain | | IN | IN | IN |
| Daphnia magna 48h EC50 (mg/L) | 0.00220011 | 0.7453111 | 1.328652 | 0.1619699 |
| Domain | | IN | IN | IN |
| Pseudokirchneriella s. 72h EC50 (mg/L) | 24.00017 | 9.340055 | 17.46523 | 1.214883 |
| Domain | | IN | IN | IN |

*DTU-developed models*

| | Fisk, Fish 96h | Daphnid 48h | Green Algae 96h |
|---|---|---|---|
| LC50 (Fisk, Fish) or EC50 (Daphnid and Algae) for Most Toxic Class (mg/L) | 1.39 | 0.003 | 14.993 |
| Max. Log Kow for Most Toxic Class | 5 | 5 | 6.4 |
| Most Toxic Class | Esters, Dithiophosphates | Esters, Dithiophosphates | Esters, Dithiophosphates |
| Note | | | |

*EPI ECOSAR models*
*ECOSAR Classes: Esters;Esters, Dithiophosphates*

Oral absorption

| | |
|---|---|
| Lipinski's Rule-of-five score (bioavailability) | 0 |
| Absorption from gastrointestinal tract for 1 mg dose (%) | 95 |
| Absorption from gastrointestinal tract for 1000 mg dose (%) | 50 |

*Leadscope model on Lipinski's Rule-of-five. Equation from literature on GI abs.*
*Lipinski scores of 0 or 1: The substance may be bioavailable. Lipinski scores of 2, 3 or 4: The substance may not be bioavailable.*

Skin absorption

| | |
|---|---|
| Dermal absorption (mg/cm2/event) | 0.00037 |

*EPI DERMWIN model*

Brain/blood Distribution

| | |
|---|---|
| Log brain/blood partition coefficient | -0.1886 |

*Equation from literature*
*Partitioning between the two tissues at equilibrium. >1: high, >0 to <1: medium, >-1 to <0, fair, <-1: low.*

Metabolism

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| CYP2C9 substrates (Human clinical data) | NEG | NEG_IN | NEG_IN | NEG_IN | POS_IN |
| CYP2D6 substrates (Human clinical data) | NEG | NEG_IN | NEG_IN | NEG_IN | NEG_IN |

*DTU-developed models*

Acute toxicity in Rodents

| | LD50 (mg/kg/d) | Reliability Index |
|---|---|---|
| Rat Oral | 1600 | 0.58 |
| Rat Intraperitoneal | 120 | 0.59 |
| Mouse Oral | 1100 | 0.39 |
| Mouse Intraperitoneal | 920 | 0.38 |
| Mouse Intravenous | 210 | 0.76 |
| Mouse Subcutaneous | 120 | 0.57 |

*ACDLabs models*
*Reliability index: <0.3 = Not reliable prediction quality; 0.3-0.5 = borderline prediction quality; 0.5-0.75 = moderate prediction quality; >0.75 = high prediction quality.*

MRDD in Humans

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| MRDD in Humans ≤ 2.69 mg/kg-bw/d | | NEG_IN | INC_OUT | NEG_IN | NEG_IN |

*DTU-developed models*
*Model based on data on pharmaceuticals. Maximum recommended daily dose in pharmaceutical clinical trials employing primarily oral route of exposure and daily treatments, usually for 3-12 months.*

Irritation and Sensitization

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| Severe Skin Irritation in Rabbit | | NEG_IN | INC_OUT | NEG_IN | NEG_IN |
| Allergic Contact Dermatitis in Guinea Pig and Human* | N/A | INC_OUT | POS_IN | NEG_IN | INC_OUT |
| Respiratory Sensitisation in Humans | | NEG_OUT | INC_OUT | NEG_IN | INC_OUT |

