

GEFÖRDERT VOM



Bundesministerium
für Bildung
und Forschung

FOR 
IDENT

an example in an analytical workflow out of the FOR-IDENT Initiative



Bayerisches Landesamt für
Umwelt



HOCHSCHULE
WEIHENSTEPHAN-TRIESDORF
UNIVERSITY OF APPLIED SCIENCES



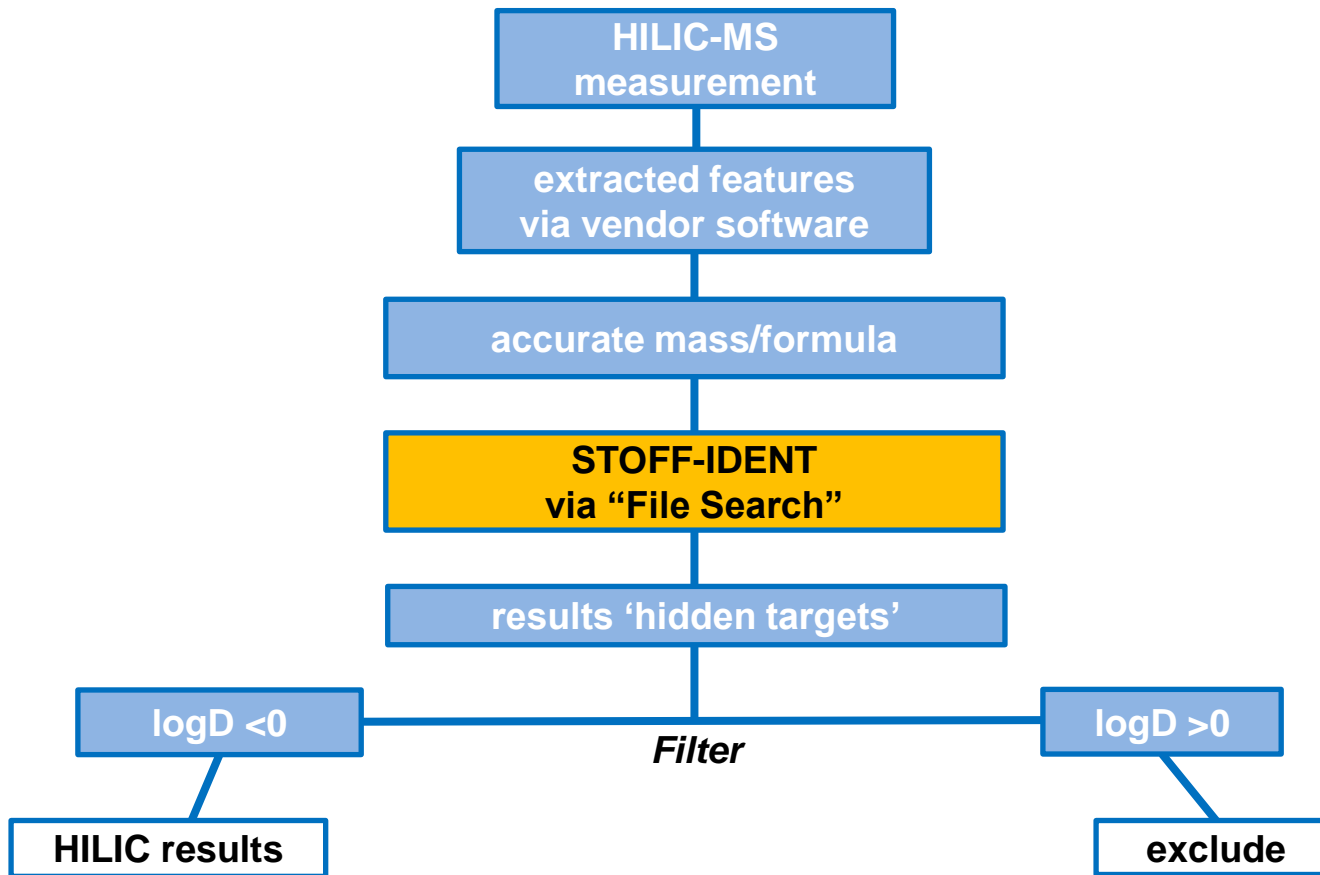
TUM

Technische Universität München

Zweckverband
Landeswasserversorgung



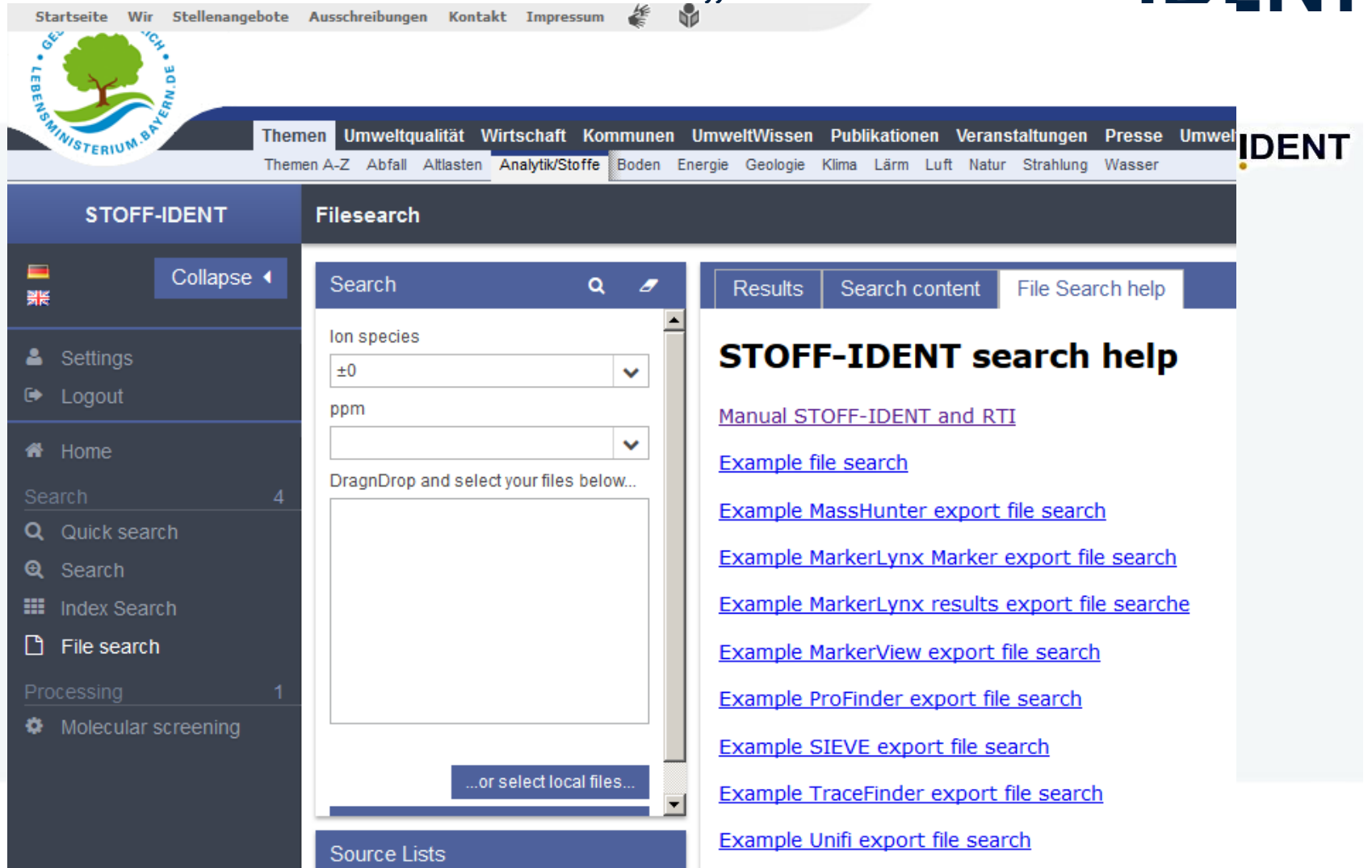
Workflow non-target/ hidden-target Screening polar molecules (HILIC)



