KnowSEC
A Web-System for Managing Data on Substances

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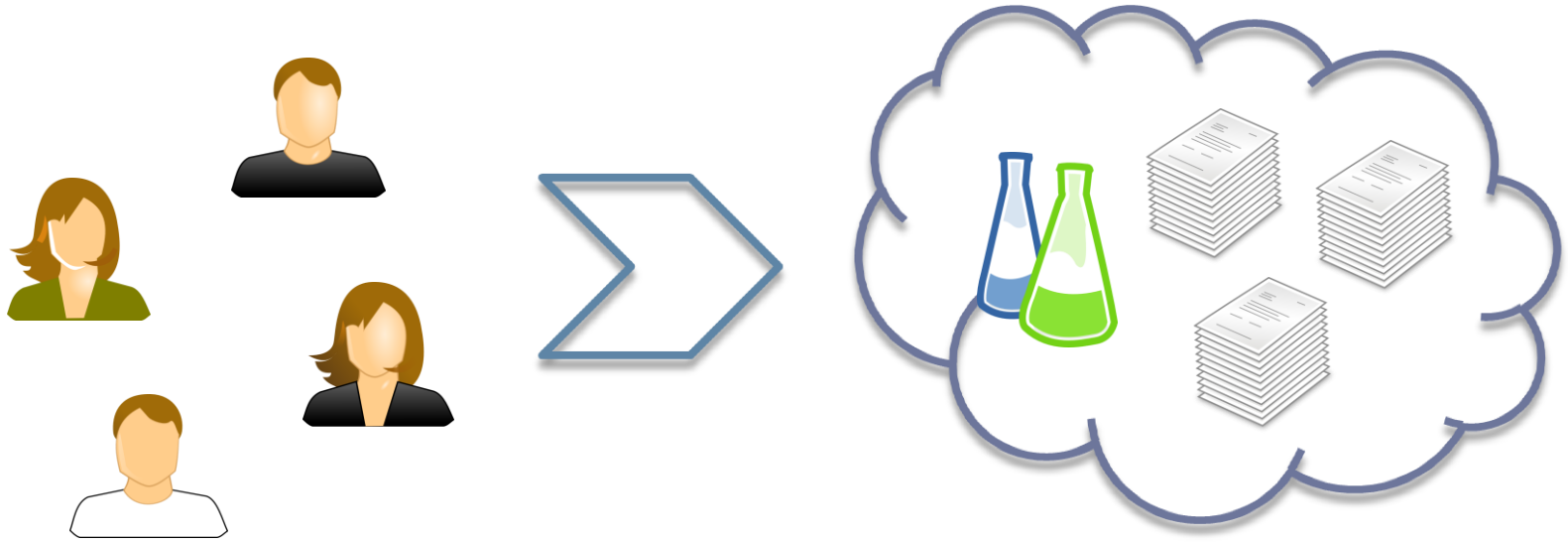
Why am I here, what is KnowSEC?

- 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

denkbares GmbH

- 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



- Large amount of task
- Collaborative
- Episodic

- Efficient
- Consistent

- Comprehensive evaluation
- Documentation

The Concept

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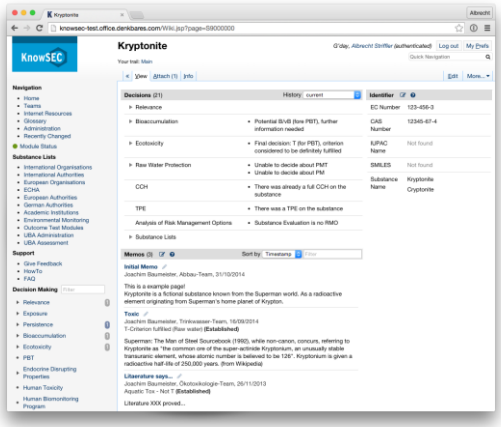
Challenges	Concept	KnowSEC
Collaborative Large amount of tasks	Centralized Document Management	
Consistent Efficient Episodic	Decision Support Memos	
Comprehensive Evaluation	Dynamic data views	



