

RISK *Identifizieren | Bewerten*

IDENT *Handeln | Kommunizieren*

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

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CONDIAS
CONDUCTIVE DIAMOND PRODUCTS



Outline

STOFF-IDENT

- database entries
- database features
- database application
- outlook

The screenshot shows the STOFF-IDENT search interface. On the left, there are input fields for CAS, Name (containing 'valsartan'), Formula, IUPAC, and SMILES. Below these is a 'Monoisotopic Mass' field with a range of '30 | >30 | 30-200' and a tolerance of '5 ppm'. The main search results area on the right displays 'found 4 entries - 4 visible' and a table with the following data:

Name	CAS	EC Number	Elemental formula	SMILES	IUPAC
valsartan	137862-53-4		C ₂₄ H ₂₉ N ₅ O ₃	CCCCC(=O)N(Cc1ccc(cc1)-c1c	3-methyl-2-[N-(
Valsartan acid	164265-78-5		C ₁₄ H ₁₀ N ₄ O ₂	OC(=O)c1ccc(cc1)-c1ccc1-c1	2'-[2H-Tetraazol
dealkylated valsartan	914465-68-2		C ₁₉ H ₂₁ N ₅ O	CCCCC(=O)NCC1ccc(cc1)-c1cc	
amino-valsartan	147225-68-1		C ₁₄ H ₁₃ N ₅	NC1ccc(cc1)-c1ccc1-c1n[n]	

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



Screening using databases: STOFF-IDENT

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	identifizier	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	Quinoxifen	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)

Suche **Suspected target screening** Über Kontakt Benutzer Ausloggen

Suspected target screening sirti_demo_3.xls sirti_demo_3.xls sirti_demo_3.xls

Hinzufügen Suche Zurücksetzen

Wichtig! Unbedingt beachten.

pH: 5.0
ppm: 5
Ionisierung: ±0
Stationäre Phase: C18
Dateien: sirti_demo_3.xls

Gefunden: 8 Einträge - 8 sichtbar Herunterladen

Filter Bereichsfilter (z.B. 1.45-2.54) Nur Beste

pH Abhängigkeit	Ziel	Beste(r) Treffer	Monoisotopische Δ Masse	Korr. logD	Korr. Δ logD	logD	Δ logD	Name	Summenformel
● (a)	Y1	X	253.0521	0.76	0.28	0.76	0.28	Sulfamethoxazole	C10H11N3O3S
● (a)	Y3	X	252.0899	2.15	-0.19	2.15	-0.19	Dilantin	C15H12N2O2
● (d)	Y3		252.0899	0.82	1.14	1.82	0.14	oxcarbazepine	C15H12N2O2
● (d)	Y3		252.0899	0.97	0.98	1.97	-0.02	Carbamazepine-10,11-epoxide	C15H12N2O2
● (a)	Y3		252.0899	2.46	-0.50	2.46	-0.50	2-Hydroxycarbamazepin	C15H12N2O2
● (a)	Y3		252.0899	2.46	-0.50	2.46	-0.50	3-Hydroxycarbamazepin	C15H12N2O2
● (d)	Y2		218.1055	0.12	0.68	1.12	-0.32	Primidone	C12H14N2O2
● (d)	Y2	X	218.1055	0.67	0.13	1.67	-0.87	mephenytoin	C12H14N2O2

↑ acquisition parameter and SI file

↑ best match

↑ RTI/logD normalization

↑ search results

mephenytoin Details Textform Herunterladen

Allgemein

Eigenschaft	Wert	Quelle	Zusatz	Editor	Letzte Änderung
Name	mephenytoin	Oberacher 2011		Anne Bayer	2014.08.29
Summenformel	C12H14N2O2	ChemAxon's JChem		Anne Bayer	2014.08.29
Monoisotopische Masse	218.105527702	calculated		Anne Bayer	2014.08.29
CAS	50-12-4	Oberacher 2011		Anne Bayer	2014.08.29