*DTU-developed models*
**Based on commercial training set*

| | VEGA | ADI |
|---|---|---|
| Skin Sensitization (CAESAR) | NEG_Low | 0 |

*CAESAR skin sensitization model is version 2.1.6 contained in VEGA command line version 1.1.2 BETA 5 with calculation core version 1.2.4*
*Prediction: POS = Sensitizer, NEG = Non-sensitizer, SUSP.POS = Suspected sensitizer, POSS.NEG = Possible Non-sensitizer, Exp = experimental value, Good = Good reliability, Mod = Moderate reliability, Low = Low reliability.*

| | |
|---|---|
| Protein binding by OASIS, alerts in: | |
| - parent only | (Thio)Phosphates |
| - metabolites from skin metabolism simulator only | (Thio)Phosphates |
| - metabolites from auto-oxidation simulator only | |
| Protein binding by OECD, alerts in: | |
| - parent only | No alert found |
| - metabolites from skin metabolism simulator only | No alert found |
| - metabolites from auto-oxidation simulator only | |
| Protein binding potency Cys (DRPA 13%), alerts in: | |
| - parent only | DPRA less than 9% (DPRA 13%) >> Non- |

| | |
|---|---|
| | Conjugated carboxylic acids and esters (non reactive) |
| - metabolites from skin metabolism simulator only | DPRA less than 9% (DPRA 13%) >> Alcohols; DPRA less than 9% (DPRA 13%) >> Non-Conjugated carboxylic acids and esters (non reactive) |
| - metabolites from auto-oxidation simulator only | |
| Protein binding potency Lys (DRPA 13%), alerts in: | |
| - parent only | DPRA less than 9% (DPRA 13%) >> Non-Conjugated carboxylic acids and esters (non reactive) |
| - metabolites from skin metabolism simulator only | DPRA less than 9% (DPRA 13%) >> Alcohols; DPRA less than 9% (DPRA 13%) >> Non-Conjugated carboxylic acids and esters (non reactive); DPRA less than 9% (DPRA 13%) >> Nonionic surfactants |
| - metabolites from auto-oxidation simulator only | |
| Keratinocyte gene expression, alerts in: | |
| - parent only | Not possible to classify according to these rules |
| - metabolites from skin metabolism simulator only | Not possible to classify according to these rules |
| - metabolites from auto-oxidation simulator only | |
| Protein binding potency GSH, alerts in: | |
| - parent only | Not possible to classify according to these rules (GSH) |

*OECD QSAR Toolbox v.4.1 profilers*

*Profiler predictions are supporting information to be used together with the relevant QSAR predictions*

Endocrine and Molecular Endpoints

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| Estrogen Receptor α Binding, Full training set (Human *in vitro*) | NEG | NEG_IN | NEG_IN | NEG_IN | POS_IN |
| Estrogen Receptor α Binding, Balanced Training Set (Human *in vitro*) | NEG | NEG_IN | NEG_IN | NEG_IN | NEG_IN |
| Estrogen Receptor α Activation (Human *in vitro*) | | NEG_IN | INC_OUT | NEG_IN | NEG_IN |
| Estrogen Receptor Activation, CERAPP data (*in vitro*) | NEG | N/A | N/A | NEG_IN | N/A |
| Androgen Receptor Inhibition | NEG | NEG_IN | NEG_IN | NEG_IN | NEG_IN |

