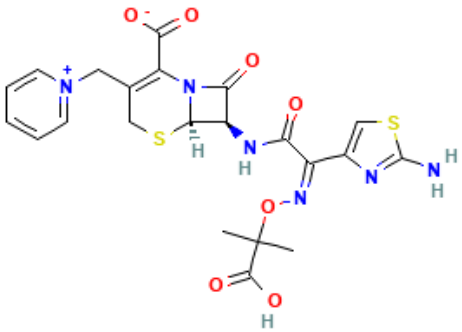
Miljø- og
Ligestillingsministeriet
Miljøstyrelsen

Fastsættelse af kvalitetskriterier for vandmiljøet

Ceftazidim

CAS nr. 72558-82-8

(inkl. ceftazidim pentahydrat, 78439-06-2)



Vandkvalitetskriterium	$VKK_{ferskvand}$	0,5 µg/l
Vandkvalitetskriterium	$VKK_{saltvand}$	0,5 µg/l
Korttidsvandkvalitetskriterium	$KVKK_{ferskvand}$	Ikke muligt
Korttidsvandkvalitetskriterium	$KVKK_{saltvand}$	Ikke muligt
Sedimentkvalitetskriterium	$SKK_{ferskvand}$	Ikke muligt
Sedimentkvalitetskriterium	$SKK_{saltvand}$	Ikke muligt
Biota-kvalitetskriterium, sekundær forgiftning	$BKK_{sek.forgiftn.}$	Ikke relevant
Biota-kvalitetskriterium, human konsum	HKK	Ikke relevant

Februar 2025

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, 2018) 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 den 22. juli 2024.

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).

AA-EQS for water
Background reports or detailed description of the data for direct effects of ceftazidime for aquatic organisms, presented in appendix A, have not been available (reliability score 4) and can therefore not be used to determined AA-EQS.

A PNEC-MIC of 0.5 µg/l has been determined for ceftazidime in a publication from Bengtsson-Palme & Larsson (2016). In comparison, they note a PNEC of 1.3 µg/l based on ecotoxicological data (NOEC of 13 µg/l for *Anavaena flos-aquae* (appendix A) and an assessment factor of 10).

Since no AA-EQS can be determined from reliable data, and since the PNEC noted in Bengtsson-Palme & Larsson (2016) is higher than the derived PNEC-MIC, AA-EQS is set equal to PNEC-MIC.

AA-EQS = PNEC-MIC = 0.5 µg/l

MAC-EQS for water
No reliable acute data is available for direct effects of ceftazidime for aquatic organisms. Therefore, no MAC-EQS can be determined.

QS for sediment
Following TGD (EU, 2018) a QS for sediment must be derived if log K_{ow} or log K_{oc} ≥3, or there is other evidence of accumulation in sediment or evidence of high toxicity towards sediment-dwelling organisms. For ceftazidime, log K_{ow} (1.15) and K_{oc} values (3.9 and 4.6) have only been found using (Q)SAR, but due to uncertainty in the (Q)SAR results (both CAS no. 72558-82-8 and 78439-06-2 give the exact same results), a QS for sediment is not derived.

QS for secondary poisoning
The criteria for setting a QS for secondary poisoning is not fulfilled since log K_{ow} < 3 and BCF (and BAF) < 100, and no other evidence has been found, that suggest a potential for secondary poisoning of ceftazidime.

QS for human health
Ceftazidime has no harmonized classifications. It has some self-classifications, where Acute Tox. 1 (H300) would be relevant if the substance also has the potential for bioaccumulation, since this is not the case for ceftazidime, the criteria for deriving a QS for human health is not met.

QS_{water} based on $QS_{sec.\ pois.}$ and $QS_{human\ health}$
Since no QS for secondary poisoning or human health has been determined no QS_{water} is calculated.

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

$AA\text{-}EQS_{freshwater}$	= 0.5 µg/l
$AA\text{-}EQS_{saltwater}$	= 0.5 µg/l
$MAC\text{-}EQS_{freshwater}$	Not possible
$MAC\text{-}EQS_{saltwater}$	Not possible
$QS_{sediment,\ freshwater}$	Not possible
$QS_{sediment,\ saltwater}$	Not possible
$QS_{sec.\ pois.}$	Not relevant
$QS_{human\ health}$	Not relevant

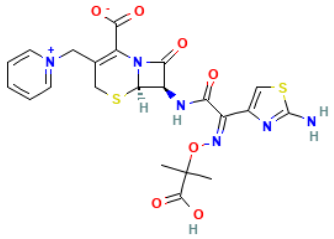
1 Indledning

Identiteten af ceftazidim fremgår af tabel 1.1.

Ceftazidim er et antibiotika, som anvendes ved behandling af svære bakterielle infektioner eks. lungebetændelse, hjernehindebetændelse, knogle- og ledinfektioner, komplicerede urinvejsinfektioner m.m.. Ceftazidim virker på både Gram-positive og Gram-negative bakterier (hører under gruppen af cephalosporiner), hvor det går ind og hæmmer/blokerer syntesen af bakteriens cellevæg, hvilket resultere i bakteriecellelyse og -død (produktresume.dk).

Ceftazidim anvendes også i kombination med aktivstoffet avibactam, en non-β-lactam β-lactamase-hæmmer, for nogle bakterielle infektioner så som komplicerede urinvejsinfektioner og lungebetændelse (erhvervet efter hospitalsindlæggelse eller efter intubering) (DrugBank.com (for stoffet avibactam); Medicin.dk (for stoffet Zavicatfa, komb. af ceftazidim og avibactam)).

