RISK İDENT

Identifizieren | Bewerten

Handeln | Kommunizieren

Screening using databases of environmentally-relevant substances: „STOFF-IDENT“

Dr. Manfred Sengl
Bavarian Environment Agency

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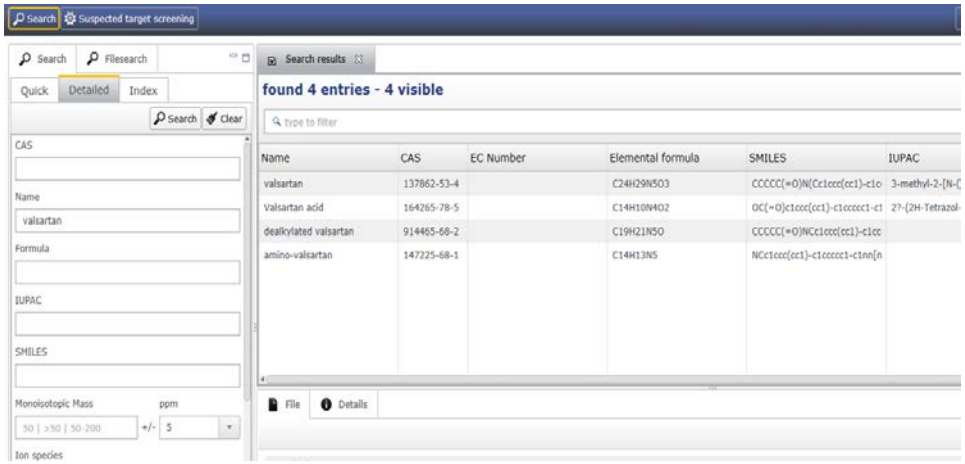
NaWaM RiSKWa FONA
Risikomanagement von neuen Schadstoffen und Krankheitserregern im Wasserkreislauf

Bayerisches Landesamt für Umwelt
HOCHSCHULE WEIHENSTEPHAN-TRIESDORF UNIVERSITY OF APPLIED SCIENCES
Technische Universität München
Zweckverband Landeswasserversorgung
CONDIAS CONDUCTIVE DIAMOND PRODUCTS

Outline

STOFF-IDENT

- database entries
- database features
- database application
- outlook



STOFF-IDENT: database of environmentally-relevant substances

data base entries:

- industrial chemicals (registered under REACH) ca. 4350
- human pharmaceuticals and metabolites ca. 1600
- (veterinary pharmaceuticals)
- pesticides and metabolites ca. 300
- biocides ca. 880
- further substances detected in the aquatic environment (e.g. from target lists of project partners)
- transformation products

▸ total: ca. 8000 entries





Fotos: LfU

REACH

registration time table:

- 1.12.2010: chemicals >1000 t/a
  + R50/53 >100 t/a
  + CMR (category 1+2) ≥1 t/a
- 1.06.2013: chemicals >100 t/a
- 1.06.2018: chemicals 1-100 t/a

- 7.12.2010: 2.992 registrations
- 1.06.2013: 6.600 registrations
- 3.12.2013: 11.766 registrations
- manual removal of anorganic substances, mixtures of substances, intermediates and complexes

STOFF-IDENT: data sets

- name
- CAS-Nr.
- EC-Nr.
- SMILES
- chemical name (IUPAC)
- molecular formula
- exact, monoisotopic mass
- log P_{OW}
- log D_{OW} at pH 3, 5, 7, 9
- volume bands according to REACH
- additional information e.g. water solubility
- substance group, application = category

How to use the database „STOFF-IDENT“ (SI)

