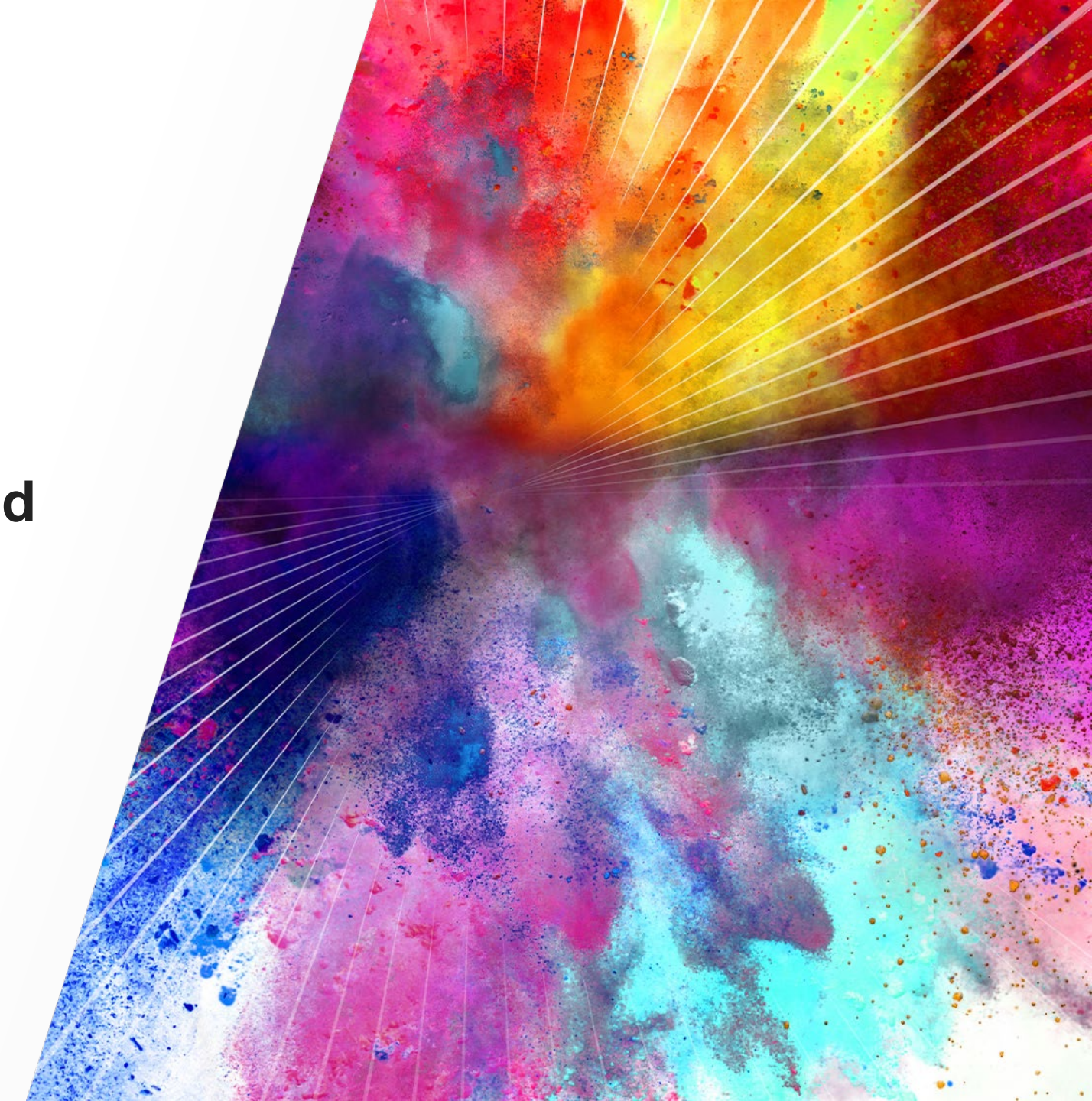
Thermo Scientific™ Compound Discoverer™ 3.5 software