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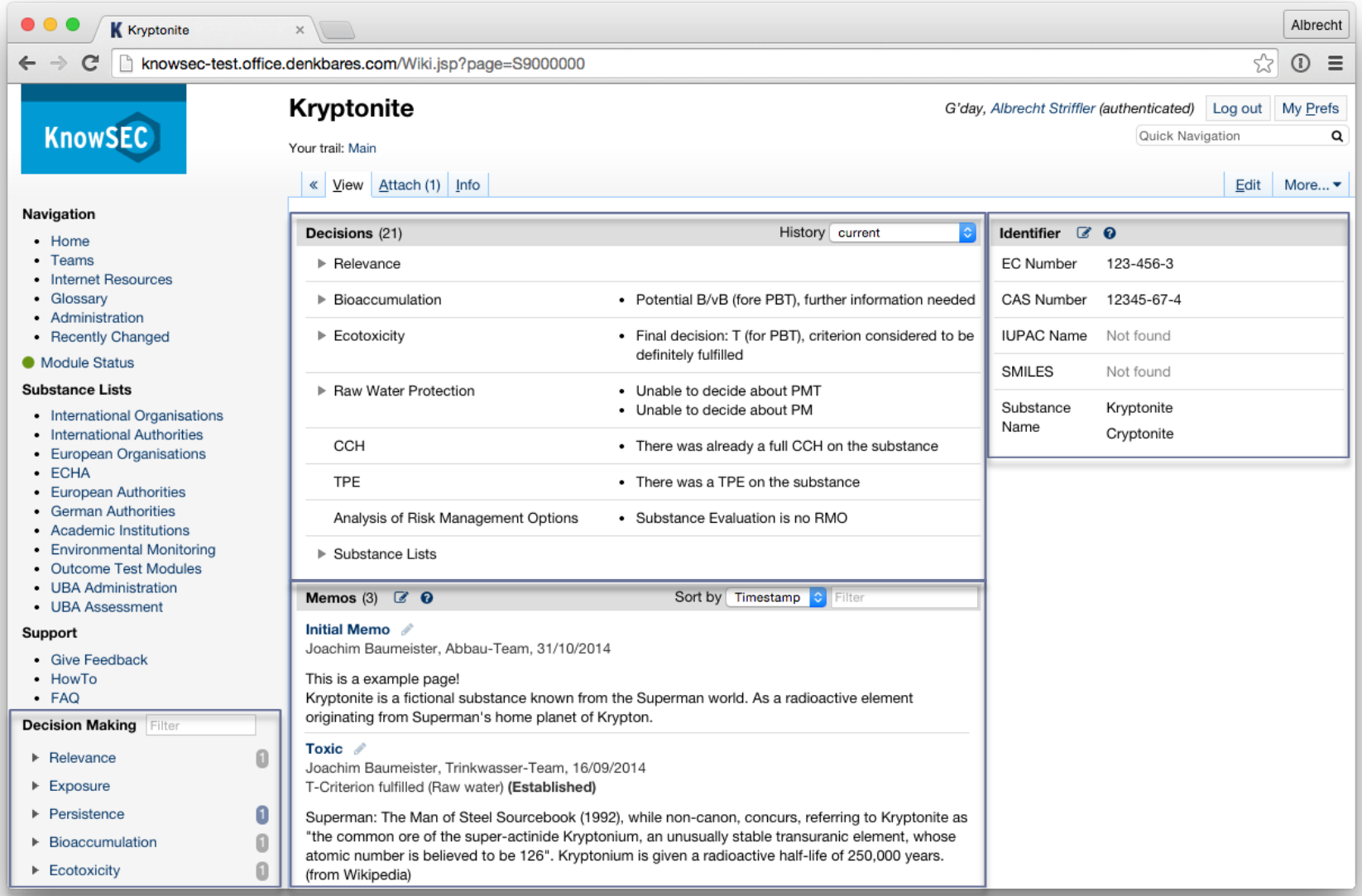
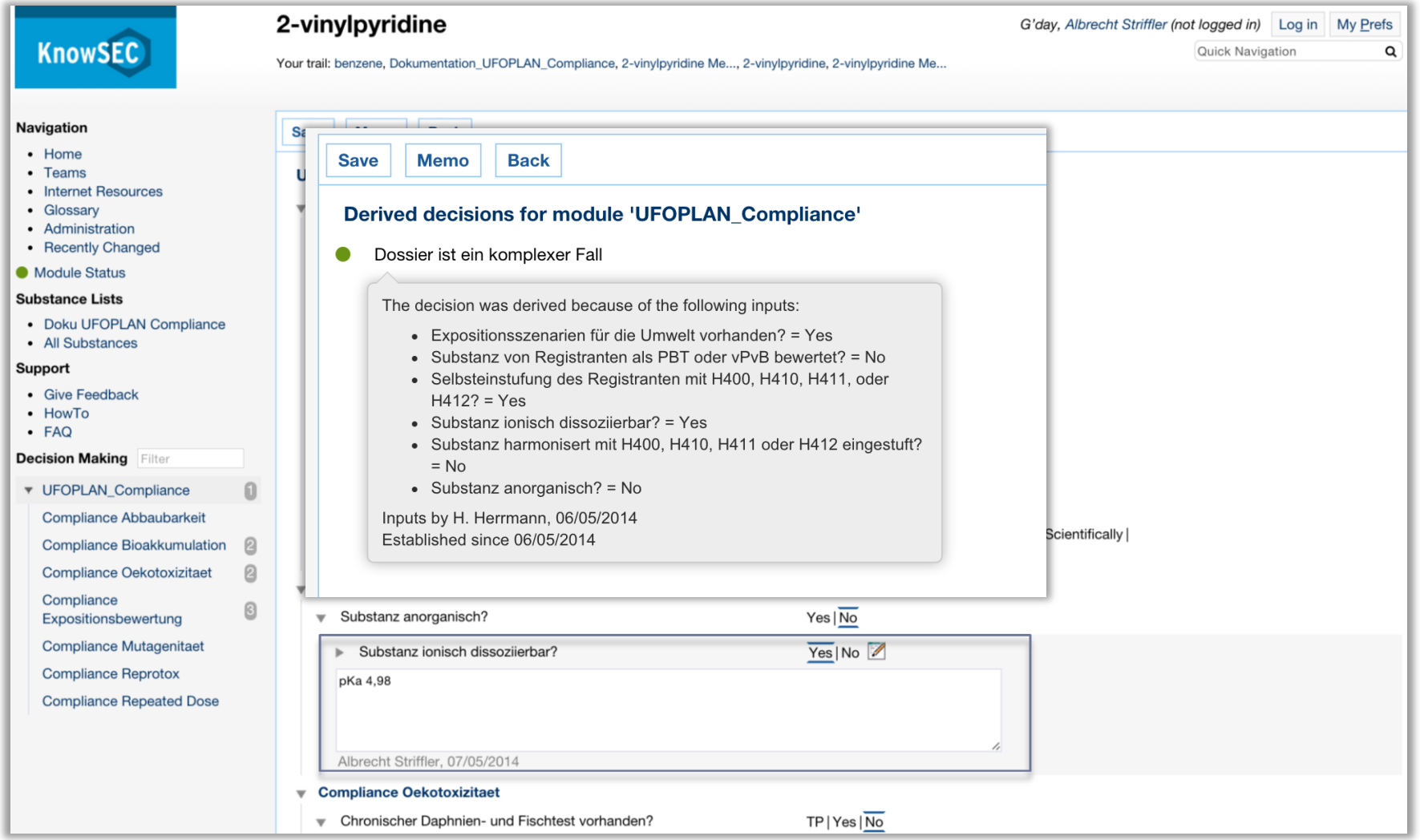