Tabel 1.1. Identitet af ceftazidim

IUPAC navn	(6R,7R)-7-[[(2Z)-2-(2-amino-1,3-thiazol-4-yl)-2-(2-carboxypropan-2-yloxyimino)acetyl]amino]-8-oxo-3-(pyridin-1-ium-1-ylmethyl)-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate
Strukturformel	
CAS nr.	72558-82-8
EINECS nr.	276-715-9
Kemisk formel	$C_{22}H_{22}N_6O_7S_2$
SMILES	CC(C)(C(=O)O)ON=C(C1=CSC(=N1)N)C(=O)NC2C3N(C2=O)C(=C(CS3)C[N+]4=CC=CC=C4)C(=O)[O-]
Harmoniseret klassificering	Ceftazidim har ikke nogen harmoniserede klassificeringer.
Selvklassificering ECHA (2023), C&L Inventory	<u>Størstedelen har angivet følgende:</u> Skin Sens. 1, H317 (Kan forårsage allergisk hudreaktion) Resp. Sens. 1, H334 (Kan forårsage allergi- eller astmasymptomer eller åndedrætsbesvær ved indånding) Acute Tox. 1, H300 (Livsfarlig ved indtagelse) <u>Et mindretal har angivet følgende:</u> Aquatic Acute 1, M-factor = 10, H400 (Meget giftig for vandlevende organismer)

	Aquatic Chronic 1, M-factor = 1, H410 (Meget giftig med langvarige virkninger for vandlevende organismer) Eye Irrit. 2, H319 (Forårsager alvorlig øjenirritation)

Ceftazidim fremgår flere steder også som ceftazidim pentahydrat (CAS 78439-06-2), som har den kemiske formel $C_{22}H_{32}N_6O_{12}S_2$. Det europæiske medicinagenturs (EMA) komite for medicinske produkter til human brug (CHMP) har foretaget vurderinger af produktet Zavicefta, som indeholder både ceftazidim og avibactam som aktivstoffer. I CHMP's vurderingsrapporter (CHMP 2016; 2020) er ceftazidim angivet med CAS 78439-06-2 (ceftazidim pentahydrat). Ligeledes angives på DrungBank.com (for stoffet ceftazidim) at ceftazidim pentahydrat er den eksakte ingrediens som ofte anvendes i lægemidler indeholdende ceftazidim. Derfor er ceftazidim pentahydrat også inkluderet i dette datablad.

2 Fysisk kemiske egenskaber

De fysisk kemiske egenskaber for ceftazidim fremgår af tabel 2.1.

Den Danske (Q)SAR Database er anvendt til at estimere de fleste fysiske-kemiske egenskaber, da der ikke er fundet øvrige data herfor i litteratursøgningen. Ved anvendelse af CAS nr. 72558-82-8 i den Danske (Q)SAR Database for ceftazidim fås resultater med molekyleformlen $C_{22}H_{23}N_6O_7S_2$, hvilket indeholder ét H-atom mere end molekyleformlen fundet øvrige steder for stoffet. Samme molekyleformel angives, hvis CAS nr. 78439-06-2 for ceftazidim pentahydrat anvendes, som ellers indeholder en del flere H-og O-atomer end ceftazidim. Derfor bør der tages et vis forbehold for (Q)SAR resultaterne.

Tabel 2.1. Fysisk kemiske egenskaber for ceftazidim [og ceftazidim pentahydrat]

Parameter	**Værdi**	**Reference**
Molekylevægt, M_w ($g \cdot mol^{-1}$)	546,6	Pubchem
Smeltepunkt, T_m (ºC)	349,84 [a]	Dansk (Q)SAR Database
Kogepunkt, T_b (ºC)	852,33 [a]	Dansk (Q)SAR Database
Damptryk, P_v (Pa)	$3{,}09 \times 10^{-19}$ [a]	Dansk (Q)SAR Database
Henry's konstant, H ($Pa \cdot m^3 \cdot mol^{-1}$)	$4{,}63 \times 10^{-18}$ [a]	Dansk (Q)SAR Database
Vandopløselighed, S_w ($mg \cdot L^{-1}$)	36,59 [a] [>1000]	Dansk (Q)SAR Database CHMP, 2016; 2020
Dissociationskonstant, pK_a	1,6 [a]	Dansk (Q)SAR Database
Octanol/vand fordelingskoefficient, log K_{ow}	1,15 [-2,2]	Dansk (Q)SAR Database CHMP, 2016; 2020
Sediment/vand fordelingskoefficient, normaliseret til organisk karbon, K_{oc} ($L \cdot kg^{-1}$)	37.050 [a,b] 7.476 [a,c] [29,2 [d]] [785 [e]]	Dansk (Q)SAR Database Dansk (Q)SAR Database CHMP, 2016; 2020 CHMP, 2016; 2020

[a] Estimeret værdi
[b] Bestemt ved MCI (first order Molecular Connectivity Index)
[c] Bestemt ud fra K_{ow}
[d] ved sediment med lav organisk karbon indhold (præcist indhold angives ikke)
[e] ved sediment med høj organisk karbon indhold (præcist indhold angives ikke)

3 Skæbne i miljøet

3.1 Nedbrydelighed

Der er ikke fundet eksperimentelle data for nedbrydelighed for ceftazidim.

For ceftazidim pentahydrat er halveringstider ved hydrolyse beregnet til 495, 433 og 35,4 timer ved 25 °C for hhv. pH 5, 7 og 9. Dertil er stoffet vurderet som ikke let bionedbrydeligt da under 2,1% blev mineraliseret ved en 28-dags test (CHMP, 2016; 2020).