Ralf Tautenhahn

Product Manager, Compound Discoverer software



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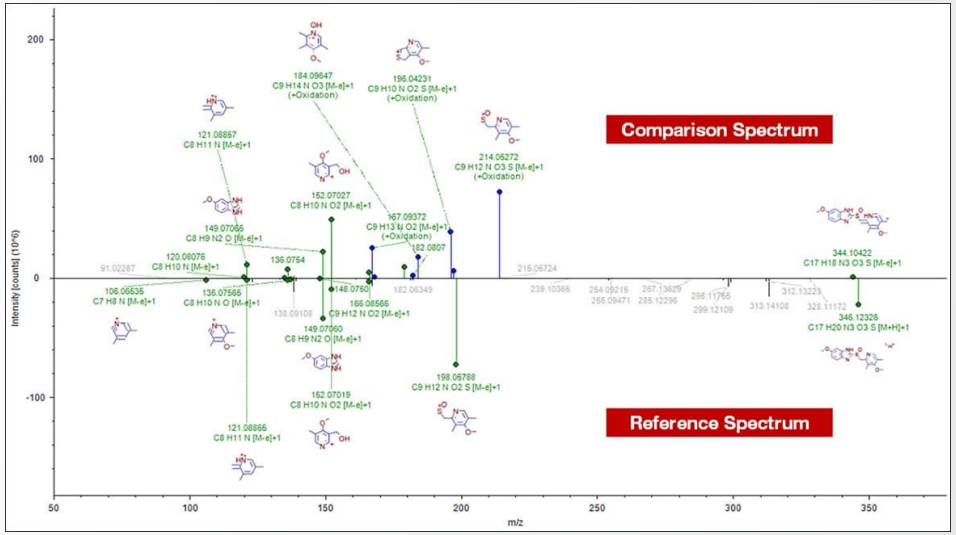
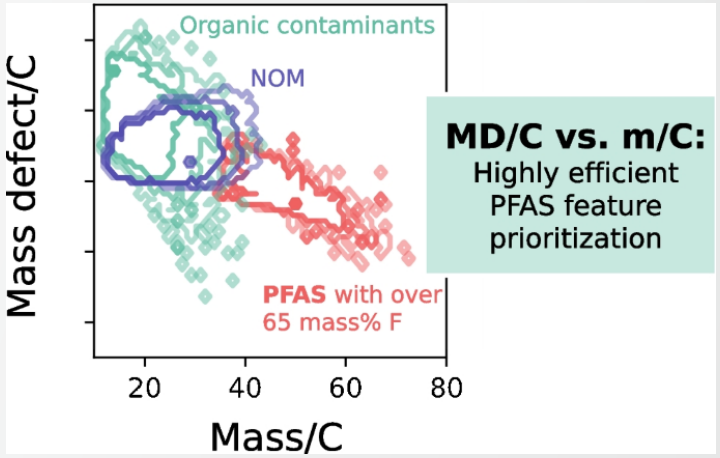
Compound Discoverer 3.5 software

- In-silico fragmentation (“FISh Scoring”) uses a new algorithm with increased coverage for negative ionization mode and increased speed of fragmentation
- Apply PFAS Scoring node for PFAS prioritization
- PFAS Plot shows the normalized mass defect (MD/C) versus normalized mass (m/C), with option for CF2-transformed
- Top-level table "Formulas", consolidates detected or predicted formulas from all annotation sources within a workflow
- Export Compounds table to Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS)
- Export GC/EI Compounds table to Chromeleon CDS
- Targeted stable isotope labeling workflow



