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

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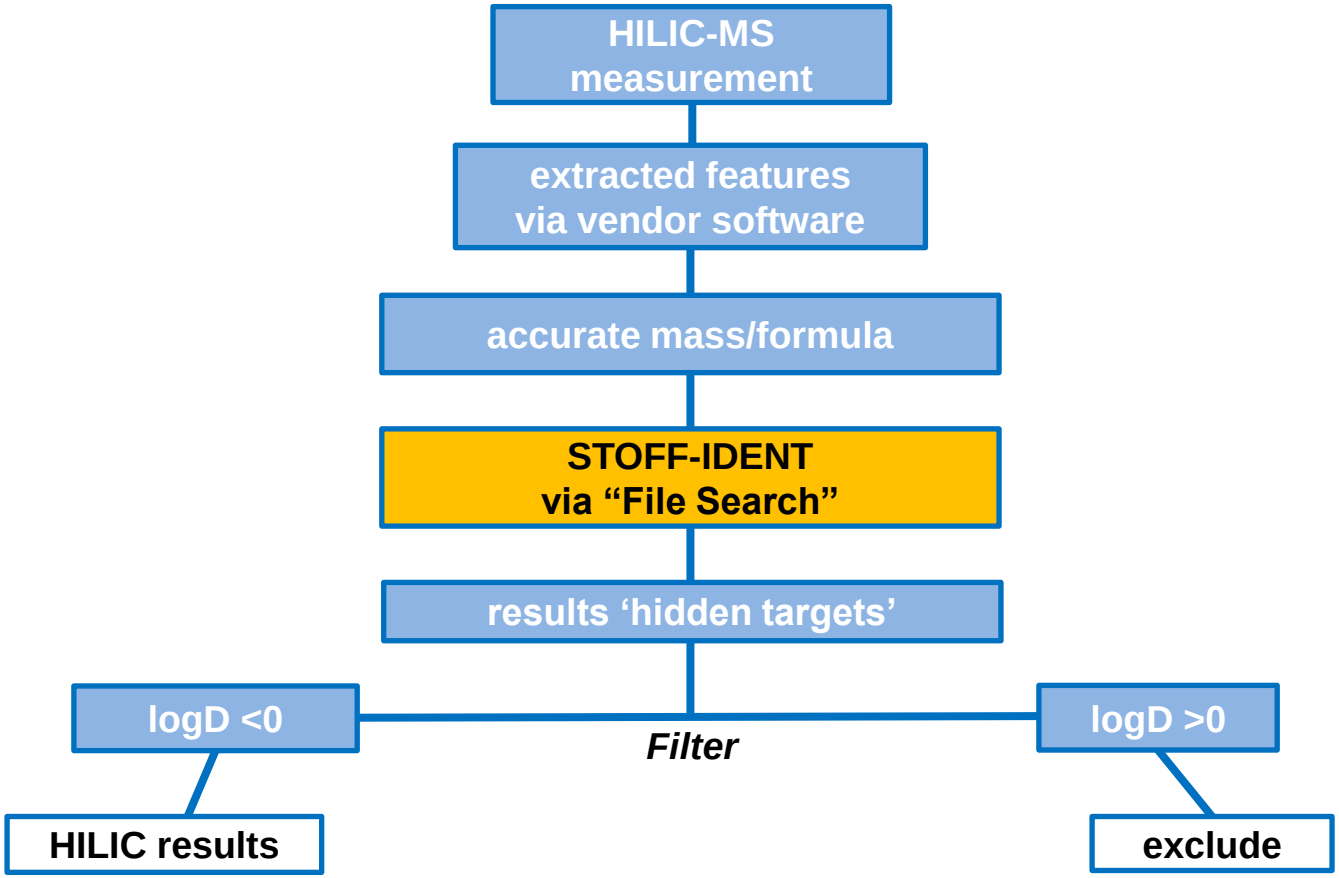
Workflow non-target/ hidden-target Screening polar molecules (HILIC)