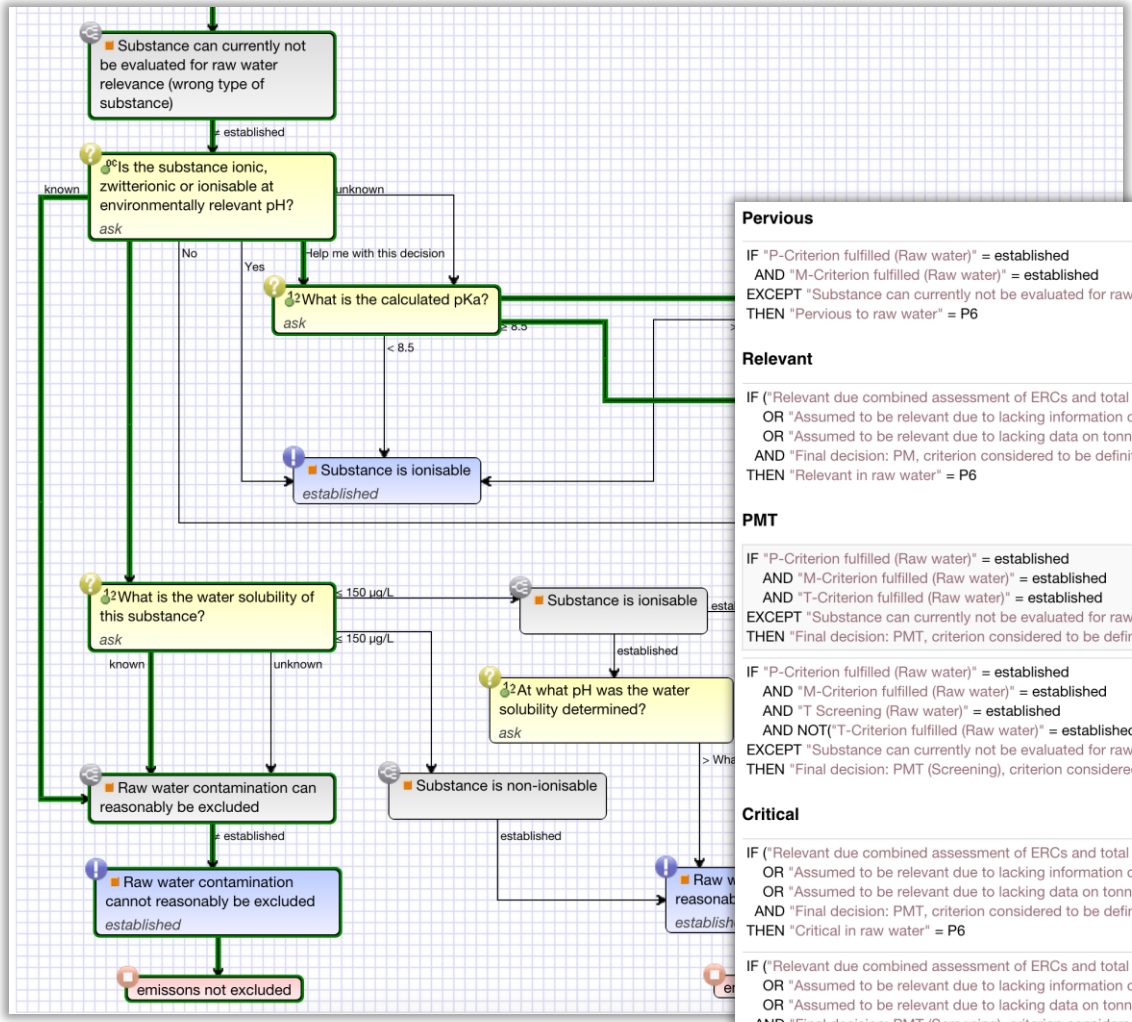