|  | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| (Human *in vitro*) |  |  |  |  |  |
| Androgen Receptor Binding, CoMPARA data (*in vitro*) | NEG | N/A | N/A | NEG_IN | N/A |
| Androgen Receptor Inhibition, CoMPARA data (*in vitro*) | NEG | N/A | N/A | NEG_IN | N/A |
| Androgen Receptor Activation, CoMPARA data (*in vitro*) | NEG | N/A | N/A | NEG_IN | N/A |
| Thyroperoxidase (TPO) inhibition QSAR1 (Rat *in vitro*) | POS | N/A | N/A | NEG_OUT | N/A |
| Thyroperoxidase (TPO) inhibition QSAR2 (Rat *in vitro*) | POS | N/A | N/A | NEG_OUT | N/A |
| Sodium/iodide symporter (NIS), higher sensitivity |  | N/A | N/A | NEG_IN | N/A |
| Sodium/iodide symporter (NIS), higher specificity |  | N/A | N/A | NEG_IN | N/A |
| Thyroid Receptor α Binding (Human *in vitro*) |  |  |  |  |  |
| mg/L |  |  | 52841.4 | 4745.745 | 951.2055 |
| µM |  |  | 159955.8 | 14365.81 | 2879.387 |
| Positive for $IC_{50} \leq 10$ µM |  |  |  |  |  |
| Positive for $IC_{50} \leq 100$ µM |  |  |  |  |  |
| Domain |  | OUT | OUT | OUT | OUT |
| Thyroid Receptor β Binding (Human *in vitro*) |  |  |  |  |  |
| mg/L |  |  | 10689.92 | 270.8846 | 142.7823 |
| µM |  |  | 32359.38 | 819.9927 | 432.2151 |
| Positive for $IC_{50} \leq 10$ µM |  |  |  |  |  |
| Positive for $IC_{50} \leq 100$ µM |  |  |  |  |  |
| Domain |  | OUT | OUT | OUT | OUT |
| Arylhydrocarbon (AhR) Activation – Rational final model (Human *in vitro*) |  | N/A | N/A | NEG_IN | N/A |
| Arylhydrocarbon (AhR) Activation – Random final model (Human *in vitro*) |  | N/A | N/A | NEG_IN | N/A |
| Pregnane X Receptor (PXR) Binding (Human *in vitro*) | N/A | INC_OUT | INC_OUT | POS_OUT | INC_OUT |
| Pregnane X Receptor (PXR) Binding (Human *in vitro*) NEW |  | N/A | N/A | INC_OUT | N/A |
| Pregnane X Receptor (PXR) Activation (Human *in vitro*) | NEG | N/A | N/A | NEG_OUT | N/A |
| Pregnane X Receptor (PXR) Activation (Rat *in vitro*) | NEG | N/A | N/A | NEG_IN | N/A |
| CYP3A4 Induction (Human *in vitro*) | NEG | N/A | N/A | NEG_IN | N/A |
| Constitutive Androstane Receptor (CAR) Activation at max. 20 µM (*in vitro*) |  | N/A | N/A | NEG_IN | N/A |

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| Constitutive Androstane Receptor (CAR) Activation at max. 50 µM (*in vitro*) | | N/A | N/A | NEG_IN | N/A |
| Constitutive Androstane Receptor (CAR) Inhibition at max. 20 µM (*in vitro*) | | N/A | N/A | NEG_IN | N/A |
| Constitutive Androstane Receptor (CAR) Inhibition at max. 50 µM (*in vitro*) | | N/A | N/A | NEG_IN | N/A |

*DTU-developed models*

| | |
|---|---|
| Estrogen Receptor Binding, alerts in: | |
| - parent only | Non binder, non cyclic structure |
| - metabolites from *in vivo* Rat metabolism simulator only | Non binder, non cyclic structure |
| - metabolites from Rat liver S9 metabolism simulator only | Non binder, non cyclic structure |
| rtER Expert System - USEPA, alerts in: | |
| - parent only | No alert found |
| - metabolites from *in vivo* Rat metabolism simulator only | No alert found |
| - metabolites from Rat liver S9 metabolism simulator only | No alert found |

*OECD QSAR Toolbox v.4.2 profilers*
*Profiler predictions are supporting information to be used together with the relevant QSAR predictions*

Developmental Toxicity

| | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|
| Teratogenic Potential in Humans | NEG_IN | NEG_IN | NEG_IN | NEG_IN |

*DTU-developed models based on commercial training set*

Genotoxicity - Structural Alerts for DNA Reactivity

| | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|
| Ashby Structural Alerts | POS_IN | POS_IN | POS_IN | POS_IN |

*DTU-developed models based on commercial training set*

| | |
|---|---|
| DNA binding by OASIS, alerts in: | |
| - parent only | Alkylphosphates, Alkylthiophosphates and Alkylphosphonates |
| DNA binding by OECD, alerts in: | |
| - parent only | No alert found |

*OECD QSAR Toolbox v.4.2 profilers*
*Profiler predictions are supporting information to be used together with the relevant QSAR predictions*

*In vitro* Genotoxicity - Bacterial Reverse Mutation Test (Ames test)