Den Danske (Q)SAR Database estimerer ligeledes, at stoffet ikke er let bionedbrydeligt.

3.2 Bioakkumulering

Der er ikke fundet eksperimentelle data for bioakkumulering for hverken ceftazidim eller ceftazidim pentahydrat.

Den Danske (Q)SAR Database estimerer en BCF på 3,16 l/kg vådvægt. Anvendes Arnot-Gobas er både BCF og BAF angivet til 1,97-2,4 l/kg vådvægt. Disse resultater viser, at stoffet har et meget lavt potentiale for at bioakkumulere.

3.3 Naturlig forekomst

Ceftazidim forekommer ikke naturligt i miljøet.

4 Toksicitetsdata

Troværdigheden af studierne er vurderet ved tildelingen af en CRED (Criteria for Reporting and Evaluating Ecotoxicity Data) score fra 1 til 4 (Moermond et al., 2016). Score 1 angiver, at studiet kan anvendes uden forbehold, mens score 2 angiver at studiet kan anvendes med forbehold, f.eks. at der er tilstrækkelige oplysninger, selvom studiet ikke er udført i forhold til guideline. Studier som ikke er tilstrækkeligt beskrevet tildeles score 3 eller 4, hvor score 4 tildeles studier, hvor det ikke er muligt at vurdere kvaliteten og dermed troværdigheden. Estimeret data ved QSAR angives ligeledes en score 4, men data herfra kan anvendes supplerende.

4.1 Toksicitet over for vandlevende organismer

I bilag A er sammenstillet data fundet for kroniske og akutte effekter af ceftazidim og ceftazidim pentahydrat over for ferskvandslevende organismer. Der er ikke fundet data for saltvandslevende organismer. Overvejende er data fundet for ceftazidim pentahydrat, og der kan derved ikke laves en sammenligning med ceftazidim. Al data er tildelt en troværdighedsscore på 4, hvorfor det ikke kan anvendes i beregningerne af et vandkvalitetskriterie (VKK).

QSAR data er ikke angivet i bilag A grundet stor usikkerhed (se afsnit 2). Den Danske (Q)SAR Database angiver eks. resultater for akvatisk akut toksicitet fra tre forskellige modeller. For både fisk og krebsdyr er resultaterne uden for domænet, men for algen er resultaterne inden for domænet, men de tre modeller giver vidt forskellige resultater (hhv. 0,76, 665,7 og 1330,7 mg/l), som øger usikkerheden ved at anvende dem.

4.2 Toksicitet over for sedimentlevende organismer

Der er ikke fundet data for sedimentlevende organismer.

4.3 Toksicitet over for pattedyr og fugle

Der er ikke fundet data for pattedyr eller fugle.

4.4 Toksicitet over for mennesker

Ceftazidim er et antibiotika, som kun anvendes, når det er nødvendigt for medicinsk behandling. Derfor foreligger der ikke nogen værdi for et acceptabelt daglig indtag (ADI), et tolerabelt daglig indtag (TDI) eller øvrige referenceværdier (RfV) for stoffet.

På produktresume.dk er der angivet en liste med mulige bivirkninger af stoffet, og også mulige effekter af en overdosering. Der er generelt set bivirkninger/effekter, som kan behandles eller som kun er af forbipasserende karakter, og derved ikke relevant for dette datablad.

5 Andre effekter

Der er ikke kendskab til andre effekter for ceftazidim eller ceftazidim pentahydrat.

6 Udledning af vandkvalitetskriterium

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

6.1 Vandkvalitetskriterium (VKK)

Der er ikke noget troværdigt kronisk data tilgængeligt for akvatiske organismer, hvorfor der ikke kan udledes et VKK for direkte effekter.

6.2 Korttidsvandkvalitetskriterium (KVKK)

Der er ikke noget troværdigt akut data tilgængeligt for akvatiske organismer, hvorfor der ikke kan udledes et KVKK.

6.3 Kvalitetskriterium for sediment (SKK)

Jf. TGD (EU, 2018) skal der udledes et sedimentkvalitetskriterie (SKK), hvis log K_{ow} eller log K_{oc} ≥3, eller der foreligger anden evidens for akkumulering i sediment eller evidens for høj toksicitet over for sedimentlevende organismer. For ceftazidim er der kun fundet log K_{ow} og K_{oc}-værdier ved brug af QSAR, hvor K_{oc} vil resultere i log værdier > 3 (hhv. 3,9 og 4,6 – se tabel 2.1). Der er ikke fundet data for sedimentlevende organismer, men (Q)SAR resultaterne kunne tale for at udlede et SKK ved brug af EqP, men grundet usikkerhed ved (Q)SAR resultaterne (se afsnit 2) beregnes der ikke et SKK. Til sammenligning har ceftazidim jf. tabel 2.1 log K_{oc}-værdier på < 3 (hhv. 1,5 og 2,9 bestemt ved lavt og højt organisk karbon indhold).

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

Jf. TGD (EU, 2018) skal der udledes et biotakvalitetskriterie for sekundær forgiftning ($BKK_{sek. forgiftn.}$), hvis BCF (BAF) ≥ 100. Der er ikke fundet eksperimentelle BCF eller BAF for ceftazidim, men ud fra det estimerede data angivet i afsnit 3.2 er BCF og BAF < 100. Dertil er der heller ikke fundet øvrige data, som viser potentiale for sekundær forgiftning. Derfor udledes $BKK_{sek. forgift.}$ ikke.