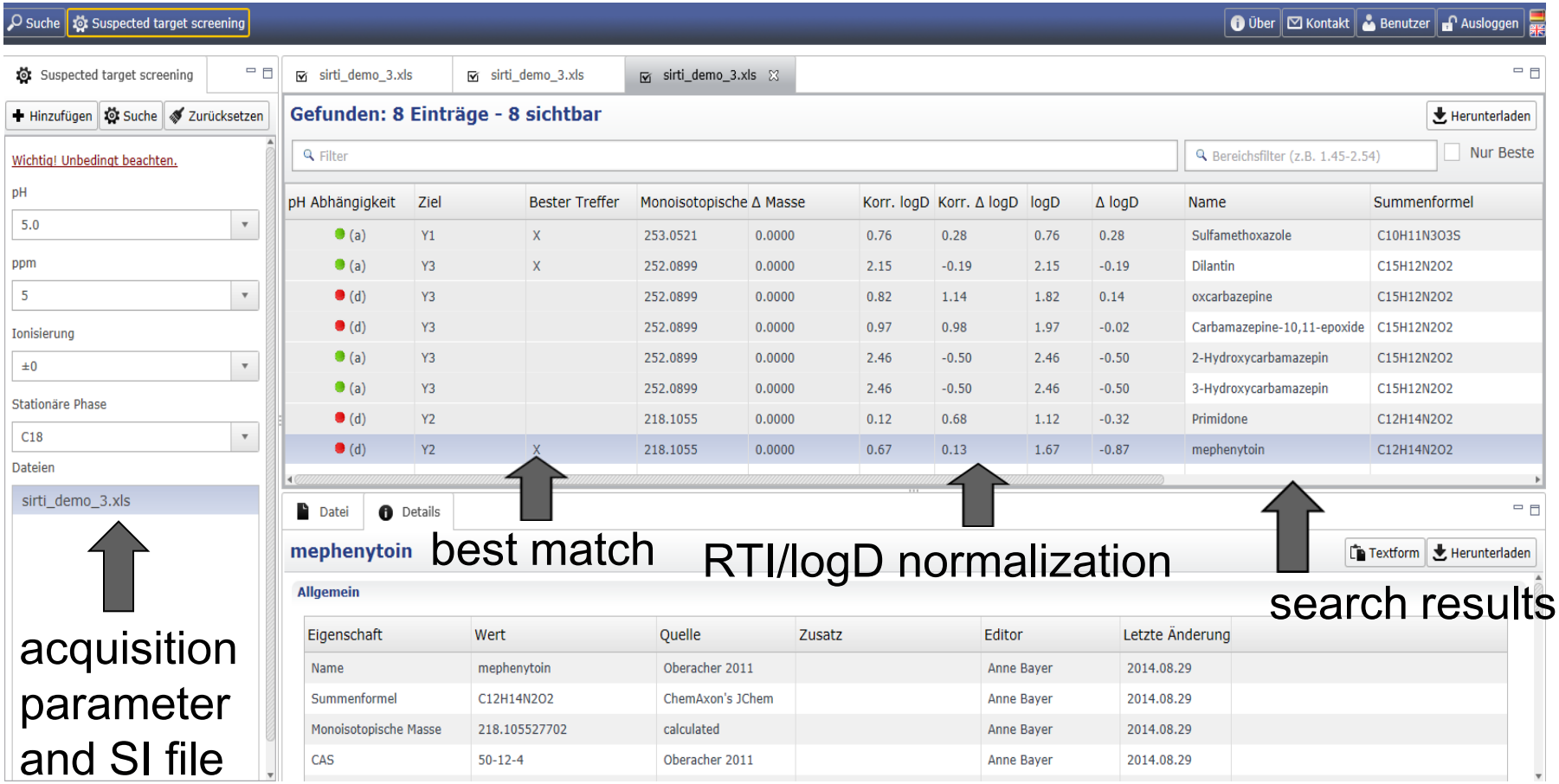
- search for single feature
- upload of search files in Excel-format together with the upload of calibration data for retention time index (RTI)

C9

	A	B	C	D
1	identifier	accurate mass	elemental formula	rt1
2				
3				
4	Y1	253,0521		12,2
5	Y2	218,1055		11,1
6	Y3	252,0898		14,7
7				
8				
9				
10				

	A	B	C	D	E
1	substance name	rt1	rt2	rt3	logP
2					
3					
4	Metformin	1,5	1,5	1,6	-1,36
5	Chloridazon	12,5	12,5	12,4	1,11
6	Carbetamide	14,0	14,1	14,0	1,65
7	Monuron	14,4	14,5	14,4	1,93
8	Metobromuron	17,5	17,6	17,6	2,24
9	Chlorbromuron	18,2	18,2	18,2	2,85
10	Metconazole	20,0	20,0	20,0	3,59
11	Diazinon	20,4	20,4	20,4	4,19
12	Quinoxyfen	22,3	22,3	22,3	4,98
13	Fenofibrate	0,0	0,0	0,0	5,28
14					

How to use the database „STOFF-IDENT“ (SI)



How to use the database „STOFF-IDENT“ (SI)

found 289 entries - 289 visible

type to filter

pH dependency	Target identifier	Best match	Monoisotopic ma	Δ mass	logD	Δ logD	Name
	DEET (N,N-Diethyl-meta-	X	191.1310	0.0005	2.50	-0.36	N,N-diethyl-m-toluamide
	DEET (N,N-Diethyl-meta-		191.1310	0.0005	-1.26	3.40	phendimetrazine
	DEET (N,N-Diethyl-meta-		191.1310	0.0005	2.65	-0.50	N-ethyl-N-(3-methylphenyl)pr
	Metolachlor	X	283.1339	0.0007	3.45	0.22	S-Metolachlor
	Terbutryn		241.1361	0.0004	0.99	1.06	Terbutryn
	Terbutryn	X	241.1361	0.0004	1.12	0.92	Prometryn
	Terbutylazin		229.1094	0.0007	2.23	0.46	propazine
	Terbutylazin		229.1094	0.0007	2.31	0.37	sebuthylazine

green indicates a neutral molecule with logD value between 0.35 – 4.00

How to use the database „STOFF-IDENT“ (SI)

found 1849 entries - 1849 visible

type to filter

pH dependency	Target identifier	Best match	Monoisotopic ma	Δ mass	logD	Δ logD	Name
	Nicosulfuron		410.1009	-0.0006	0.75	1.27	Nicosulfuron
	Oxazepam		286.0509	-0.0001	2.92	-0.45	oxazepam
	Oxazepam		286.0509	-0.0001	1.33	1.15	demoxepam
	Acesulfam		162.9939	-0.0001	-1.71	1.16	Acesulfam-H
	Alachlor-ESA +Acetochl		315.1138	0.0001	3.33	-3.17	bumetrizole
	Alachlor-OXA+Acetochl		265.1314	0.0003	1.95	0.20	CGA 62826 / NOA 409045 (R-I
	2-Naphthalinsulfonsae		208.0194	0.0001	-0.23	1.42	Naphthalin-2-sulfonsäure