HILIC- Detected Masses

P12		f_x			
	A	B	C	D	E
1	Compound	Formula	Mass	RT	CAS ID
2			224.0223	5.16	
3			167.018	5.16	
4			267.9731	5.18	
5			443.2352	5.98	
6			192.134	6	
7			485.2456	6	
8			266.1711	6.03	
9			286.0748	6.05	
10			231.1825	6.05	
11			327.2252	6.06	

HILIC- STOFF-IDENT „Filesearch“



The screenshot shows the STOFF-IDENT Filesearch interface. At the top, there is a navigation bar with links: Startseite, Wir, Stellenangebote, Ausschreibungen, Kontakt, Impressum. Below this is a logo for the LEBENS-MINISTERIUM BAYERN DE. The main navigation bar includes: Themen, Umweltqualität, Wirtschaft, Kommunen, UmweltWissen, Publikationen, Veranstaltungen, Presse, Umwelt. A secondary bar lists: Themen A-Z, Abfall, Altlasten, Analytik/Stoffe, Boden, Energie, Geologie, Klima, Lärm, Luft, Natur, Strahlung, Wasser.

The interface is divided into two main sections:

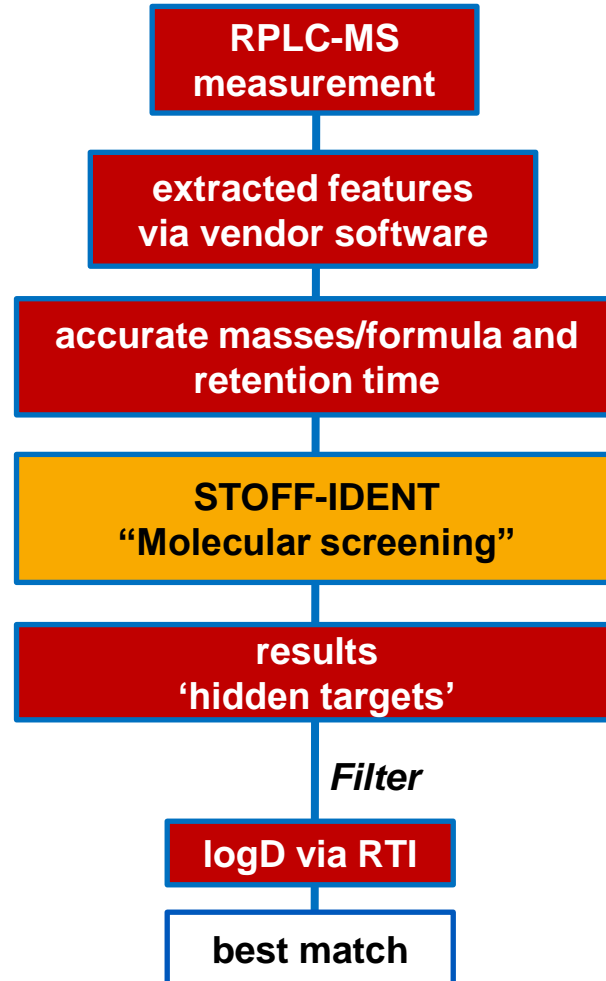
- Left Sidebar (STOFF-IDENT):** Contains a language selector (German, English), a 'Collapse' button, and a menu with items: Settings, Logout, Home, Search (4), Quick search, Search, Index Search, File search, Processing (1), and Molecular screening.
- Main Content Area (Filesearch):**
 - Search bar with a magnifying glass icon.
 - Input fields for 'Ion species' (value: ±0) and 'ppm'.
 - A 'DragDrop and select your files below...' area with a large empty box.
 - A button labeled '...or select local files...'.
 - A 'Source Lists' section at the bottom.
- Right Panel (STOFF-IDENT search help):** Contains a 'Results' tab, a 'Search content' tab, and a 'File Search help' link. Below this is a list of example search results:
 - [Manual STOFF-IDENT and RTI](#)
 - [Example file search](#)
 - [Example MassHunter export file search](#)
 - [Example MarkerLynx Marker export file search](#)
 - [Example MarkerLynx results export file searche](#)
 - [Example MarkerView export file search](#)
 - [Example ProFinder export file search](#)
 - [Example SIEVE export file search](#)
 - [Example TraceFinder export file search](#)
 - [Example Unifi export file search](#)