FISh Scoring

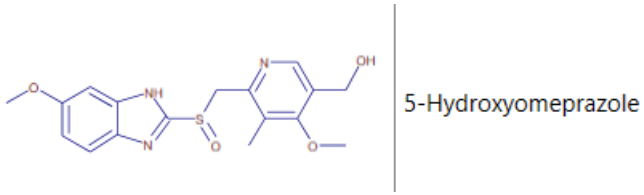


PFAS Plot

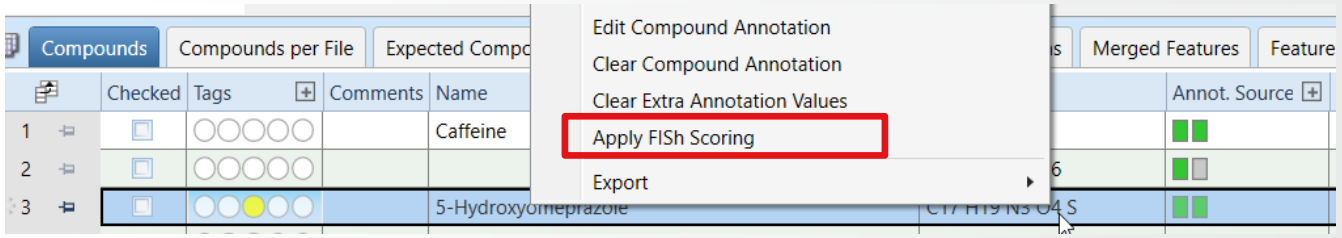
Compound Discoverer 3.5 software

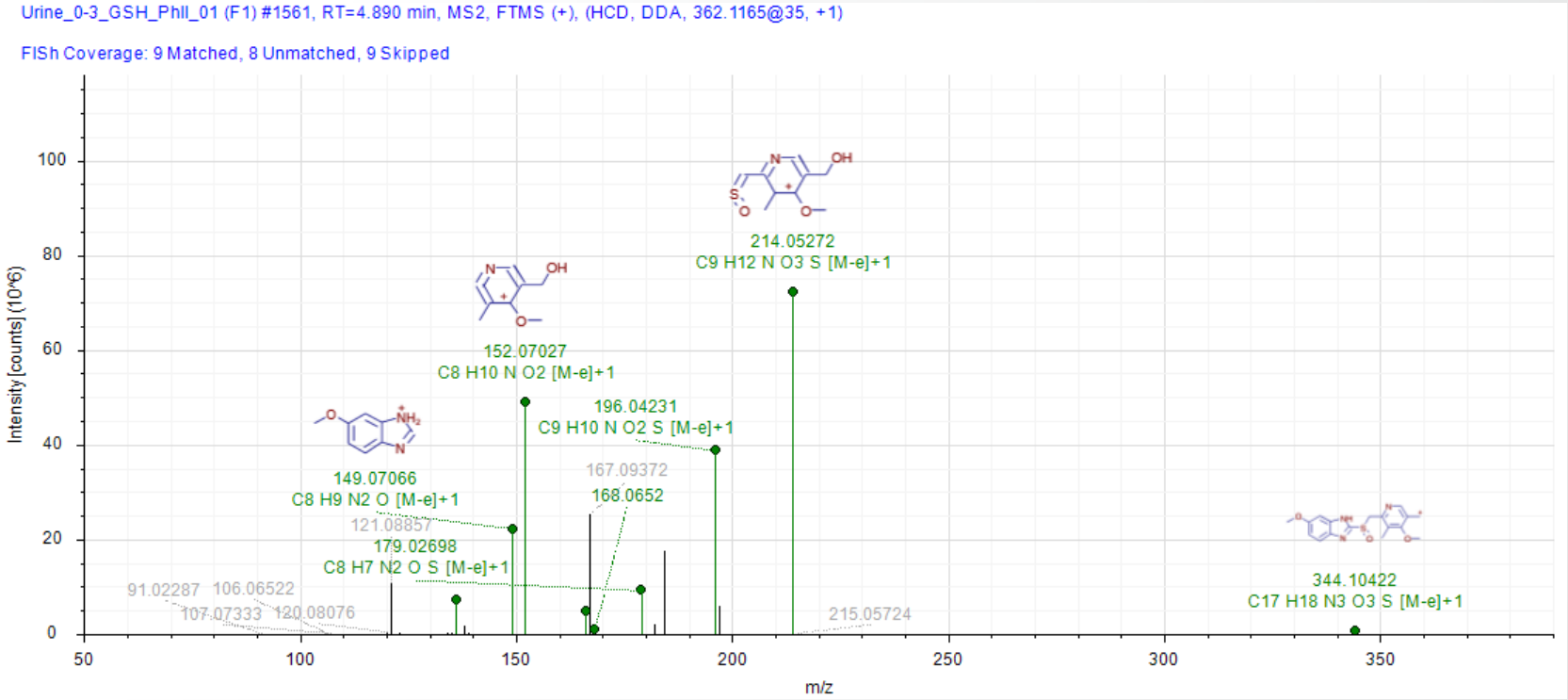
Improved FISh scoring

In-silico fragmentation (“FISh Scoring”) uses a new algorithm with increased coverage for negative ionization mode and increased speed of fragmentation



