

The logo for KnowSEC, featuring the text "KnowSEC" in white on a blue background with a hexagonal icon to the right.

KnowSEC

A Web-System for Managing Data on Substances

Albrecht Striffler, Dirk Wassermann, denkbares GmbH, 2015-03-02



Why am I here, what is KnowSEC?

- ▶ KnowSEC, a software for prioritization, evaluation, and documentation of substance related work
- ▶ Developed since 2011 for UBA, by denkbares GmbH
- ▶ KnowSEC was used to help with the systematic analysis of data availability



„Uba2005“ von Martin Förster, 06846
Dessau, vegoh@gmx.de. Licensed CC-by-sa
2.0/de

- ▶ 2009 founded by Volker Belli (formerly: denkbar/cc since 2007)
- ▶ > 15 years of expertise in conception, implementation, and maintenance of knowledge systems
- ▶ Currently 10 employees + students
- ▶ Areas:
 - ▶ Mechanical engineering (CLAAS, Heidelberger Druckmaschinen, SHL, Bosch, etc.)
 - ▶ Environmental protection (UBA)
 - ▶ Medicine (Dräger)
 - ▶ Defense (Krauss-Maffei Wegmann)



The Challenge



DENKBARES
KM & AI SOLUTIONS



- Large amount of task
- Collaborative
- Episodic
- Efficient
- Consistent
- Comprehensive evaluation
- Documentation



The Concept

Challenges

Collaborative
Large amount
of tasks

Consistent
Efficient
Episodic

Comprehensive
Evaluation

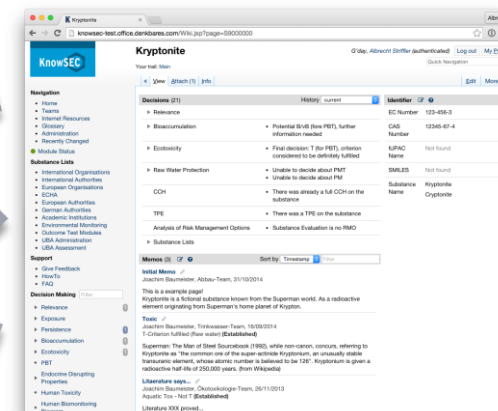
Concept

Centralized
Document
Management

Decision
Support
Memos

Dynamic data
views

KnowSEC





Kryptonite

G'day, Albrecht Striffler (authenticated)
Log out
My Prefs

Your trail: Main
Quick Navigation

<< View Attach (1) Info
Edit More...

Navigation

- Home
- Teams
- Internet Resources
- Glossary
- Administration
- Recently Changed
- Module Status

Substance Lists

- International Organisations
- International Authorities
- European Organisations
- ECHA
- European Authorities
- German Authorities
- Academic Institutions
- Environmental Monitoring
- Outcome Test Modules
- UBA Administration
- UBA Assessment

Support

- Give Feedback
- HowTo
- FAQ

Decision Making

- ▶ Relevance 1
- ▶ Exposure
- ▶ Persistence 1
- ▶ Bioaccumulation 1
- ▶ Ecotoxicity 1

Decisions (21) History current

- ▶ Relevance
- ▶ Bioaccumulation
 - Potential B/vB (fore PBT), further information needed
- ▶ Ecotoxicity
 - Final decision: T (for PBT), criterion considered to be definitely fulfilled
- ▶ Raw Water Protection
 - Unable to decide about PMT
 - Unable to decide about PM
- CCH
 - There was already a full CCH on the substance
- TPE
 - There was a TPE on the substance
- Analysis of Risk Management Options
 - Substance Evaluation is no RMO
- ▶ Substance Lists

Memos (3) Sort by Timestamp Filter

Initial Memo

Joachim Baumeister, Abbau-Team, 31/10/2014

This is a example page!
Kryptonite is a fictional substance known from the Superman world. As a radioactive element originating from Superman's home planet of Krypton.