HILIC- LogD Filter

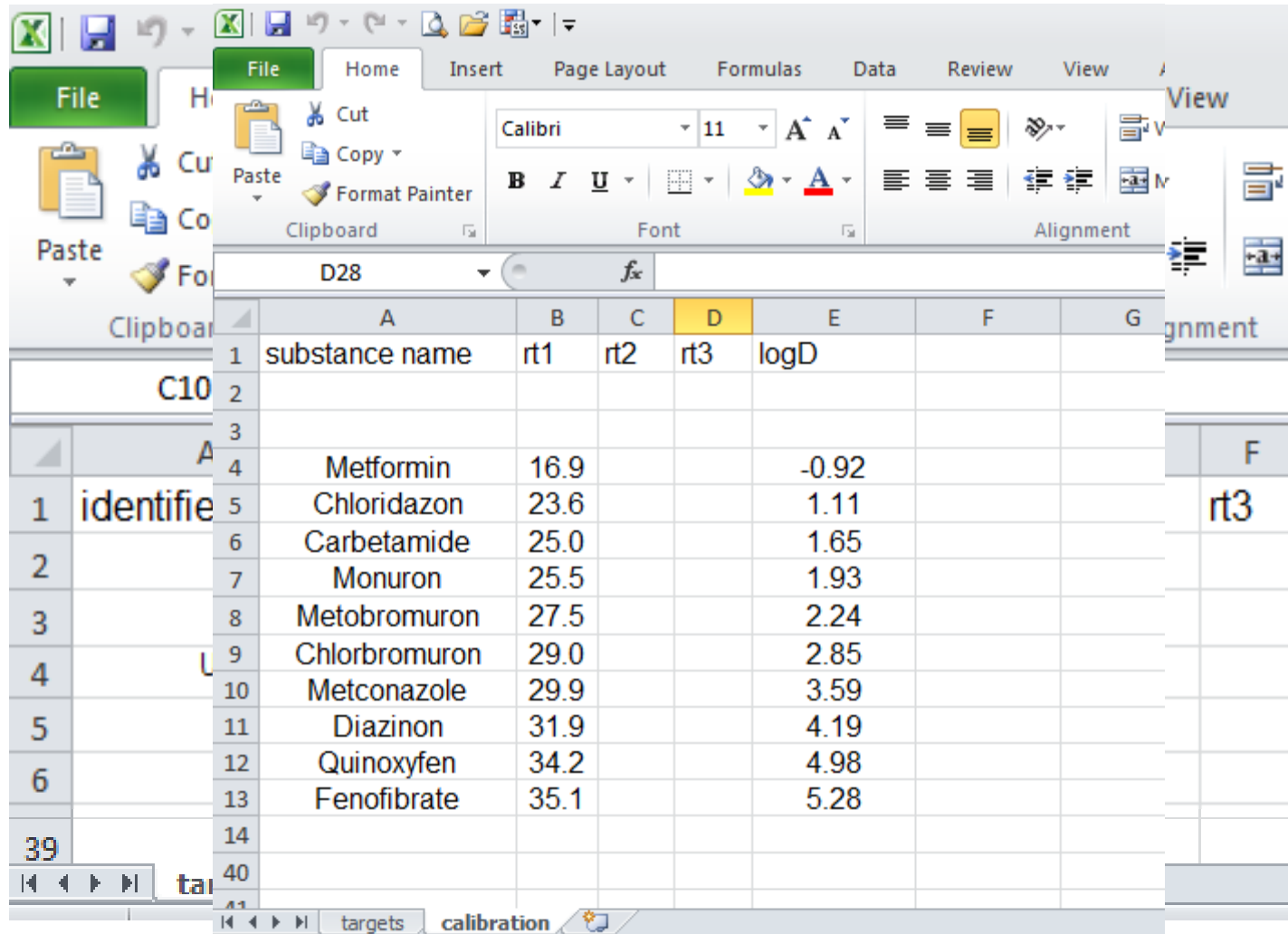
	A	B	C	D	E	F
1		Ziel	Δ Masse	CAS	logD	Name
2	14	SI generated 57	0.0006	108-80-5	-1.1	1,3,5-triazinane-2,4,6-trione
3	33	SI generated 146	-0.0003	1852-17-1	-1	perhydropyrimidin-2-one
4	96	SI generated 347	0.0004	459-73-4	-1	ethyl glycinate
5	10	SI generated 28	0.0003		-0.3	2-[(dimethylamino)methyl]cyclo
6	31	SI generated 144	0.0002		-0.3	2-[(dimethylamino)methyl]cyclo
7	9	SI generated 28	0.0003	826-36-8	-0.3	2,2,6,6-tetramethyl-4-piperidone
8	30	SI generated 144	0.0002	826-36-8	-0.3	2,2,6,6-tetramethyl-4-piperidone
9	16	SI generated 79	-0.0004	69-89-6	-0.3	xanthine
10	2	SI generated 8	0.0002	143-24-8	-0.1	tetraglyme
11	5	SI generated 24	-0.0005	1672-58-8	0.11	N-Formyl-4-aminoantipyrin
12	26	SI generated 117	0.0008	75-05-8	0.12	N-(dimethylvinylsilyl)-1,1-dimeth
13	7	SI generated 23	-0.0003	75-05-8	0.15	N-Acetyl-4-aminoantipyrin
14	22	SI generated 116	-0.0003	818-61-1	0.22	2-hydroxyethyl acrylate