5-Hydroxyomeprazole

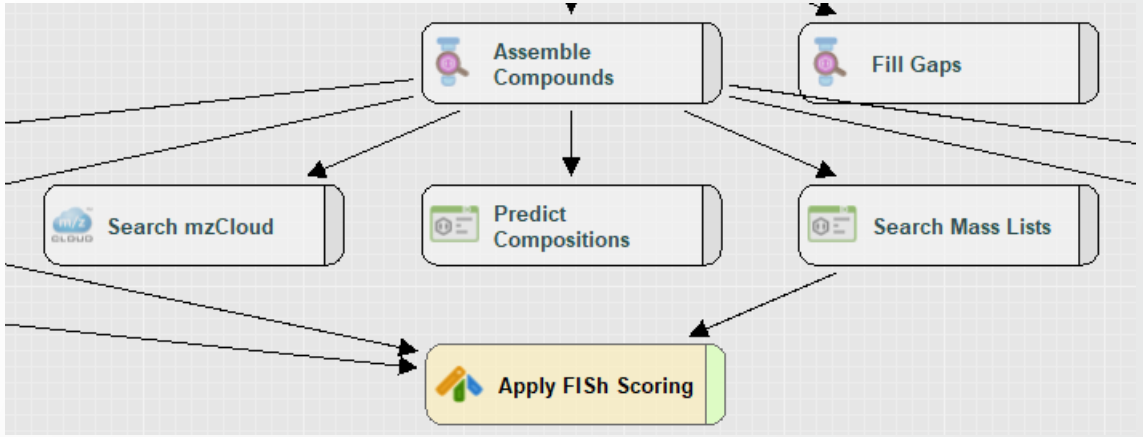




Compound Discoverer 3.5 software

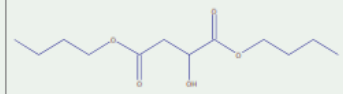
Improved FISh scoring

In-silico fragmentation (“FISh Scoring”) uses a new algorithm (“sledgehammer”, also in MassFrontier 8.1) with increased coverage for negative ionization mode and increased speed of fragmentation (~3x)



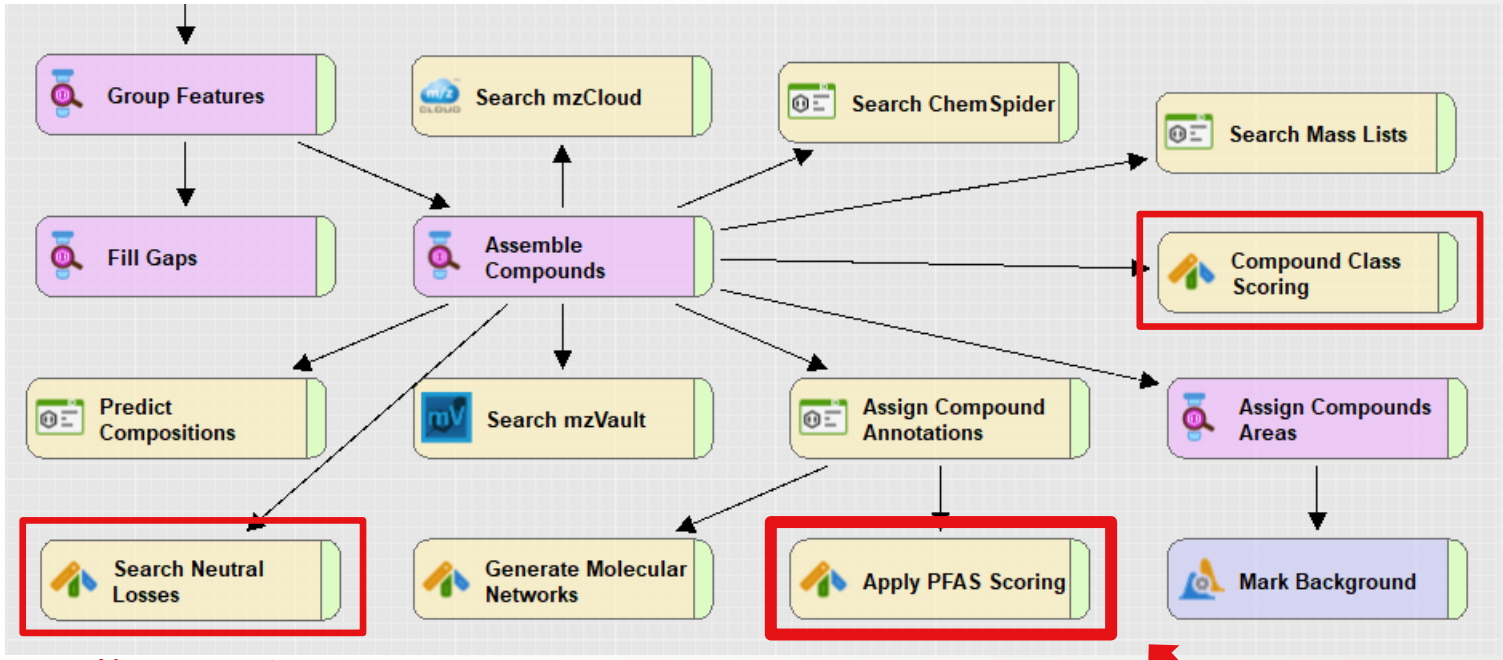
	3-Hydroxydodecanedioic acid	C12 H22 O5		1	0	0	2	2	-0.00027	-1.09	246.14646	229.14318	+H-H2O]+1	6.729	2707560788