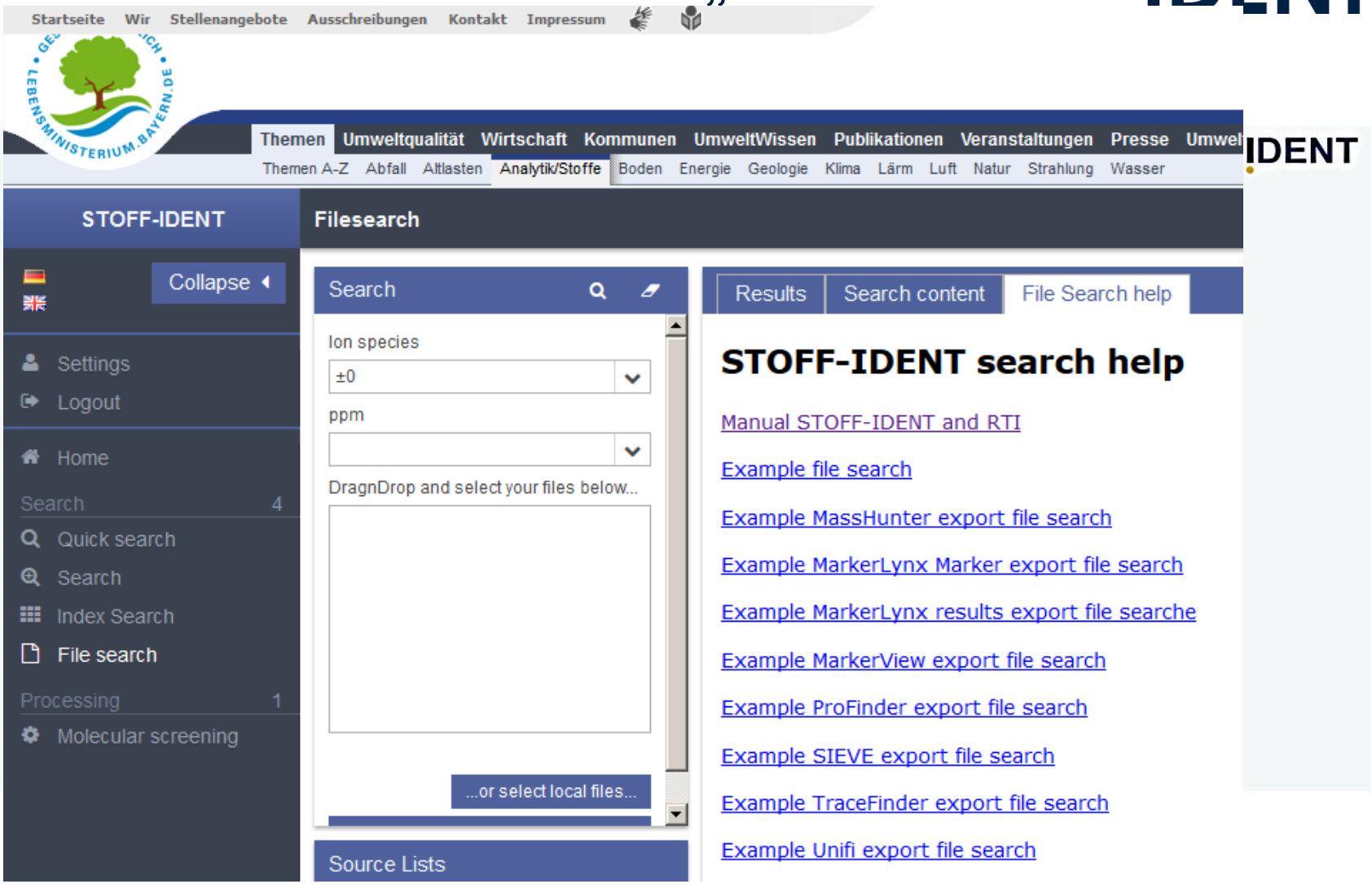


HILIC- Detected Masses

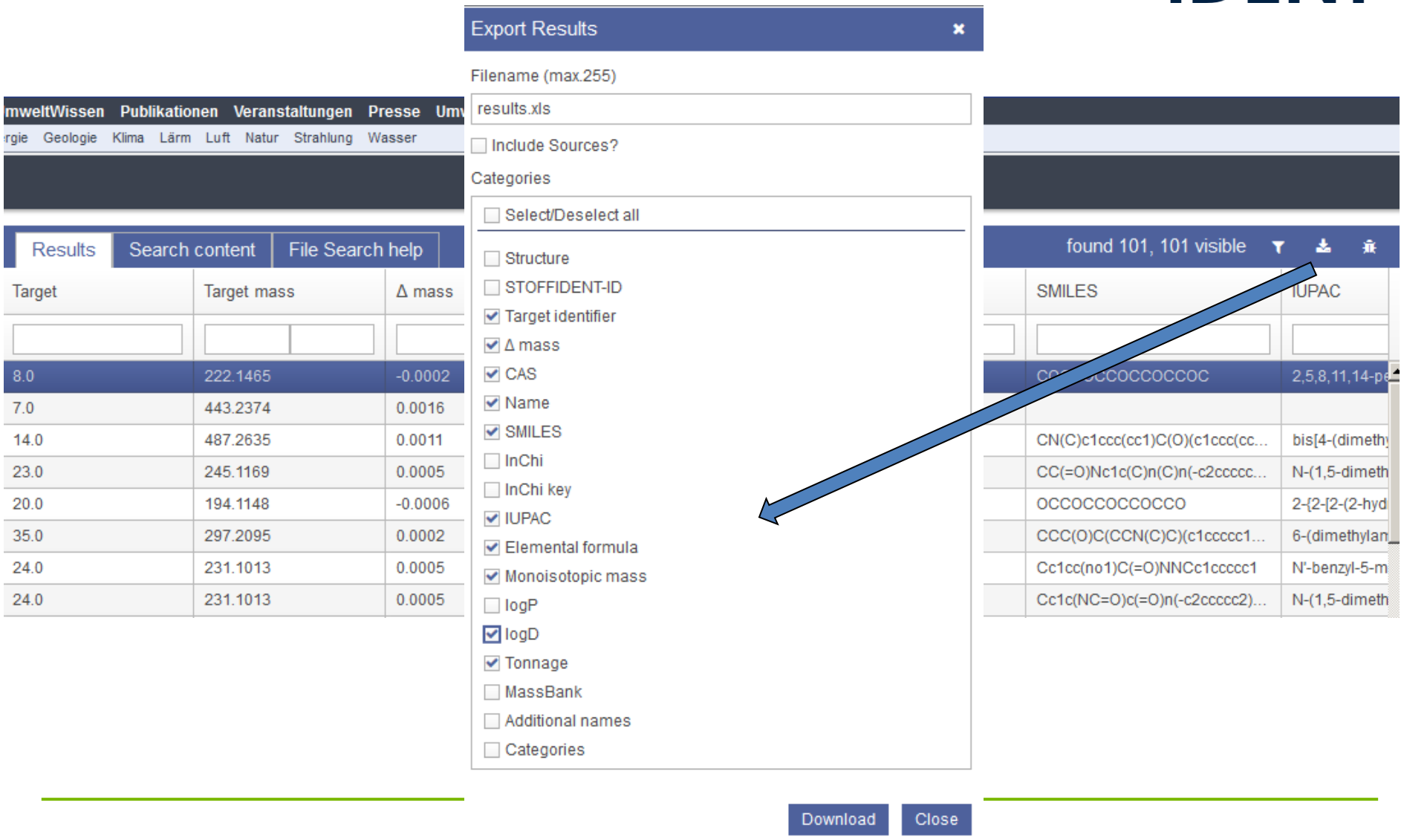
P12

	A	B	C	D	E
1	Compoun	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“



HILIC- Results and Download