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

found 289 entries - 289 visible

type to filter

pH dependency	Target identifier	Best match	Monoisotopic mass	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 m _r	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	5.33	-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 negatively charged

Δ logD: subtract 1 logD value

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

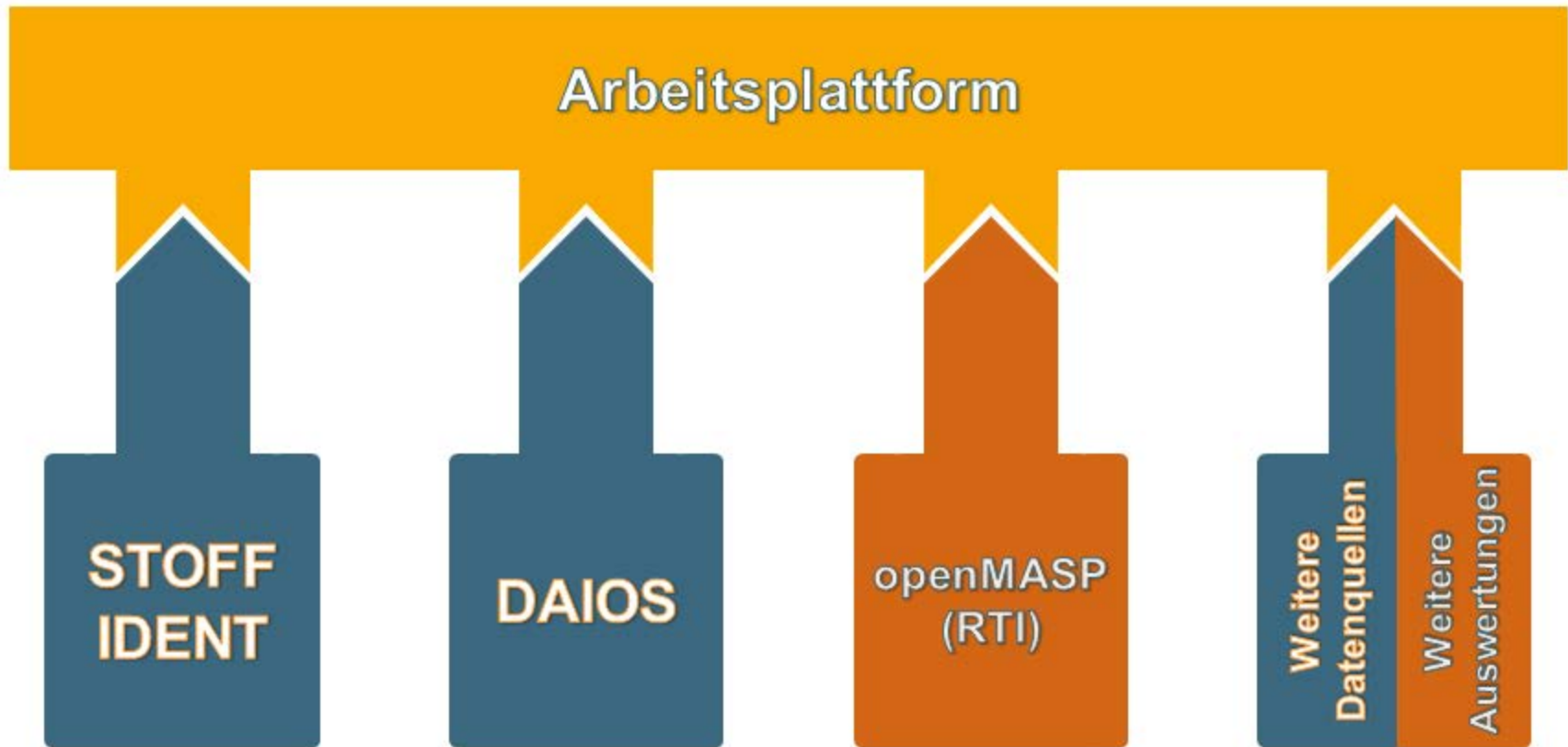
Additional features

- 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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