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| Ames test in S. typhimurium (*in vitro*) | NEG | NEG_IN | NEG_IN | NEG_IN | NEG_OUT |
| *Direct Acting Mutagens (without S9) | N/A | POS_OUT | INC_OUT | POS_IN | NEG_OUT |
| *Base-Pair Ames Mutagens | N/A | NEG_IN | INC_OUT | NEG_IN | NEG_IN |
| *Frameshift Ames Mutagens | N/A | NEG_OUT | INC_OUT | INC_OUT | NEG_IN |
| *Potent Ames Mutagens, Reversions ≥ 10 Times Controls | N/A | INC_OUT | INC_OUT | INC_OUT | INC_OUT |

*DTU-developed models*
* The four models (Direct Acting mutagens (without S9), Base-Pair Ames Mutagens, Frameshift Ames Mutagens, Potent Ames Mutagens) should not be used to determine if substances are Ames mutagens, but can be used for indication of mechanism or potency for cases where the main Ames model (Ames test in S. typhimurium (*in vitro*)) is POS_IN.

| | VEGA | Mut. / Non-mut. scores | Used models |
|---|---|---|---|
| Mutagenicity consensus | NEG | 0 / 1 | 3 |

*Mutagenicity (Ames) consensus model version 1.0.2 contained in VEGA version 1.1.4 with calculation core version 1.2.4*
*Prediction: POS = Mutagenic, NEG = Non-mutagenic.*

VEGA

| ISS | CAESAR | SarPy | KNN |
|---|---|---|---|
| NEG_Exp | NEG_Exp | NEG_Exp | NEG_Low |

*Four individual models in mutagenicity consensus model version 1.0.2 contained in VEGA version 1.1.4 with calculation core version 1.2.4*
*Prediction: POS = Mutagenic, NEG = Non-mutagenic, SUSP.POS = Suspected mutagenic, POSS.NEG = Possible Non-mutagenic, Exp = experimental value, Good = Good reliability, Mod = Moderate reliability, Low = Low reliability.*

| DNA alerts for AMES by OASIS, alerts in: | |
|---|---|
| - parent only | No alert found |
| *In vitro* mutagenicity (Ames test) alerts by ISS, alerts in: | |
| - parent only | No alert found |

*OECD QSAR Toolbox v.4.2 profilers*
*Profiler predictions are supporting information to be used together with the relevant QSAR predictions*

Other *in vitro* Genotoxicity Endpoints

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| Chromosome Aberrations in Chinese Hamster Ovary (CHO) Cells* | N/A | POS_IN | POS_IN | NEG_IN | POS_IN |
| Chromosome Aberrations in Chinese Hamster Lung (CHL) Cells | POS | POS_IN | POS_IN | NEG_OUT | POS_IN |
| Mutations in Thymidine Kinase Locus in Mouse Lymphoma Cells | | NEG_OUT | INC_OUT | NEG_IN | INC_OUT |
| Mutations in HGPRT Locus in Chinese Hamster Ovary (CHO) Cells | | INC_OUT | INC_OUT | NEG_IN | POS_IN |
| Unscheduled DNA Synthesis (UDS) in Rat Hepatocytes | | NEG_OUT | INC_OUT | INC_OUT | NEG_IN |
| Syrian Hamster Embryo (SHE) Cell Transformation | | INC_OUT | INC_OUT | NEG_IN | POS_IN |

*DTU-developed models*
**Based on commercial training set*
*HGPRT: Hypoxanthine-guanine phosphoribosyltransferase*

| | |
|---|---|
| DNA alerts for CA and MNT by OASIS, alerts in: | |
| - parent only | Alkylphosphates, Alkylthiophosphates and Alkylphosphonates |
| Protein binding alerts for Chromosomal aberration by OASIS, alerts in: | |
| - parent only | No alert found |

*OECD QSAR Toolbox v.4.2 profilers*
*CA: Chromosomal aberration, MNT: Micronucleus test*
*Profiler predictions are supporting information to be used together with the relevant QSAR predictions*