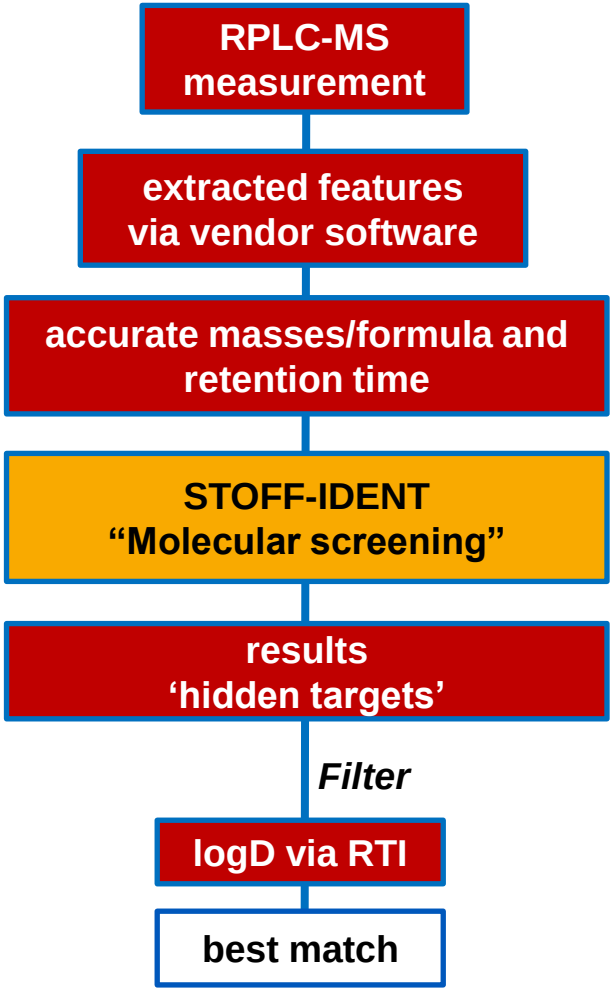


HILIC- LogD Filter

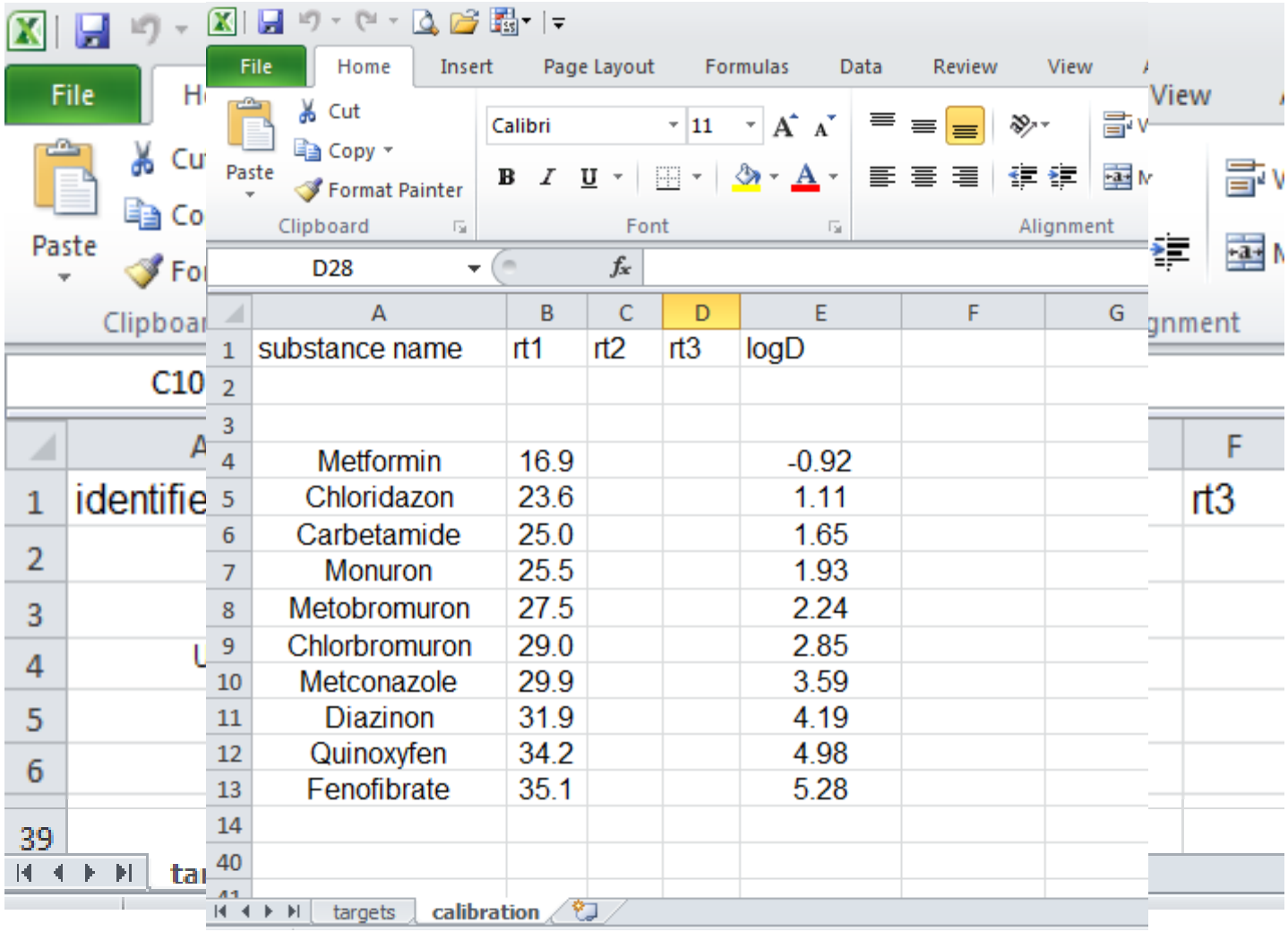
	A	B	C	D	E	F
1		Ziel	Δ Masse	CAS	logD	Name
2	14	SI generated 57	0.0006	108-80-5	-1.1	1,3,5-triazinane-2,4,6-trione
3	33	SI generated 146	-0.0003	1852-17-1	-1	perhydropyrimidin-2-one
4	96	SI generated 347	0.0004	459-73-4	-1	ethyl glycinate
5	10	SI generated 28	0.0003		-0.3	2-[(dimethylamino)methyl]cyclc
6	31	SI generated 144	0.0002		-0.3	2-[(dimethylamino)methyl]cyclc
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		0.12	N-(dimethylvinylsilyl)-1,1-dimeth
13	7	SI generated 23			0.15	N-Acetyl-4-aminoantipyrin
14	22	SI generated 116		818-61-1	0.22	2-hydroxyethyl acrylate