red indicates an ionizable molecule

⟹ if the molecule is <u>negatively</u> charged

Δ logD: substract 1 logD value

⟹ i.e. Δ logD = 1.16 - 1.00 = **0.16**

Additional features

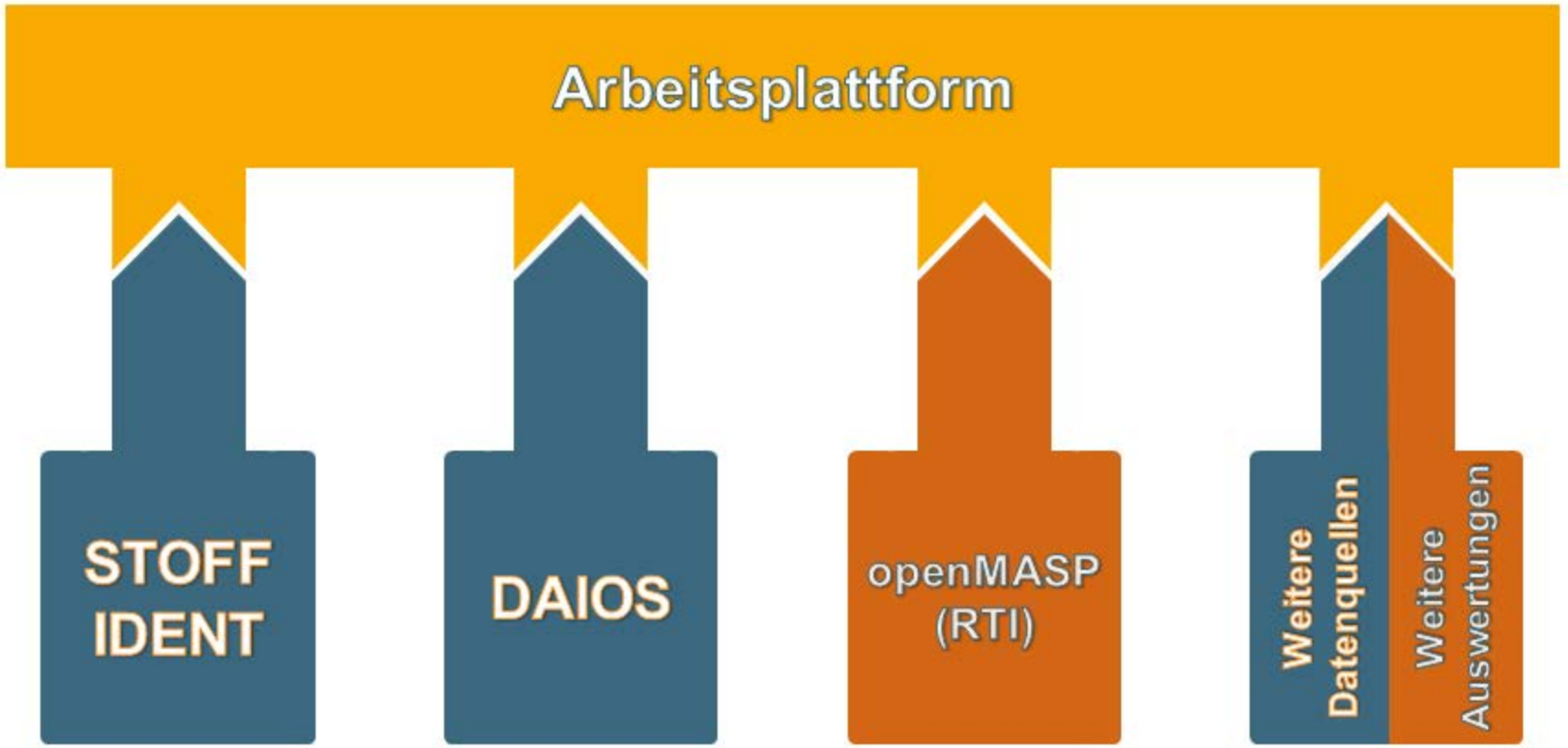
- Links to

  - MassBank data set via MassBank ID
  - chemicalize.org (further physico-chemical properties etc.)
  - ECHA REACH homepage – but no direct link to respective data sheet possible
  - DAIOS (planned)

Outlook

- STOFF-IDENT will be publicly available (homepage LfU) in 2015
- at the moment: login-data can be requested directly at: marco.luthardt@hswt.de
- new REACH chemicals will be inserted on a regular basis
- a follow-up project is planned to create a larger working platform to integrate different tools for non-target analysis (open-source solution)

Outlook: STOFF-IDENT – a part of a greater open-source platform



RISK-IDENT project team February 2014

Thank you very much for your attention!

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