Toxic

Joachim Baumeister, Trinkwasser-Team, 16/09/2014
T-Criterion fulfilled (Raw water) **(Established)**

Superman: The Man of Steel Sourcebook (1992), while non-canon, concurs, referring to Kryptonite as "the common ore of the super-actinide Kryptonium, an unusually stable transuranic element, whose atomic number is believed to be 126". Kryptonium is given a radioactive half-life of 250,000 years. (from Wikipedia)

Identifier

EC Number	123-456-3
CAS Number	12345-67-4
IUPAC Name	Not found
SMILES	Not found
Substance Name	Kryptonite
	Cryptonite

KnowSEC – Decision Support



DENKBARES
KM & AI SOLUTIONS

KnowSEC

2-vinylpyridine

Your trail: benzene, Dokumentation_UFOPLAN_Compliance, 2-vinylpyridine Me..., 2-vinylpyridine, 2-vinylpyridine Me...

G'day, Albrecht Striffler (not logged in) [Log in](#) [My Prefs](#)

Quick Navigation

Navigation

- Home
- Teams
- Internet Resources
- Glossary
- Administration
- Recently Changed
- Module Status

Substance Lists

- Doku UFOPLAN Compliance
- All Substances

Support

- Give Feedback
- HowTo
- FAQ

Decision Making

- ▼ UFOPLAN_Compliance 1
 - Compliance Abbaubarkeit
 - Compliance Bioakkumulation 2
 - Compliance Oekotoxizitaet 2
 - Compliance Expositionsbewertung 3
 - Compliance Mutagenitaet
 - Compliance Reptox
 - Compliance Repeated Dose

Derived decisions for module 'UFOPLAN_Compliance'

- Dossier ist ein komplexer Fall

The decision was derived because of the following inputs:

- Expositionsszenarien für die Umwelt vorhanden? = Yes
- Substanz von Registranten als PBT oder vPvB bewertet? = No
- Selbsteinstufung des Registranten mit H400, H410, H411, oder H412? = Yes
- Substanz ionisch dissoziiierbar? = Yes
- Substanz harmonisiert mit H400, H410, H411 oder H412 eingestuft? = No
- Substanz anorganisch? = No