6.5 Kvalitetskriterium for human konsum af vandlevende organismer (HKK)

Ceftazidim har ikke nogen harmoniserede klassificeringer, som opfylder de angivne triggers jævnfør afsnit 2.4.3.2 i TGD (EU, 2018). Der er nogle selvklassificeringer for stoffet, hvoraf Acute Tox. 1 (H300) vil være relevant for fastsættelsen af et kriterie for human sundhed (HKK), dog kun hvis stoffet også har et potentiale for at bioakkumulere, hvilket umiddelbart ikke er tilfældet for ceftazidim. Derfor udledes der ikke et HKK.

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

Jævnfør TGD (EU, 2018) 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 af fiskeriprodukter.

Da der ikke er fastsat nogen biotakvalitetskriterier foretages der ikke en tilbageregning.

6.7 Bidrag af ceftazidim til antimikrobiel resistens

Ceftazidim er som nævnt i afsnit 1 et antibiotika, som anvendes til bekæmpelse af bakterielle infektioner. Da det er et antibiotika vil det også være relevant at medtage antimikrobiel resistens i overvejelserne ved fastsættelse af vandkvalitetskriterier (VKK).

Bengtsson-Palme & Larsson (2016) har udledt PNEC-værdier for forskellige antibiotika ved at anvende Minimum Inhibitory Concentrations (MIC) fra European Committee on Antimicrobial Susceptibility Testing database (EUCAST).

Bestemmelsen af PNEC-MIC er baseret på antagelsen om, at den selektive koncentration af antibiotika skal være lavere end koncentrationen, som hæmmer væksten af bakterier. PNEC-MIC er derfor bestemt ved anvendelse af den laveste MIC-værdi og en usikkerhedsfaktor på 10 i betragtningen af, at den selektive koncentration skal være lavere end den hæmmende koncentration. PNEC-MIC sammenlignes med værdien for VKK, og for at sikre beskyttelse af både menneskers sundhed og miljøet anbefales det at anvende den laveste af de to værdier (AMR Alliance, 2018; Tell et al., 2019).

For ceftazidim kommer Bengtsson-Palme & Larsson (2016) frem til en PNEC-MIC på 0,5 µg/l, som er lavere end den PNEC-værdi (1,3 µg/l), som de kommer frem til, ved brug af økotoksikologisk data (NOEC på 13 for *Anabaena flos-aquae*).

I dette datablad er VKK ikke beregnet på direkte effekter, da data ikke har været tilgængelig for en troværdighedsvurdering, hvortil en score 4 er tildelt (se bilag A). CHMP (2016; 2020) kommer dog også frem til en PNEC for overfladevand på 1,3 µg/l (NOEC på 13 µg/l for *Anabaena flos-aquae* (bilag A) og en usikkerhedsfaktor på 10, ligesom Bengtsson-Palme & Larsson (2016). For ceftazidim vælges derfor at sætte VKK = PNEC-MIC, da der ikke kan fastsættes et VKK på baggrund af troværdighedsvurderet økotoksikologiske data.

7 Konklusion

Følgende kvalitetskriterier for vandmiljøet er udregnet for ceftazidim:

Vandkvalitetskriterium

$VKK_{ferskvand}$	0,5 µg/l
$VKK_{saltvand}$	0,5 µg/l

Korttidsvandkvalitetskriterium

$KVKK_{ferskvand}$	Ikke muligt
$KVKK_{saltvand}$	Ikke muligt

Sedimentkvalitetskriterium

$SKK_{ferskvand}$	Ikke muligt
$SKK_{saltvand}$	Ikke muligt

Biotakvalitetskriterium, sekundær forgiftning

$BKK_{sek.forgiftn.}$	Ikke relevant

Biotakvalitetskriterium, human konsum

HKK	Ikke relevant

8 Referencer

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DrugBank.dk.

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Bilag A

Toksicitet over for vandorganismer (EC_x, LC_x, NOEC, osv.)

Ferskvandsorganismer

Akut toksicitet

	Form/salt	Målt	Varighed	Effekt	Værdi (mg/l)	Bemærkning	Reference	Troværdighed (1-4)
Fisk								
Zebrafisk, WT [a] (embryoer, 6 hpf [b])			3 dage	LD_{50} (dødelighed)	30.200	Det noteres, at kunstigt havvand anvendes, men promillen kan beregnes til 0,25 ppt [c].	Zhang et al., 2015	4
Zebrafisk, WT [a] (larver, 3 dpf [d])			3 dage	LD_{50} (dødelighed)	3.900	Det noteres, at kunstigt havvand anvendes, men promillen kan beregnes til 0,25 ppt [c].	Zhang et al., 2015	4

[a] WT = wild type

[b] hpf = hours post fertilization eller timer efter befrugtning

[c] 20 g salt opløses i 80 liter (= 80.000 g) omvendt osmose vand. Formel for at beregne salinitet: Salinitet [ppt] = masse af salt [g] / masse af vand [g] * 1000. For ferskvand ligger promillen på under 0,5.