delete

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

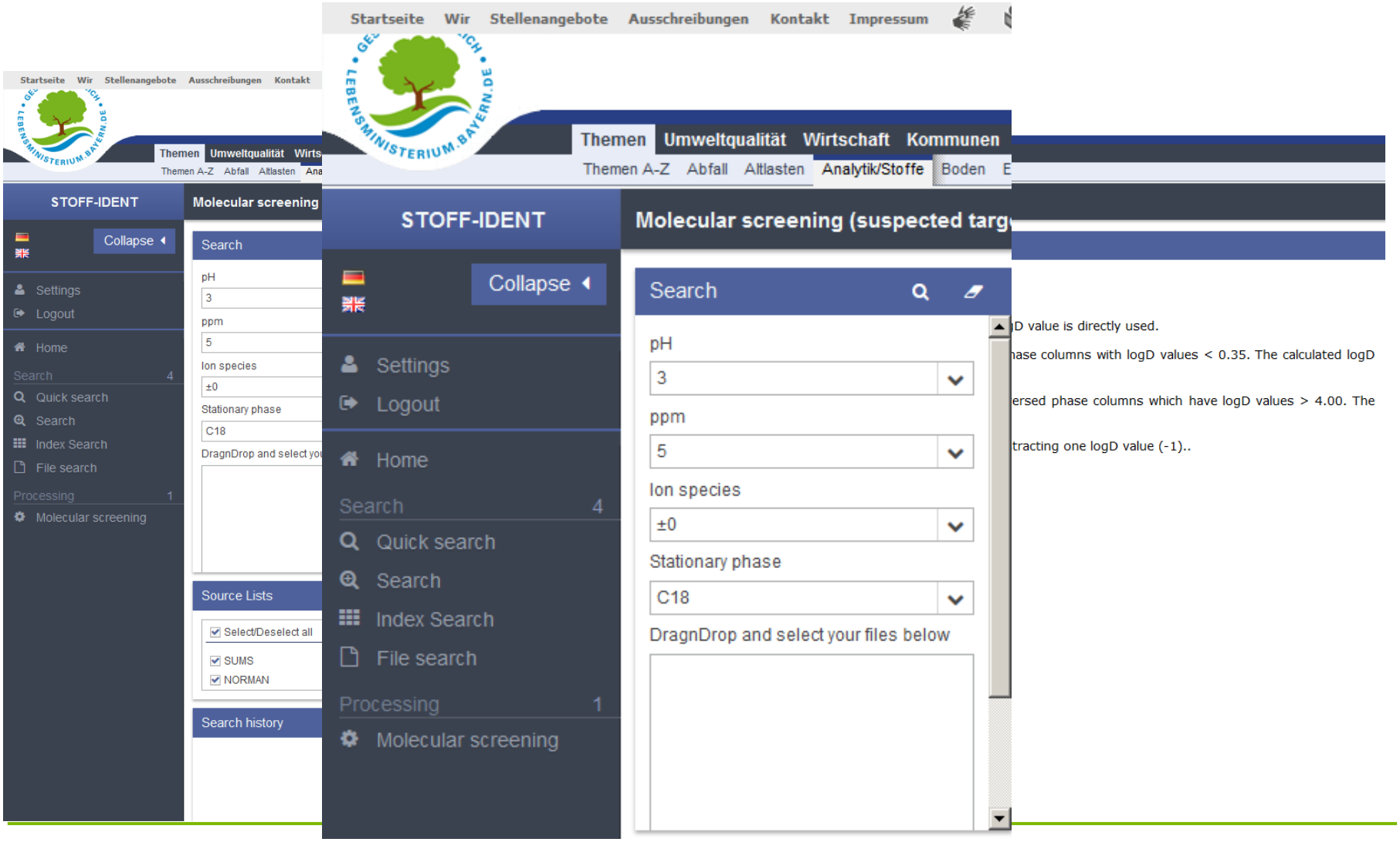


RPLC- Deteced Masses and retention time



	A	B	C	D	E	F	G
1	substance name	rt1	rt2	rt3	logD		
2							
3							
4	Metformin	16.9			-0.92		
5	Chloridazon	23.6			1.11		
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							
40							

RPLC- STOFF-IDENT „molecular screening“



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
Unknown Y	23.6	●	▬	●	164.0950	0.0099	82.7
Unknown Y	23.6	●	▬		164.0950	0.0252	82.7
Unknown Y	23.6	●	▬		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 substracting 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 substracting 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)
Unknown Y	23.6				0.09	1.11	1.02
Unknown Y	23.6				3.73	1.11	-2.62
Unknown Y	23.6				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 substracting 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 substracting one logD value (-1)..
- Red indicates positively charged molecules. The calculated logD value is directly used.