Inputs by H. Herrmann, 06/05/2014
Established since 06/05/2014

Substanz anorganisch? Yes | No

Substanz ionisch dissoziiierbar? Yes | No

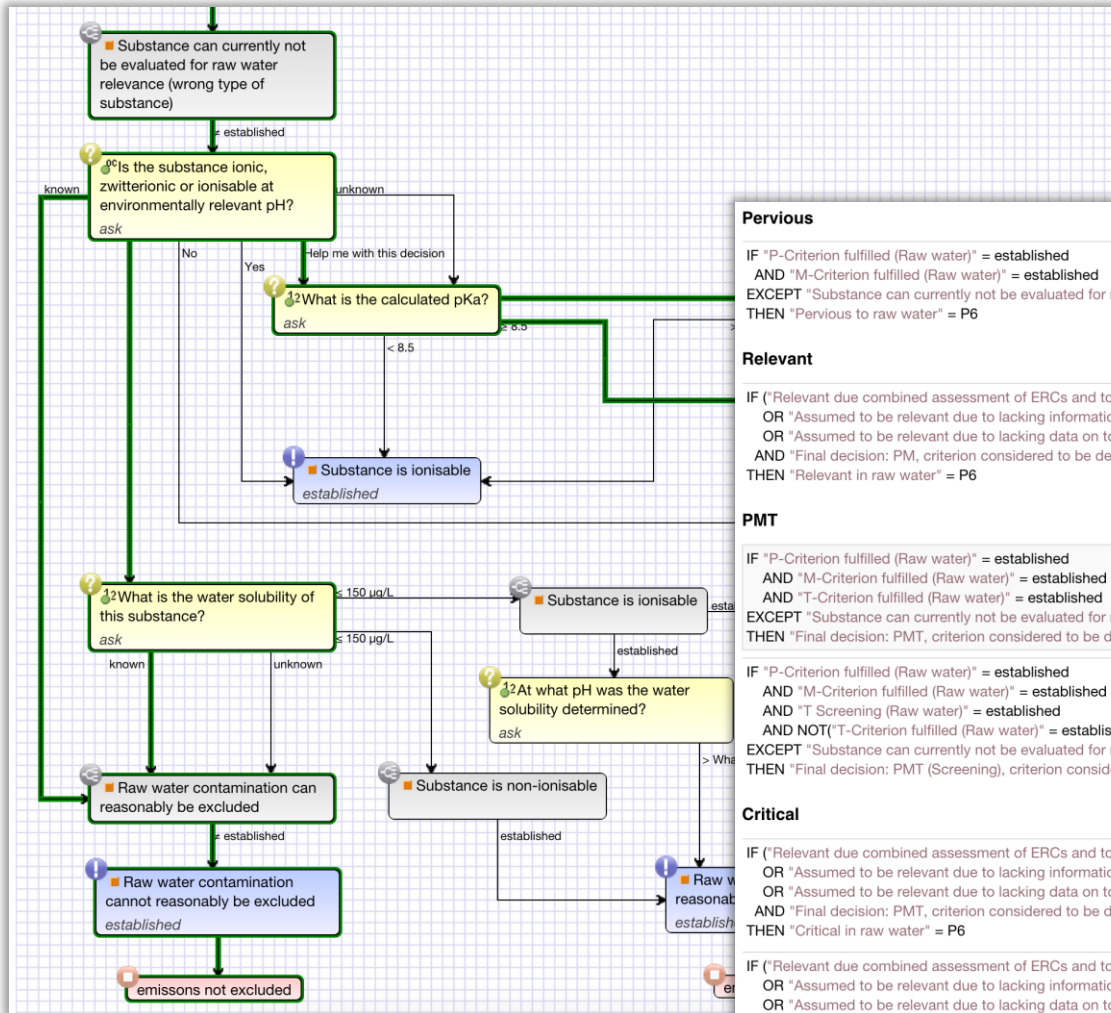
pKa 4,98

Albrecht Striffler, 07/05/2014

Compliance Oekotoxizitaet

Chronischer Daphnien- und Fischtest vorhanden? TP | Yes | No

KnowSEC – Decision Support



Pervious

```

IF "P-Criterion fulfilled (Raw water)" = established
AND "M-Criterion fulfilled (Raw water)" = established
EXCEPT "Substance can currently not be evaluated for raw water relevance (wrong type of substance)" = established
THEN "Pervious to raw water" = P6
    
```

Relevant

```

IF ("Relevant due combined assessment of ERCs and total tonnage" = established
OR "Assumed to be relevant due to lacking information on environmental release" = established
OR "Assumed to be relevant due to lacking data on tonnage" = established)
AND "Final decision: PM, criterion considered to be definitely fulfilled" = established
THEN "Relevant in raw water" = P6
    
```

PMT

```

IF "P-Criterion fulfilled (Raw water)" = established
AND "M-Criterion fulfilled (Raw water)" = established
AND "T-Criterion fulfilled (Raw water)" = established
EXCEPT "Substance can currently not be evaluated for raw water relevance (wrong type of substance)" = established
THEN "Final decision: PMT, criterion considered to be definitely fulfilled" = P6
    
```

```

IF "P-Criterion fulfilled (Raw water)" = established
AND "M-Criterion fulfilled (Raw water)" = established
AND "T Screening (Raw water)" = established
AND NOT("T-Criterion fulfilled (Raw water)" = established)
EXCEPT "Substance can currently not be evaluated for raw water relevance (wrong type of substance)" = established
THEN "Final decision: PMT (Screening), criterion considered to be definitely fulfilled" = P6
    
```

Critical

```

IF ("Relevant due combined assessment of ERCs and total tonnage" = established
OR "Assumed to be relevant due to lacking information on environmental release" = established
OR "Assumed to be relevant due to lacking data on tonnage" = established)
AND "Final decision: PMT, criterion considered to be definitely fulfilled" = established
THEN "Critical in raw water" = P6
    
```

```

IF ("Relevant due combined assessment of ERCs and total tonnage" = established
OR "Assumed to be relevant due to lacking information on environmental release" = established
OR "Assumed to be relevant due to lacking data on tonnage" = established)
AND "Final decision: PMT (Screening), criterion considered to be definitely fulfilled" = established
THEN "Critical in raw water (Screening)" = P6
    
```


KnowSEC – Dynamic Views



DENKBARES
KM & AI SOLUTIONS

Critical outcome Test Module Raw Water Protection

G'day, Albrecht Striffler (authenticated) [Log out](#) [My Prefs](#)

Your trail: [Main](#), [Substance Lists for Outcome Test Modules](#)

« [View](#) [Attach](#) [Info](#)

[Edit Mode](#) [Edit](#) [More...](#)