[d] dpf = days post fertilization eller dage efter befrugtning

Ferskvandsorganismer
Kronisk toksicitet

	Form/salt	Målt	Varighed	Effekt	Værdi (mg/l)	Bemærkning	Reference	Troværdighed (1-4)
Cyanobakterier								
Anavaena flos-aquae	Pentahydrat		72 timer	NOEC (vækst)	0,013	OECD 201	CHMP, 2016; 2020	4
Anavaena flos-aquae	Pentahydrat		72 timer	LOEC (vækst)	0,025	OECD 201	CHMP, 2016; 2020	4
Alger								
Raphidocelis subcapitata	Pentahydrat		72 timer	NOEC (vækst)	120	OECD 201	CHMP, 2016; 2020	4
Raphidocelis subcapitata	Pentahydrat		72 timer	LOEC (vækst)	>120	OECD 201	CHMP, 2016; 2020	4
Krebsdyr								
Daphnia magna	Pentahydrat		21 dage	NOEC (reproduktion)	9,2	OECD 211	CHMP, 2016; 2020	4
Daphnia magna	Pentahydrat		21 dage	LOEC (reproduktion)	>9,2	OECD 211	CHMP, 2016; 2020	4
Insekter								
Chrinomus riparius	Pentahydrat		28 dage	NOEC (fremkomst)	100	OECD 218		
Chrinomus riparius	Pentahydrat		28 dage	LOEC (fremkomst)	>100	OECD 218		
Fisk								
Pimephales promelas	Pentahydrat		32 dage	NOEC (reproduktion)	8,0	OECD 210	CHMP, 2016; 2020	4
Pimephales promelas	Pentahydrat		32 dage	LOEC (reproduktion)	>8,0	OECD 210	CHMP, 2016; 2020	4

Saltvandsorganismer
Akut toksicitet
Ingen data tilgængeligt.

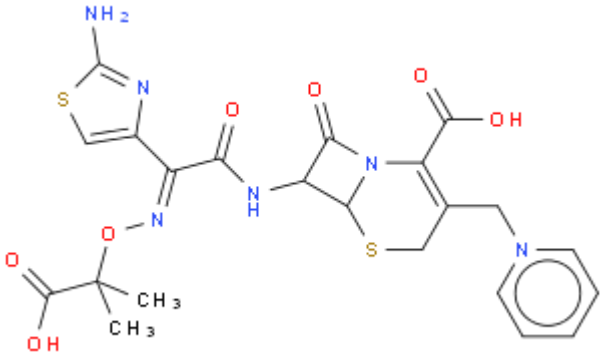
Saltvandsorganismer
Kronisk toksicitet
Ingen data tilgængeligt.

Bilag B

Danish (Q)SAR Database, https://qsar.food.dtu.dk Date: 17-07-2024

(Q)SAR predicted profile

8.1 Structure (as used for QSAR prediction):



SMILES (used for QSAR prediction):
C(=O)(C(C1=CSC(N)=N1)=NOC(C)(C)C(=O)O)NC1C(=O)N2C(C(=O)O)=C(Cn3ccccc3)CSC12

8.2 ID

Registry Number	72558-82-8	PubChem CID	
REACH EC Number (pre-registration, by 2013)	276-715-9	REACH EC Number (registration, 2019 or 2022)	
REACH registration (2022)		REACH registration cumulated minimum annual tonnage (2022)	
EU CLP Harmonized Classification*		DK-EPA / DTU QSAR-based CLP Advisory Classification	Aquatic Chronic 3
EU Biocide active substances		EU Pesticide active substances	
EU EFSA Botanical substances		US TSCA (Oct. 2021)	
Tox21 (2019)		ToxCast (Oct. 2021)	
Molecular Formula	C22 H23 N6 O7 S2	Molecular weight (g/mole)	547.58
Chemical Name			

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

8.3 Melting point, Boiling point and Vapour pressure

Melting Point (deg C)	349.84	Melting Point Experimental (deg C)	
Boiling Point (deg C)	852.33	Boiling Point Experimental (deg C)	
Vapour Pressure (atm)		Vapour Pressure Experimental (atm)	
Vapour Pressure (mm Hg)	2.32E-021	Vapour Pressure Experimental (mm Hg)	
Vapour Pressure (Pa)	3.093E-019	Vapour pressure Subcooled Liquid (Pa)	1.58E-015

EPI MPBPVP models

8.4 Henry's Law Constant

HLC Bond Method (atm-m3/mole)	2.463E-028	HLC Group Method (atm-m3/mole)	
HLC Via VP/WSol (atm-m3/mole)	4.568E-023	HLC Via VP/WSol (Pa-m3/mole)	4.629E-018
Henrys Law Const. Exp db (Pa-m3/mole)		Henrys Law Const. Exp db (atm-m3/mole)	

EPI HENRYWIN models

8.5 Water Solubility

Water solubility from Kow (mg/L)	36.59	Water solubility from Fragments (mg/L)	1000000
Water solubility Exp (mg/L)		Water solubility Exp Ref	

EPI WATERNT model

	Exp	Prediction	Domain
Water solubility v1.0.1 (mg/L)			

VEGA model

8.6 Hydrolysis

Hydrolysis Ka half-life pH 7		Hydrolysis Kb half-life pH 7	
Hydrolysis Ka half-life pH 8		Hydrolysis Kb half-life pH 8	

EPI HYDROWIN model

8.7 pKa

pKa Acid	1.6
- Standard deviation (±)	0.5
pKa Base	9.8
- Standard deviation (±)	0.9

ACDLabs model

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

8.8 Partition coefficients

pH	1	4	5	6	7	8	9
LogD	-3.7	-2.84	-3.06	-3.1	-3.11	-3.11	

Minimum LogD in the pH interval 4-9	-3.11	Maximum LogD in the pH interval 4-9	-2.84

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	27.148	Log Kaw	-25.998

EPI KOAWIN models

Koa: octanol-air partition coefficient. Kaw: air-water partition coefficient.