delete

Workflow non-target/ hidden-target Screening nonpolar molecules (RPLC)

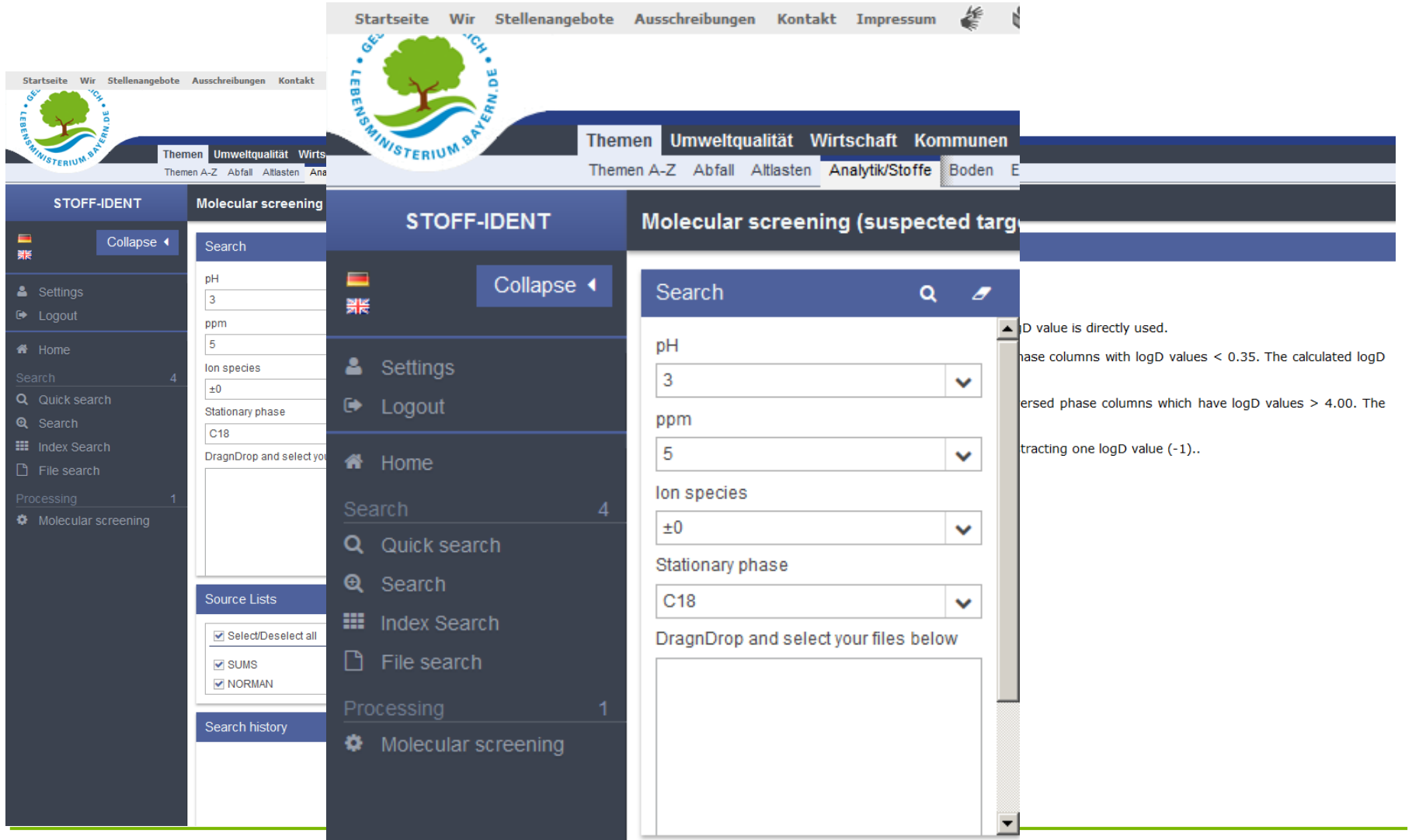


RPLC- Deteced Masses and retention time



	A	B	C	D	E	F	G
1	substance name	rt1	rt2	rt3	logD		
2							
3							
4	Metformin	16.9			-0.92		F
5	Chloridazon	23.6			1.11		rt3
6	Carbetamide	25.0			1.65		
7	Monuron	25.5			1.93		
8	Metobromuron	27.5			2.24		
9	Chlorbromuron	29.0			2.85		
10	Metconazole	29.9			3.59		
11	Diazinon	31.9			4.19		
12	Quinoxyfen	34.2			4.98		
13	Fenofibrate	35.1			5.28		
14							
15							
16							
17							
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41							

RPLC- STOFF-IDENT „molecular screening“



The screenshot displays the RPLC-STOFF-IDENT molecular screening interface. The main search area includes the following parameters:

- pH:** 3
- ppm:** 5
- Ion species:** ±0
- Stationary phase:** C18

The interface also features a sidebar menu with the following items:

- Settings
- Logout
- Home
- Search (4)
- Quick search
- Search
- Index Search
- File search
- Processing (1)
- Molecular screening

Below the search parameters, there is a section for **Source Lists** with the following options:

- Select/Deselect all
- SUMS
- NORMAN

At the bottom of the interface, there is a **Search history** section.

logD value is directly used.
 phase columns with logD values < 0.35. The calculated logD
 reversed phase columns which have logD values > 4.00. The