*In vivo* Genotoxicity Endpoints

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| Sex-Linked Recessive Lethal (SLRL) Test in Drosophila m. | NEG | NEG_IN | NEG_IN | NEG_OUT | NEG_IN |
| Micronucleus Test in Mouse Erythrocytes | POS | POS_IN | POS_IN | NEG_IN | POS_IN |
| Dominant Lethal Mutations in Rodents | | POS_IN | INC_OUT | POS_IN | POS_IN |
| Sister Chromatid Exchange in Mouse Bone Marrow Cells | | INC_OUT | INC_OUT | NEG_IN | POS_IN |
| Comet Assay in Mouse | | INC_OUT | INC_OUT | NEG_IN | POS_IN |

*DTU-developed models*

| *In vivo* mutagenicity (Micronucleus) alerts by ISS, alerts in: | |
|---|---|
| - parent only | H-acceptor-path3-H-acceptor |

*OECD QSAR Toolbox v.4.2 profilers*
*Profiler predictions are supporting information to be used together with the relevant QSAR predictions*

Carcinogenicity

| | E Ultra | Leadscope |
|---|---|---|
| FDA RCA Cancer Male Rat | NEG_IN | NEG_IN |
| FDA RCA Cancer Female Rat | NEG_IN | NEG_IN |
| FDA RCA Cancer Rat | NEG_IN | NEG_IN |
| FDA RCA Cancer Male Mouse | INC_IN | NEG_IN |
| FDA RCA Cancer Female Mouse | NEG_IN | NEG_IN |
| FDA RCA Cancer Mouse | NEG_IN | NEG_IN |
| FDA RCA Cancer Rodent | NEG_IN | NEG_IN |

*Commercial models from CASE Ultra and Leadscope*
*FDA RCA: Data from US Food and Drug Administration as part of Research Cooperation Agreement*

| Carcinogenicity (genotox and nongenotox) alerts by ISS, alerts in: | |
|---|---|
| - parent only | No alert found |
| Oncologic Primary Classification, alerts in: | |
| - parent only | Organophosphorus Type Compounds |

*OECD QSAR Toolbox v.4.2 profilers*
*Profiler predictions are supporting information to be used together with the relevant QSAR predictions*

| | Exp | Battery | CASE Ultra | Leadscope | SciQSAR |
|---|---|---|---|---|---|
| Liver Specific Cancer in Rat or Mouse | | INC_OUT | INC_OUT | NEG_IN | POS_IN |

*DTU-developed models*

Abbreviations
INC: inconclusive. A definite call within the defined applicability domain could not be made.
NEG: negative
POS: positive
IN: inside applicability domain
OUT: outside applicability domain
Exp: Experimental values, from EpiSuite experimental databases or DK DTU QSAR models training sets.
N/A: Not applicable, either because training set data cannot be released for commercial or proprietary models / training sets, or because the model was not developed in a given QSAR software (i.e. a given prediction is not available as the model version does not exist).

Important notes
This is an automatically generated report from the Danish (Q)SAR Database, http://qsar.food.dtu.dk.

For predictions from CASE Ultra, Leadscope, SciQSAR as well as the Acute toxicity in rodent from ACDLabs information on the software versions can be found in the QMRFs. For the other predicted properties the software versions are:
EPI MPBPWIN v1.43
EPI HENRYWIN v3.20
EPI WSKOW v1.42
EPI WATERNT v1.01
EPI KOAWIN v1.10
EPI AEROWIN v1.00
EPI KOCWIN v2.00
EPI Level III Fugacity Model (EPI Suite v4.11)
EPI STPWIN (EPI Suite v4.11)
EPI AOPWIN v1.92
EPI BIOWIN v4.10
EPI BCFBAF v3.01
EPI ECOSAR v1.11
EPI DERMWIN v2.02
ACD/ ToxSuite 2.95.1 Ionization\pKa
ACD/ ToxSuite 2.95.1 Ionization\ LogD
ACD/ ToxSuite 2.95.1

It is recommended to run the latest version of the EPI Suite Programs in preference of the predictions given in this document when these endpoints are of importance and new versions have been released from the United States Environmental Protection Agency in comparisons. EPI Suite can be downloaded from the US EPA homepage: http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm
For further information on the applied systems, see the following homepages:
Case Ultra: http://www.multicase.com/case-ultra
Leadscope: http://www.leadscope.com/
SciQSAR: http://lhasa-llc.com/
ToxSuite: http://www.acdlabs.com/

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