> [Back to Overview](#)

Show 20 lines of 34 << < Lines 1 to 20 >

Substance	CAS	EC	Name	RawWater
S8101911	107-06-2	203-458-1	1,2-Dichlorethan	- Pervious to raw water - Critical in raw water - Final decision: PMT, criterion considered to be definitely fulfilled
S1106578	834-12-8	212-634-7	1,3,5-Triazine-2,4-diamine, N-ethyl-N'-(1-methylethyl)-6-(methylthio)-	- Pervious to raw water - Final decision: PM, criterion considered to be definitely fulfilled - Final decision: Not PMT - Not critical in raw water - Not relevant in raw water
S3872585	41098-56-0	255-217-5	1,4-Benzenedisulfonic acid, 2,2'-[1,2-ethenediylbis[(3-sulfo-4,1-phenylene)imino[6-(diethylamino)-1,3,5-triazine-4,2-diy]]imino]]bis-, hexasodium salt	- Pervious to raw water - Final decision: PM, criterion considered to be definitely fulfilled - Relevant in raw water - Final decision: Not PMT
S1885654	68971-49-3	273-468-9	1,4-Benzenedisulfonic acid, 2,2'-[1,2-ethenediylbis[(3-sulfo-4,1-phenylene)imino[6-bis(2-hydroxyethyl)amino]-1,3,5-triazine-4,2-diy]]imino]]bis-, hexasodium salt	- Pervious to raw water - Final decision: PM, criterion considered to be definitely fulfilled - Relevant in raw water - Final decision: Not PMT
S9148855	371756-75-1	609-336-8	1,4-Benzenedisulfonic acid, 2,2'-[1,2-ethenediylbis[(3-sulfo-4,1-phenylene)imino[6-bis(2-hydroxypropyl)amino]-1,3,5-triazine-4,2-diy]]imino]]bis-, hexasodium salt	- Pervious to raw water - Final decision: PM, criterion considered to be definitely fulfilled - Relevant in raw water - Final decision: Not PMT
S4083191	1671-49-4	430-550-0	1-methyl-4-(methylsulfonyl)-2-nitrobenzene	- Pervious to raw water - Final decision: PMT, criterion considered to be definitely fulfilled - Not critical in raw water - Not relevant in raw water
S3633245	95-14-7	202-394-1	1H-Benzotriazol	- Pervious to raw water - Final decision: PM, criterion considered to be definitely fulfilled - Relevant in raw water - Final decision: Not PMT

Navigation

- Home
- Teams
- Internet Resources
- Glossary
- Administration
- Recently Changed
- Module Status

Substance Lists

- International Organisations
- International Authorities
- European Organisations
- ECHA
- European Authorities
- German Authorities
- Academic Institutions
- Environmental Monitoring
- Outcome Test Modules
- UBA Administration
- UBA Assessment