RPLC- Results and Download

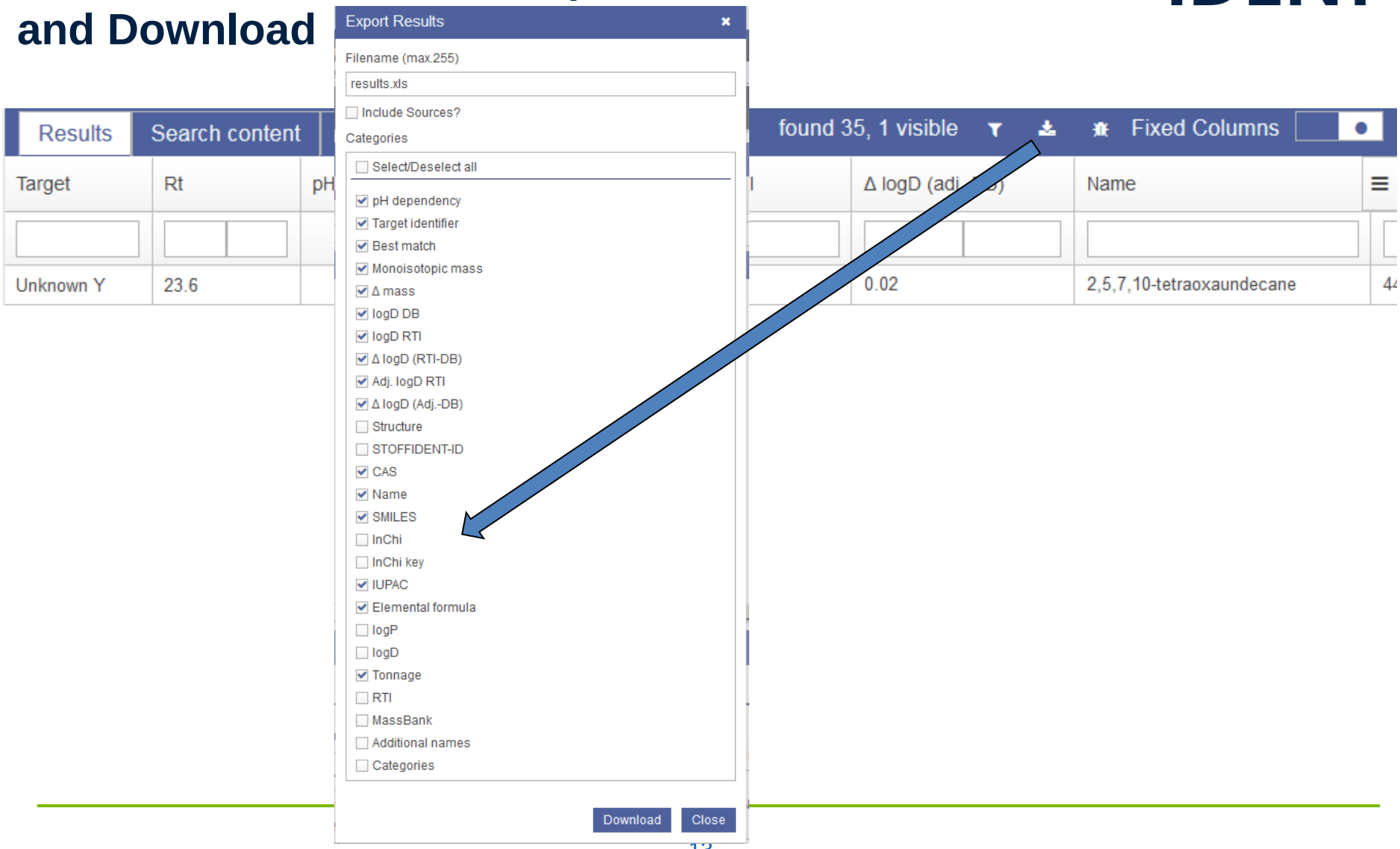
Results | Search content | Help | found 35, 35 visible | Fixed Columns