 subtracting one logD value (-1)..

RPLC- Results and Download

Results		Search content		Help		found 35, 35 visible		Fixed Co	
Target	Rt	pH dep	Score	Best	Target mass	Δ mass	RTI		
<input type="text"/>	<input type="text"/>			<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
Unknown Y	23.6	●	<div style="width: 100%; height: 10px; background-color: green;"></div>	●	164.0950	0.0099	82.7		
Unknown Y	23.6	●	<div style="width: 90%; height: 10px; background-color: green;"></div>		164.0950	0.0252	82.7		
Unknown Y	23.6	●	<div style="width: 90%; height: 10px; background-color: green;"></div>		164.0950	0.0252	82.7		

Please note:

- Green indicates neutral molecules with logD values between 0.35 – 4.00. The calculated logD value is directly used.
- Yellow indicates neutral molecules but they are in the lower hydrophobicity of reversed phase columns with logD values < 0.35. The calculated logD value is corrected by subtracting one logD value (-1).
- Purple indicates neutral molecules but they are in the higher hydrophobicity range of reversed phase columns which have logD values > 4.00. The calculated logD value is corrected by adding one logD value (+1).
- Blue indicates negatively charged molecules. The calculated logD value is corrected by subtracting one logD value (-1)..
- Red indicates positively charged molecules. The calculated logD value is directly used.