Support

- Give Feedback
- HowTo
- FAQ

Decision Making

No substance selected

KnowSEC – Dynamic Views



DENKBARES
KM & AI SOLUTIONS

Gesamtergebnisse

Show 20 lines of 1814 | 4 Lines 1 to 20 Spa

BfR	Substance	Dossier	EC	Name	Overall	Muta	Reprotox	RepDose	Abbaubarkeit	Bioakkumulation	Ökotox	ExpoEnv
BfR0001	S1171400		200-315-5	urea	Dossier ist ein komplexer Fall	UC Mutagenitaet: Komplexer Fall UCM-CX2: Komplex, weil Waiving für 1 oder 2 Studien (in vitro und/oder in vivo) vorliegt.	UC Reprotox: Komplexer Fall UCR: UCR-CX6: Komplex, weil je ein waiving für DevTox und für ReproTox -oder Ergebnisse für ReproTox an einer Nichtnagerspezies-vorliegen (2 waiver oder 1 waiver/1 Studie).	UC Repeated Dose: Komplexer Fall UCRD: UCRD-CX3: Komplex, weil Waiving je für 28d Studie und 90d Studie vorliegt.	UC Abiotische Abbaubarkeit: Komplexer Fall UC Biotische Abbaubarkeit: Komplexer Fall UCABA: Komplex, weil Waiving, aber kein Bezug auf Annex VIII UCBA: Komplex, weil nicht richtige Testmethode	UC Bioakkumulation: Compliant UCB: Compliant, weil Waiving mit Bezug auf Annex IX (log KOW <= 3)	UC Oekotoxizitaet: Komplexer Fall UCOT: Komplex, weil Waiving	UC Expositionsbewertung: Compliant UCEXO: Compliant, weil Substanz ohne Einstufung und nicht PBT/vPvB
BfR0002	S1367641		292-966-7	Fatty acids, C16-18, lead salts	Dossier ist non-compliant	UC Mutagenitaet: Komplexer Fall UCM-CX2: Komplex, weil Waiving für 1 oder 2 Studien (in vitro und/oder in vivo) vorliegt.	UC Reprotox: Non-compliant UCR: UCR-NC4: NC, weil Waiving für DevTox und/oder ReproTox -oder Ergebnisse für ReproTox an Nichtnager- fehlt.	UC Repeated Dose: Komplexer Fall UCRD: UCRD-CX3: Komplex, weil Waiving je für 28d Studie und 90d Studie vorliegt.	UC Abiotische Abbaubarkeit: Komplexer Fall UC Biotische Abbaubarkeit: Compliant UCABA: Komplex, weil Waiving, aber kein Bezug auf Annex VIII UCBA: Compliant, weil Substanz anorganisch	UC Bioakkumulation: Komplexer Fall UCB: Komplex, weil anorganisch	UC Oekotoxizitaet: Non-compliant UCOT: NC, weil Waivingbegründung fehlt oder falsch	UC Expositionsbewertung: Komplexer Fall UCEXO: Komplex, weil Expo-Szenarien für Umwelt vorhanden UCEXO: relevante Einstufung vorhanden
BfR0003	S4047452		235-252-2	trilead dioxide phosphonate	Dossier ist non-compliant	UC Mutagenitaet: Komplexer Fall UCM-CX2: Komplex, weil Waiving für 1 oder 2 Studien (in vitro und/oder in vivo) vorliegt.	UC Reprotox: Non-compliant UCR: UCR-NC4: NC, weil Waiving für DevTox und/oder ReproTox -oder Ergebnisse für ReproTox an Nichtnager- fehlt.	UC Repeated Dose: Komplexer Fall UCRD: UCRD-CX3: Komplex, weil Waiving je für 28d Studie und 90d Studie vorliegt.	UC Abiotische Abbaubarkeit: Komplexer Fall UC Biotische Abbaubarkeit: Compliant UCABA: Komplex, weil Waiving, aber kein Bezug auf Annex VIII UCBA: Compliant, weil Substanz anorganisch	UC Bioakkumulation: Komplexer Fall UCB: Komplex, weil anorganisch	UC Oekotoxizitaet: Non-compliant UCOT: NC, weil Waivingbegründung fehlt oder falsch	UC Expositionsbewertung: Komplexer Fall UCEXO: Komplex, weil Expo-Szenarien für Umwelt vorhanden UCEXO: relevante Einstufung vorhanden



How did KnowSEC help BfR?

New decision support module “UFOPLAN compliance”

Generation of ~2000 dossier pages via Excel import

Structured evaluation and input of data by BfR employees

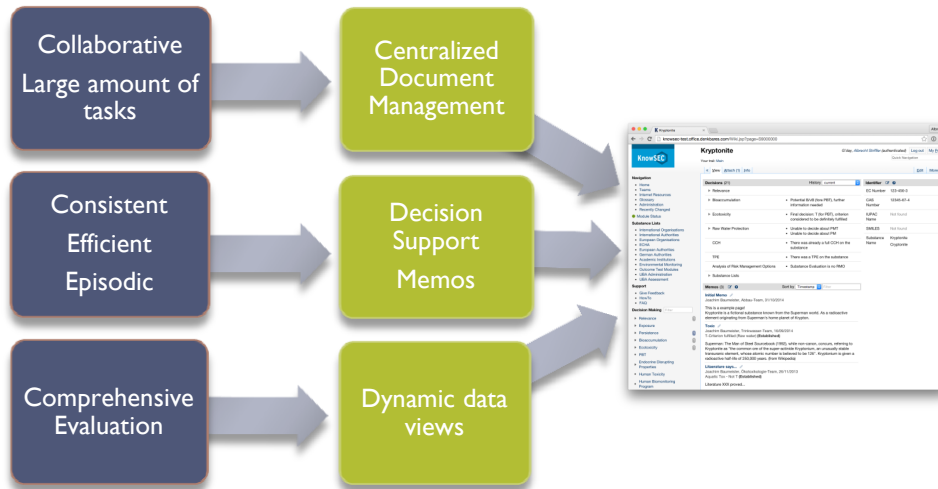
Comprehensive views of data input, memos, and derived decisions