Log Kow	1.15		
Log Kow Exp		Log Kow Exp Ref	

EPI WSKOW model

LogKow: log octanol-water partition coefficient

Kp (m3/ug) Mackay-based	1.89E009	Kp (m3/ug) Koa-based	3.45E014
Phi Junge-Pankow-based	1	Phi Mackay-based	1
Phi Koa-based	1		

EPI AEROWIN models

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

Koc from MCI (L/kg)	37050	Log Koc from MCI	4.5688
Koc from Kow (L/kg)	7.476	Log Koc from Kow	0.8737

EPI KOCWIN models

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

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

	Air	Water	Soil	Sediment
Mass Amount (%)	3.6E-010	8.34	74.3	17.4
Half-Life (hr)	1.35	900	1800	8100
Emissions (kg/hr)	1000	1000	1000	0

EPI Level III Fugacity Model

Persistence time (hr)	2210
Persistence time (days)	

EPI Level III Fugacity Model

8.10 Level III Fugacity Environmental Partitioning, emission only to water

	Air	Water	Soil	Sediment
Mass Amount (%)	1.85E-033	32.4	1.8E-022	67.6
Half-Life (hr)	1.35	900	1800	8100
Emissions (kg/hr)	0	1000	0	0

EPI Level III Fugacity Model

Persistence time (hr)	1550
Persistence time (days)	64.58334

EPI Level III Fugacity Model

8.11 Air Half-Life

	Exp	Prediction	Domain
Air Half-Life (CORAL) v1.0.1 (hr)			

VEGA model

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

	Total removal	Biodegradation	Sludge Adsorption	Volatilization
(%)	1.9	0.09	1.81	0

EPI STPWIN model

8.13 Atmospheric oxidation (25 deg C)

	OH	Ozone
Half-Life (d)	0.08831	0.155
Half-Life (hr)	1.06	3.72
Overall Rate Const. (OH: E-12 cm3/molecule-sec and OZ: E-17 cm3/molecule-sec)	121.1205	7.39375

EPI AOPWIN models

8.14 Biodegradation

Biowin1 (linear model) Probability of Rapid Biodegradation	0.6349
Biowin2 (non-linear model) Probability of Rapid Biodegradation	0.1508
Biowin3 Expert Survey Ultimate Biodegradation	2.2628
Biowin3 Expert Survey Ultimate Timeframe	weeks-months
Biowin4 Expert Survey Primary Biodegradation	3.9779
Biowin4 Exp. Survey Primary Timeframe	days
Biowin5 (MITI linear model) Biodegradation Probability	-0.2473
Biowin6 (MITI non-linear model) Biodegradation Probability	0.0001
Biowin7 (Anaerobic Linear) Biodegradation Probability	-1.285
Petroleum Hydrocarbon Biodegradation Half-Life (days)	

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".
Biowin7: ≥0.5: "Fast", <0.5: "Slow"

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Not Ready Biodegradability		INC_OUT		NEG_OUT	INC_OUT

DTU-developed models
POS=Not Ready

.	Exp	Prediction_Domain
Not Ready Biodegradability		

v1.0.10

VEGA model
POS=Not Ready

8.15 Bioaccumulation

BCF (L/kg wet-wt)	3.162
Log BCF (L/kg wet-wt)	0.5
Whole Body Primary Biotransformation Fish Half-Life (days)	0.06869
BCF Arnot-Gobas (upper trophic) Including Biotransformation (L/kg wet-wt)	1.968
BCF Arnot-Gobas (upper trophic) Zero Biotransformation (L/kg wet-wt)	2.414
BAF Arnot-Gobas (upper trophic) Including Biotransformation (L/kg wet-wt)	1.968
BAF Arnot-Gobas (upper trophic) Zero Biotransformation (L/kg wet-wt)	2.436

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

	Exp	Prediction	Domain
Log BCF (CAESAR) v2.1.15 (L/kg)			

VEGA model

8.16 Aquatic toxicity

Exp	Battery	Leadscope	SciQSAR
Fathead minnow 96h LC50 (mg/L)		48.35013	3.025712
Domain	OUT	OUT	OUT
Daphnia magna 48h EC50 (mg/L)		2.635497	12.1101
Domain	OUT	OUT	OUT
Pseudokirchneriella s. 72h EC50 (mg/L)	665.7124	1330.662	0.7629
Domain	IN	IN	IN

DTU-developed models

	Exp	Prediction	Domain
Daphnia magna 48h EC50 v1.0.1 (mg/L)			
Daphnia magna 21d NOEC v1.0.1 (mg/L)			
Algae Acute 72h ErC50 v1.0.1 (mg/L)			
Sludge Classification, 3h EC50 < 100 mg/L v1.0.1*			See prediction

Sludge 3h EC50 v1.0.1 (mg/L)

VEGA models

** The quantitative model should only be applied when the Sludge classification model is POS_IN*

MOA Toxicity classification (EPA T.E.S.T) v1.0.2
- predicted Mode of action
- Domain
- Exp, if part of training set

VEGA model

Qualitative estimation of MOA for Fathead minnow 96h

	Fish 96h	Daphnid 48h	Green Algae 96h
LC50 (Fish) or EC50 (Daphnid and Algae) for Most Toxic Class (mg/L)	2592.637	39.882	99.114
Max. Log Kow for Most Toxic Class	5	>3	>4
Most Toxic Class	Neutral Organic SAR	Anilines (Unhindered)-acid	Anilines (Unhindered)-acid
Note	Chemical may not be soluble enough	Chemical may not be soluble enough	Chemical may not be soluble enough

EPI ECOSAR models

ECOSAR Classes: Aliphatic Amines-acid; Anilines (Unhindered)-acid; Amides -acid

8.17 Oral absorption

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

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.