RPLC- Results and Download

Results		Search content	Help	found 35, 35 visible					Fixed Columns
Target	Rt	pH dep	Score	Best	logD DB	logD RTI	Δ logD (RTI-DB)		
<input type="text"/>	<input type="text"/>			<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	
Unknown Y	23.6	●	<div style="width: 100%; height: 10px; background-color: green;"></div>	●	0.09	1.11	1.02		
Unknown Y	23.6	●	<div style="width: 90%; height: 10px; background-color: green;"></div>		3.73	1.11	-2.62		
Unknown Y	23.6	●	<div style="width: 90%; height: 10px; background-color: green;"></div>		3.73	1.11	-2.62		






Please note:

- Green indicates neutral molecules with logD values between 0.35 – 4.00. The calculated logD value is directly used.
- Yellow indicates neutral molecules but they are in the lower hydrophobicity of reversed phase columns with logD values < 0.35. The calculated logD value is corrected by subtracting one logD value (-1).
- Purple indicates neutral molecules but they are in the higher hydrophobicity range of reversed phase columns which have logD values > 4.00. The calculated logD value is corrected by adding one logD value (+1).
- Blue indicates negatively charged molecules. The calculated logD value is corrected by subtracting one logD value (-1)..
- Red indicates positively charged molecules. The calculated logD value is directly used.

RPLC- Results and Download

Results	Search content	Help	found 35, 35 visible					Fixed Columns
Target	Rt	pH dep	Score	Best	adj. logD RTI	Δ logD (adj.-DB)	Name	
Unknown Y	23.6				0.11	0.02	2,5,7,10-tetraoxaundecane	
Unknown Y	23.6				1.11	-2.62	6-tert-butyl-m-cresol	
Unknown Y	23.6				1.11	-2.62	2-tert-butyl-p-cresol	

Please note:

-  Green indicates neutral molecules with logD values between 0.35 – 4.00. The calculated logD value is directly used.
-  Yellow indicates neutral molecules but they are in the lower hydrophobicity of reversed phase columns with logD values < 0.35. The calculated logD value is corrected by subtracting one logD value (-1).
-  Purple indicates neutral molecules but they are in the higher hydrophobicity range of reversed phase columns which have logD values > 4.00. The calculated logD value is corrected by adding one logD value (+1).
-  Blue indicates negatively charged molecules. The calculated logD value is corrected by subtracting one logD value (-1)..
-  Red indicates positively charged molecules. The calculated logD value is directly used.

RPLC- Results- Score, Proposed Best match and Download

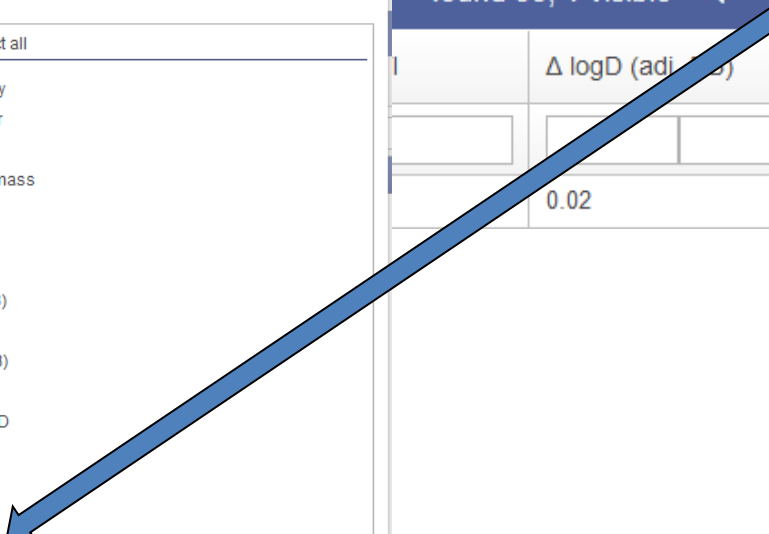
Results	Search content	pH
Unknown Y	23.6	

Export Results

Filename (max.255)
results.xls

Include Sources?