Export to Excel for further evaluation and sharing

	D	E	G	H	I	J	K	L	M	N	2C
1	Name	Decisions	1	M1	2	M2	2A	M2A	2B	M2B	2C
2	1,3,5-triazine-2,4,6-triamine phosphate	UC Mutagenitaet: Komplexer Fall	No	No							
3	2,2',6,6'-Tetrabrom-4,4'-isopropylidendiphenol	UC Mutagenitaet: Komplexer Fall	No	No							
4	2,6-di-tert-butyl-p-cresol	UC Mutagenitaet: Non-compliant	No	No							
5	2-chlorotoluene	UC Mutagenitaet: Non-compliant	No	No							
6	2-chlorotoluene	UC Mutagenitaet: Compliant	No	No							
7	2-vinylpyridine	UC Mutagenitaet: Komplexer Fall	No	No							
8	4,4'-Isopropylidenediphenol, oligomeric reaction	UC Mutagenitaet: Non-compliant	No	No							
9	Decahydronaphthalene	UC Mutagenitaet: Compliant	No	No					Yes		
10	N-(hydroxymethyl)acrylamide	UC Mutagenitaet: Compliant	No	Yes		Yes			Yes		
11	N-(hydroxymethyl)acrylamide	UC Mutagenitaet: Compliant	No	Yes		Yes			Yes		
12	acetylene	UC Mutagenitaet: Compliant	No	No							
13	aluminium	UC Mutagenitaet: Non-compliant	No	No							
14	benzene	UC Mutagenitaet: Compliant	Yes						Yes		
15	butyric acid	UC Mutagenitaet: Compliant	No	No							
16	butyric acid	UC Mutagenitaet: Compliant	No	No							
17	chromium trioxide/chromic acid	UC Mutagenitaet: Komplexer Fall	Yes					No		Yes	
18	cobalt carbonate	UC Mutagenitaet: Komplexer Fall	No	No							
19	copper oxide	UC Mutagenitaet: Non-compliant	No	No							
20	dibutyl phthalate	UC Mutagenitaet: Komplexer Fall	No	No							
21	dicumyl peroxide	UC Mutagenitaet: Compliant	No	No							
22	diisopropyl ether	UC Mutagenitaet: Compliant	No	No							
23	ethylene oxide	UC Mutagenitaet: Komplexer Fall	Yes						No		Yes
24	formaldehyde	UC Mutagenitaet: Komplexer Fall	No	No							
25	glyoxal	UC Mutagenitaet: Compliant	No	No						Yes	
26	glyoxal	UC Mutagenitaet: Compliant	No	No						Yes	
27	isodecyl diphenyl phosphate	UC Mutagenitaet: Compliant	No	No						Yes	
28	lead monoxide	UC Mutagenitaet: Komplexer Fall	No	No							
29	lead monoxide	UC Mutagenitaet: Komplexer Fall	No	No							
30	lithium carbonate	UC Mutagenitaet: Komplexer Fall	No	No							
31	methanol	UC Mutagenitaet: Komplexer Fall	No	No							
32	n-hexane	UC Mutagenitaet: Non-compliant	No	Yes		No					
33	orthophosphoric acid	UC Mutagenitaet: Compliant	No	No							
34	orthophosphoric acid	UC Mutagenitaet: Compliant	No	No							
35	propane/isobutane	UC Mutagenitaet: Non-compliant	No	No							
36	silicon dioxide	UC Mutagenitaet: Compliant	No	No							
37	sodium nitrite	UC Mutagenitaet: Komplexer Fall	No	No							
38	sodium nitrite	UC Mutagenitaet: Non-compliant	No	No							



Summary & Benefits



- ▶ Reduction of working hours
- ▶ Improved quality of results
- ▶ Powerful documentation

Happy to take questions!



Albrecht Striffler



Dirk Wassermann

firstname.lastname@denkbares.com