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

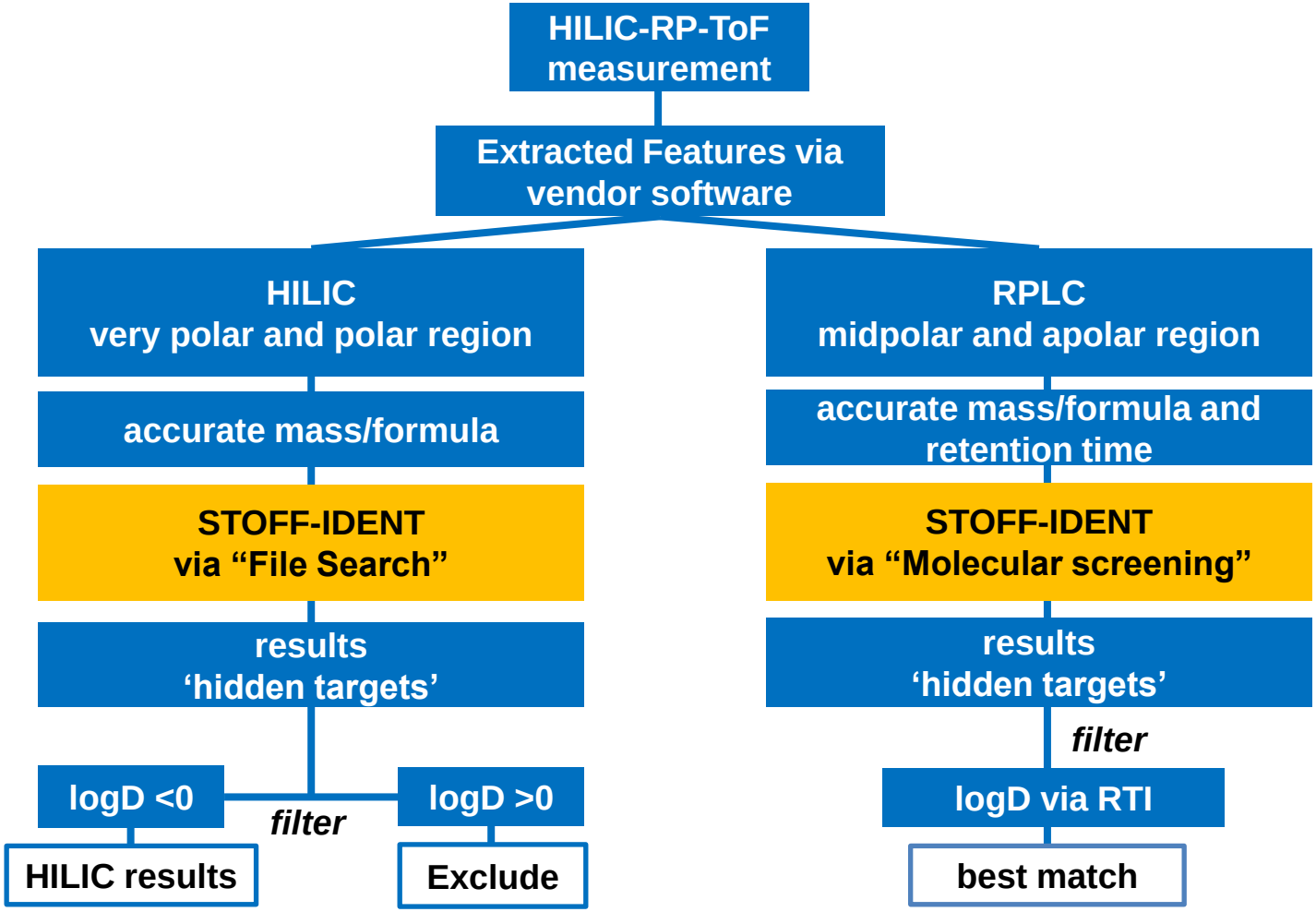
Please note:

- 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 substracting 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 substracting one logD value (-1)..
- Red indicates positively charged molecules. The calculated logD value is directly used.

RPLC- Results- Score, Proposed Best match and Download



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



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