8.18 Skin absorption

Dermal absorption (mg/cm2/event)

EPI DERMWIN model

8.19 Brain/blood Distribution

Log brain/blood partition coefficient

Equation from literature

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

8.20 Metabolism

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
CYP2C9 substrates (Human clinical data)		NEG_IN		NEG_IN	NEG_IN
CYP2D6 substrates (Human clinical data)		NEG_IN		NEG_IN	NEG_IN

DTU-developed models

8.21 Acute toxicity in Rodents

	LD50 (mg/kg/d)	Reliability Index
Rat Oral	2100	0.25
Rat Intraperitoneal	6900	0.18
Mouse Oral	8900	0.46
Mouse Intraperitoneal	2000	0.26
Mouse Intravenous	2000	0.52
Mouse Subcutaneous	9100	0.29

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.

8.22 Effects in Humans

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

.	Exp	Prediction_Domain
Hepatotoxicity v1.0.1		

VEGA model

Profiler-type of predictions to be used as supporting information together with relevant QSAR predictions.

8.23 Irritation and Sensitization

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Severe Skin Irritation in Rabbit		NEG_OUT		NEG_OUT	NEG_IN
Skin sensitisation GHS/CLP at least Cat. 1, LLNA-based (open data only)				NEG_OUT	
Skin sensitisation GHS/CLP at least Cat. 1, LLNA-based (open data and REACH-registrations)	N/A			NEG_IN	
Skin sensitisation GHS/CLP at least Cat. 1, LLNA-based, only negative predictions (open data only)				N/A	
Skin sensitisation GHS/CLP Cat. 1A, LLNA-based (open data only)				INC_OUT	
Skin sensitisation GHS/CLP Cat. 1A, LLNA-based (open data and REACH-registrations)	N/A			NEG_IN	
Skin sensitisation GHS/CLP Cat. 1A, LLNA-based, only positive predictions (open data and REACH-registrations)	N/A			N/A	
Allergic Contact Dermatitis in Guinea Pig and Human*	N/A	POS_IN		POS_IN	POS_IN
Respiratory Sensitisation in Humans		POS_IN		POS_IN	POS_IN

DTU-developed models

**Based on commercial training set*

Protein binding by OASIS, alerts in:					
- parent only		N/A			
- metabolites from skin metabolism simulator only					
- metabolites from auto-oxidation simulator only					
Protein binding by OECD, alerts in:					
- parent only		N/A			
- metabolites from skin metabolism simulator only					
- metabolites from auto-oxidation simulator only					
Protein binding potency Cys (DRPA 13%), alerts in:					
- parent only		N/A			
- metabolites from skin metabolism simulator only					
- metabolites from auto-oxidation simulator only					
Protein binding potency Lys (DRPA 13%), alerts in:					
- parent only		N/A			
- metabolites from skin metabolism simulator only					
- metabolites from auto-oxidation simulator only					
Keratinocyte gene expression, alerts in:					

- parent only	N/A
- metabolites from skin metabolism simulator only	
- metabolites from auto-oxidation simulator only	
Protein binding potency GSH, alerts in:	
- parent only	N/A

OECD QSAR Toolbox v.4.1 profilers

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

8.24 Endocrine and Molecular Endpoints

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Estrogen Receptor α Binding, Full training set (Human *in vitro*)		INC_OUT		NEG_OUT	NEG_OUT
Estrogen Receptor α Binding, Balanced Training Set (Human *in vitro*)		POS_OUT		NEG_OUT	POS_IN
Estrogen Receptor α Activation (Human *in vitro*)		NEG_OUT		NEG_OUT	NEG_IN
Estrogen Receptor Activation, CERAPP data (*in vitro*)		N/A	N/A	INC_OUT	N/A
Androgen Receptor Inhibition (Human *in vitro*)		NEG_IN		NEG_IN	NEG_IN
Androgen Receptor Binding, CoMPARA data (*in vitro*)		N/A	N/A	INC_OUT	N/A
Androgen Receptor Inhibition, CoMPARA data (*in vitro*)		N/A	N/A	INC_OUT	N/A
Androgen Receptor Activation, CoMPARA data (*in vitro*)		N/A	N/A	INC_OUT	N/A
Thyroperoxidase (TPO) inhibition QSAR1 (Rat *in vitro*)		N/A	N/A	INC_OUT	N/A
Thyroperoxidase (TPO) inhibition QSAR2 (Rat *in vitro*)		N/A	N/A	INC_OUT	N/A
Sodium/iodide symporter (NIS), higher sensitivity		N/A	N/A	INC_OUT	N/A
Sodium/iodide symporter (NIS), higher specificity		N/A	N/A	INC_OUT	N/A
Thyroid Receptor α Binding (Human *in vitro*)					
- mg/L				87790.5	
- μM				160324.5	
- Positive for IC_{50} ≤ 10 μM					
- Positive for IC_{50} ≤ 100 μM					
- Domain				OUT	
Thyroid Receptor β Binding (Human *in vitro*)					
- mg/L				17418.38	