KnowSEC – Decision Support



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

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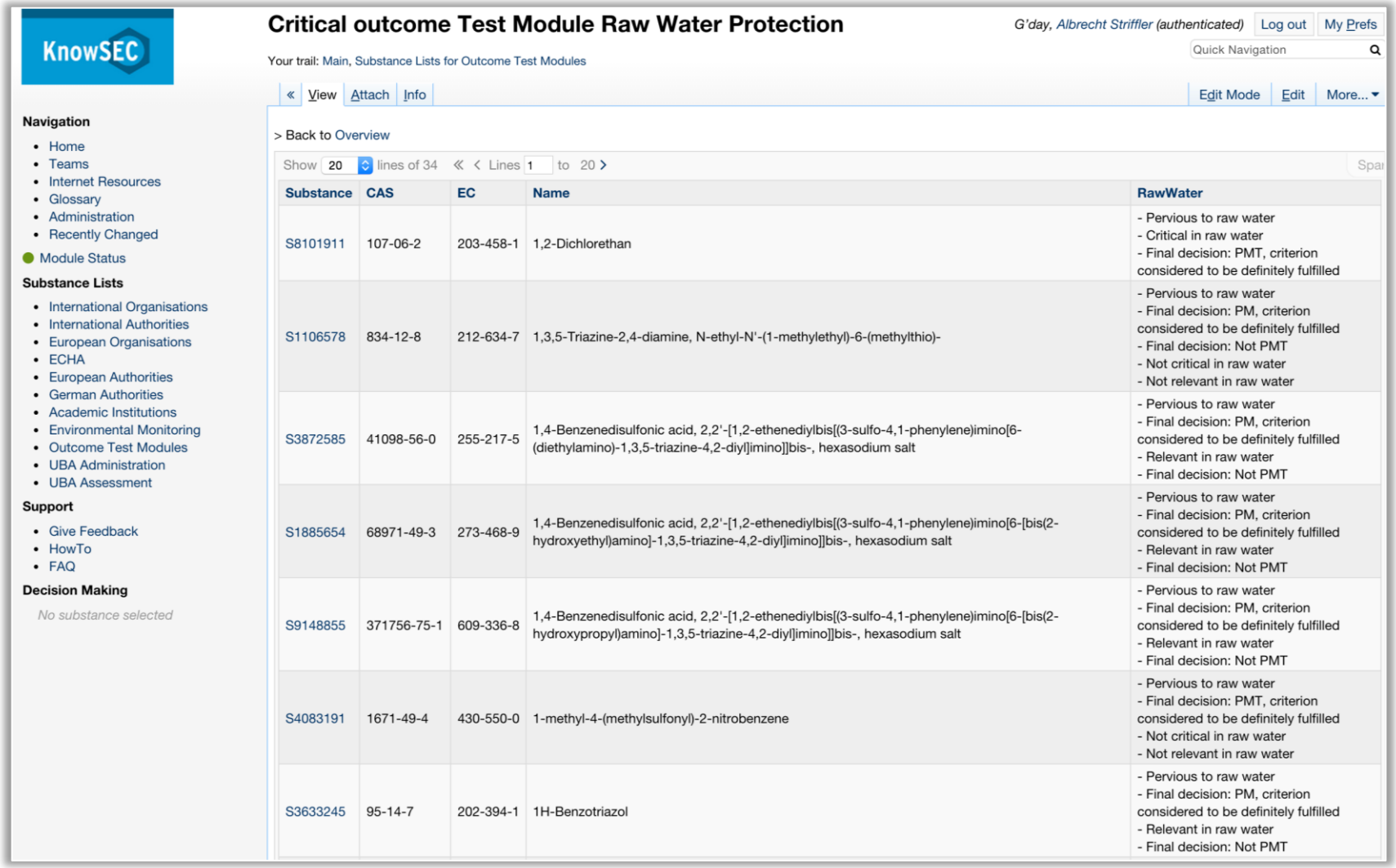

Substance	CAS	EC	Name	RawWater
S8101911	107-06-2	203-458-1	1,2-Dichlorethan	- Pervious to raw water - Critical in raw water - Final decision: PMT, criterion considered to be definitely fulfilled
S1106578	834-12-8	212-634-7	1,3,5-Triazine-2,4-diamine, N-ethyl-N'-(1-methylethyl)-6-(methylthio)-	- Pervious 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-diyl]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-diyl]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-diyl]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

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Gesamtergebnisse

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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 Stude).	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 UCEXPO: 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 UCEXPO: Komplex, weil Expo-Szenarien für Umwelt vorhanden UCEXPO: 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 UCEXPO: Komplex, weil Expo-Szenarien für Umwelt vorhanden UCEXPO: relevante Einstufung vorhanden

How did KnowSEC help BfR?