Categories

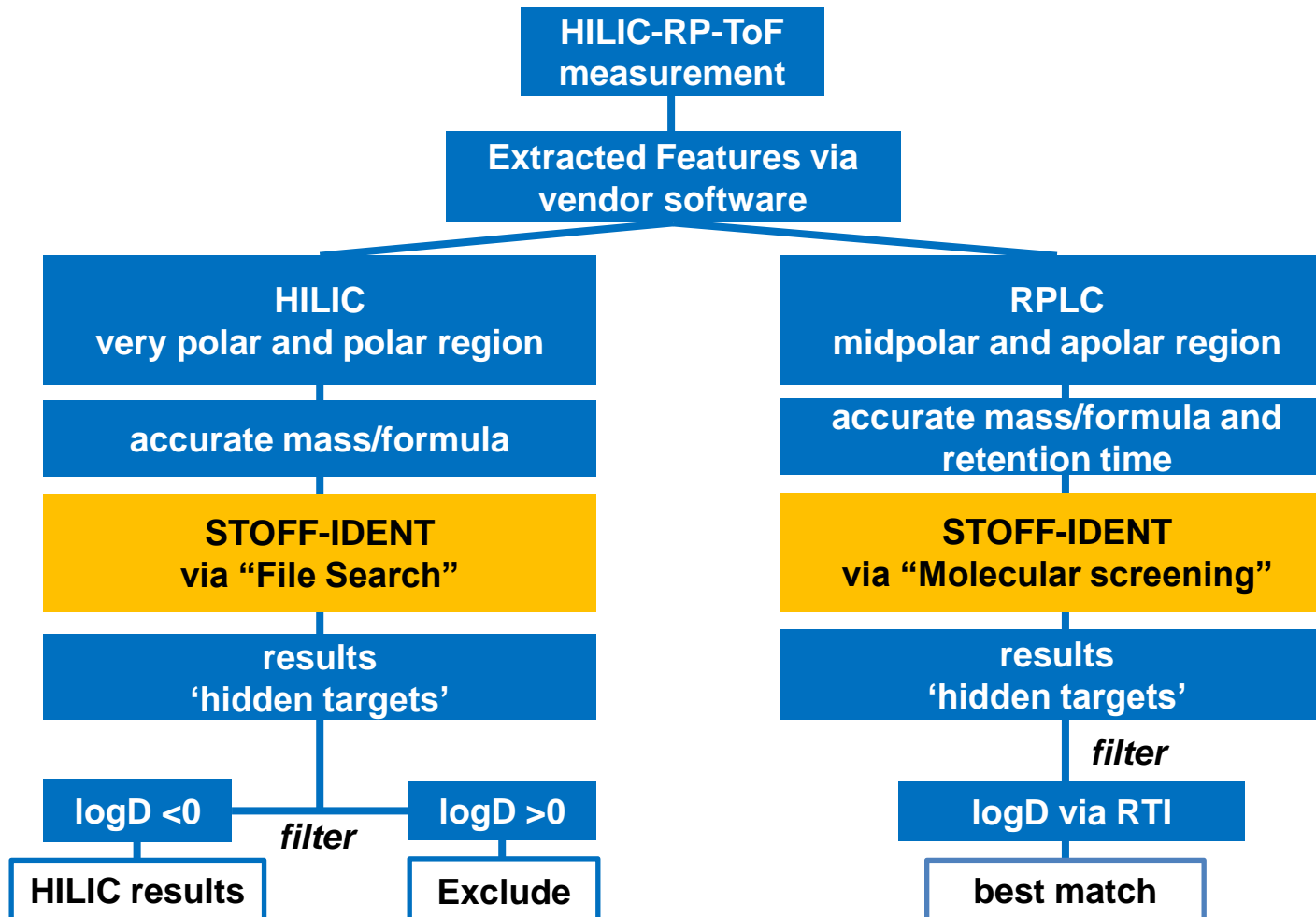
- Select/Deselect all
- pH dependency
- Target identifier
- Best match
- Monoisotopic mass
- Δ mass
- logD DB
- logD RTI
- Δ logD (RTI-DB)
- Adj. logD RTI
- Δ logD (Adj.-DB)
- Structure
- STOFFIDENT-ID
- CAS
- Name
- SMILES 
- InChi
- InChi key
- IUPAC
- Elemental formula
- logP
- logD
- Tonnage
- RTI
- MassBank
- Additional names
- Categories

Download Close

found 35, 1 visible

Δ logD (adj. DB)	Name
0.02	2,5,7,10-tetraoxaundecane

Workflow non-target/ hidden-target Screening polar molecules (HILIC) and nonpolar molecules (RPLC)



Open-Access Platform ,FOR-IDENT‘