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
- μM				31809.74	
- Positive for IC_{50} ≤ 10 μM					
- Positive for IC_{50} ≤ 100 μM					
- Domain				OUT	
Peroxisome Proliferator-Activated Receptor gamma (PPAR-γ) Inhibition at max. 10 μM (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
Peroxisome Proliferator-Activated Receptor gamma (PPAR-γ) Inhibition at any concentration (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
Retinoic Acid Receptor (RAR) inhibition at max. 10 μM (Human *in vitro*)		N/A	N/A	NEG_IN	N/A
Arylhydrocarbon Receptor (AhR) Activation – Rational final model (Human *in vitro*)		N/A	N/A	NEG_IN	N/A
Arylhydrocarbon Receptor (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	POS_IN		POS_IN	POS_IN
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_IN	N/A
Pregnane X Receptor (PXR) Activation (Rat *in vitro*)	NEG	N/A	N/A	INC_OUT	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 (Human *in vitro*)		N/A	N/A	NEG_IN	N/A
Constitutive Androstane Receptor (CAR) Activation at max. 50 μM (Human *in vitro*)		N/A	N/A	NEG_IN	N/A
Constitutive Androstane Receptor (CAR) Inhibition at max. 20 μM (Human *in vitro*)		N/A	N/A	NEG_IN	N/A
Constitutive Androstane Receptor (CAR) Inhibition at max. 50 μM (Human *in vitro*)		N/A	N/A	INC_OUT	N/A
DTU-developed models					
Estrogen Receptor Binding, alerts in:					
- parent only		N/A			
- metabolites from *in vivo* Rat metabolism simulator only					

- metabolites from Rat liver S9 metabolism simulator only	
rtER Expert System - USEPA, alerts in:	
- parent only	N/A
- metabolites from *in vivo* Rat metabolism simulator only	
- metabolites from Rat liver S9 metabolism simulator only	

OECD QSAR Toolbox v.4.2 profilers

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

8.25 Developmental Toxicity

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

DTU-developed models based on commercial training set

.	Exp	Prediction_Domain
Developmental/Reproductive Toxicity library (PG) v1.1.2		

VEGA model

Profiler-type of predictions to be used as supporting information together with relevant QSAR predictions

8.26 Genotoxicity - Structural Alerts for DNA Reactivity

	Battery	CASE Ultra	Leadscope	SciQSAR
Ashby Structural Alerts	INC_OUT		NEG_IN	POS_IN

DTU-developed models based on commercial training set

DNA binding by OASIS, alerts in:	
- parent only	N/A
DNA binding by OECD, alerts in:	
- parent only	N/A

OECD QSAR Toolbox v.4.2 profilers

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

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

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR

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

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.

Consensus	Mut. / Non-mut. Scores	Used models
Ames test Consensus	/	

VEGA model

Mutagenicity (Ames) consensus model version 1.0.4 contained in VEGA version 1.4.3 with calculation core version 1.3.14

	Exp	Prediction
Ames test (ISS) v1.0.3		
Ames test (CAESAR) - v2.1.13		
Ames test (SarPy) v1.0.8		
Ames test (KNN/Read-Across) v1.0.1		

VEGA models

DNA alerts for AMES by OASIS, alerts in:	
- parent only	N/A
In vitro mutagenicity (Ames test) alerts by ISS, alerts in:	
- parent only	N/A

OECD QSAR Toolbox v.4.2 profilers

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

8.28 Other *in vitro* Genotoxicity Endpoints

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Chromosome Aberrations in Chinese Hamster Ovary (CHO) Cells*	N/A	NEG_IN		NEG_IN	NEG_IN
Chromosome Aberrations in Chinese Hamster Lung (CHL) Cells		INC_OUT		NEG_IN	POS_IN

	Exp	Battery	CASE Ultra	Leadscope	SciQSAR
Mutations in Thymidine Kinase Locus in Mouse Lymphoma Cells		NEG_OUT		NEG_IN	NEG_OUT
Mutations in HGPRT Locus in Chinese Hamster Ovary (CHO) Cells		POS_OUT		NEG_OUT	POS_IN
Unscheduled DNA Synthesis (UDS) in Rat Hepatocytes		INC_OUT		POS_OUT	INC_OUT
Syrian Hamster Embryo (SHE) Cell Transformation		NEG_OUT		NEG_OUT	NEG_IN

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

HGPRT: Hypoxanthine-guanine phosphoribosyltransferase

.	Exp	Prediction_Domain
Micronucleus (VERMEER) v1.0.1		

VEGA model

DNA alerts for CA and MNT by OASIS, alerts in:	
- parent only	N/A
Protein binding alerts for Chromosomal aberration by OASIS, alerts in:	
- parent only	N/A

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

8.29 *In vivo* Genotoxicity Endpoints

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

DTU-developed models

In vivo mutagenicity (Micronucleus) alerts by ISS, alerts in:	
- parent only	N/A

OECD QSAR Toolbox v.4.2 profilers

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

8.30 Carcinogenicity

	E Ultra	Leadscope
FDA RCA Cancer Male Rat		NEG_IN
FDA RCA Cancer Female Rat		NEG_IN
FDA RCA Cancer Rat		NEG_IN
FDA RCA Cancer Male Mouse		NEG_IN
FDA RCA Cancer Female Mouse		NEG_IN
FDA RCA Cancer Mouse		NEG_IN
FDA RCA Cancer Rodent		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	N/A
Oncologic Primary Classification, alerts in:	
- parent only	N/A

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		NEG_OUT		NEG_OUT	NEG_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 from 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, VEGA 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: https://www.multicase.com/case-ultra

Leadscope: https://www.leadscope.com/

VEGA: https://vegahub.it

ToxSuite: https://www.acdlabs.com/

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All access to the database should happen through the provided client-side software and without any use of automated workflow or scripting.

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