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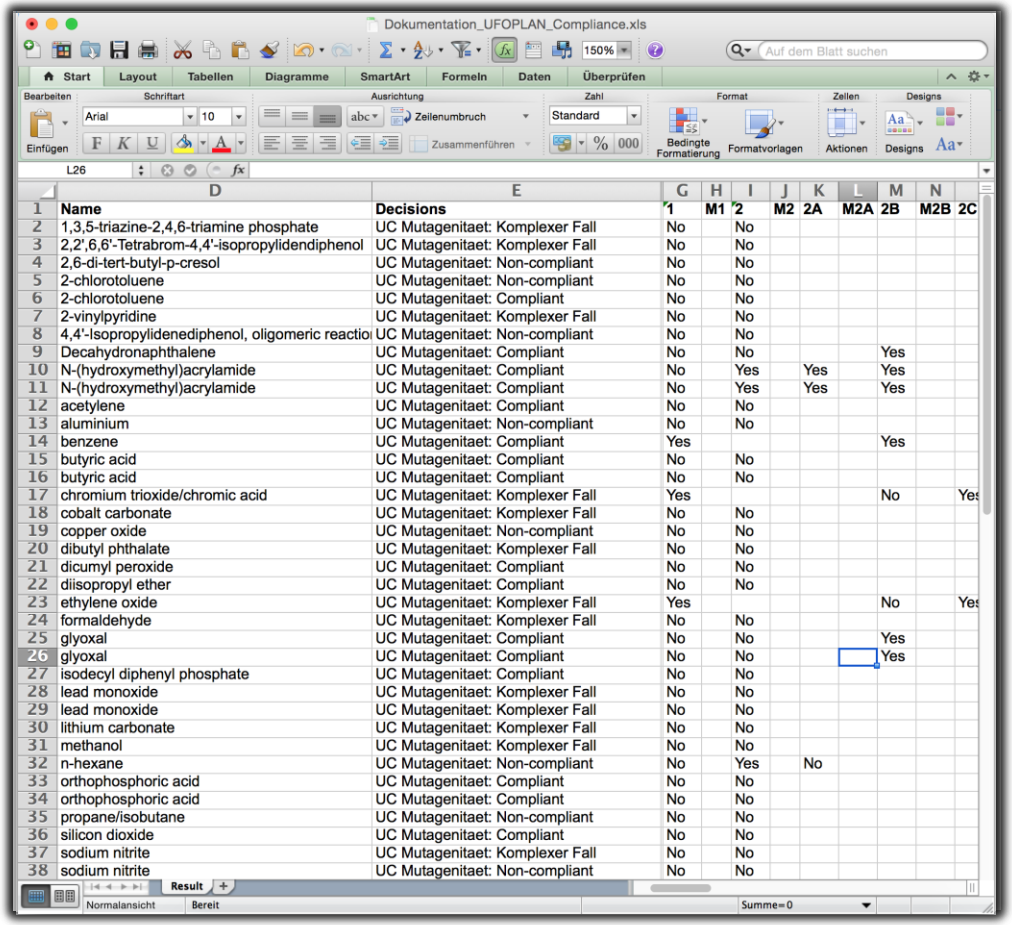
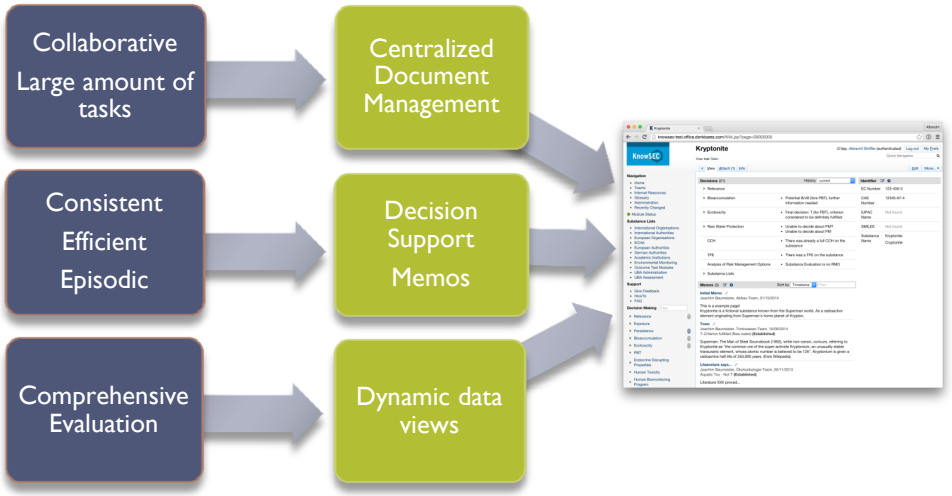
- New decision support module "UFOPLAN compliance"
- Generation of ~2000 dossier pages via Excel import
- Structured evaluation and input of data by BfR employees
- Comprehensive views of data input, memos, and derived decisions
- Export to Excel for further evaluation and sharing



	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 reactio	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						
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!

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