per File | Predicted Compositions | Features | Formulas | mzCloud Results | Metabolika Results | ChemSpider Results | Mass List Search Results | Metabolika Pathways

Compound Match	Structure	Name	Formula	Molecular Weight	ΔMass [Da]	ΔMass [ppm]	CSID	FISh Coverage	# References
		3-Hydroxydodecanedioic acid	C12 H22 O5	246.14672	-0.00027	-1.09	13628081	87.50	38
		Dibutyl malate	C12 H22 O5	246.14672	-0.00027	-1.09	86081	50.00	55

Compound Discoverer 3.5 software

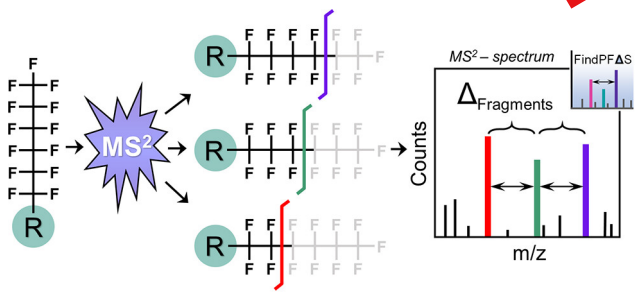
Updated NTA PFAS workflow

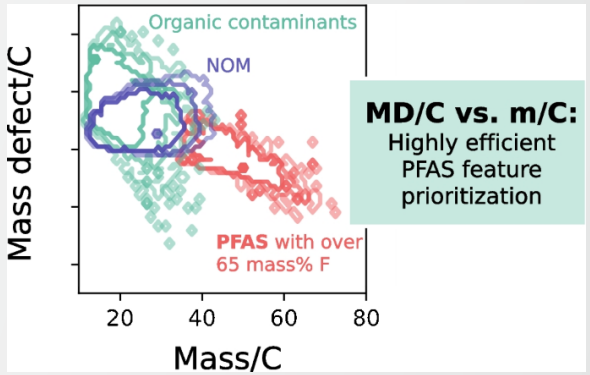


Updated database

Now supports Internal Loss Search

New PFAS Scoring node



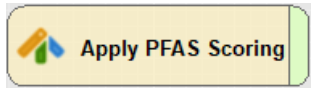


Zweigle et al. *Efficient PFAS prioritization in non-target HRMS data: systematic evaluation of the novel MD/C-m/C approach*. 2023 link.springer.com/article/10.1007/s00216-023-04601-1

Zweigle et al, FindPFΔS: Non-Target Screening for PFAS—Comprehensive Data Mining for MS2 Fragment Mass Differences, 2022, pubs.acs.org/doi/10.1021/acs.analchem.2c01521

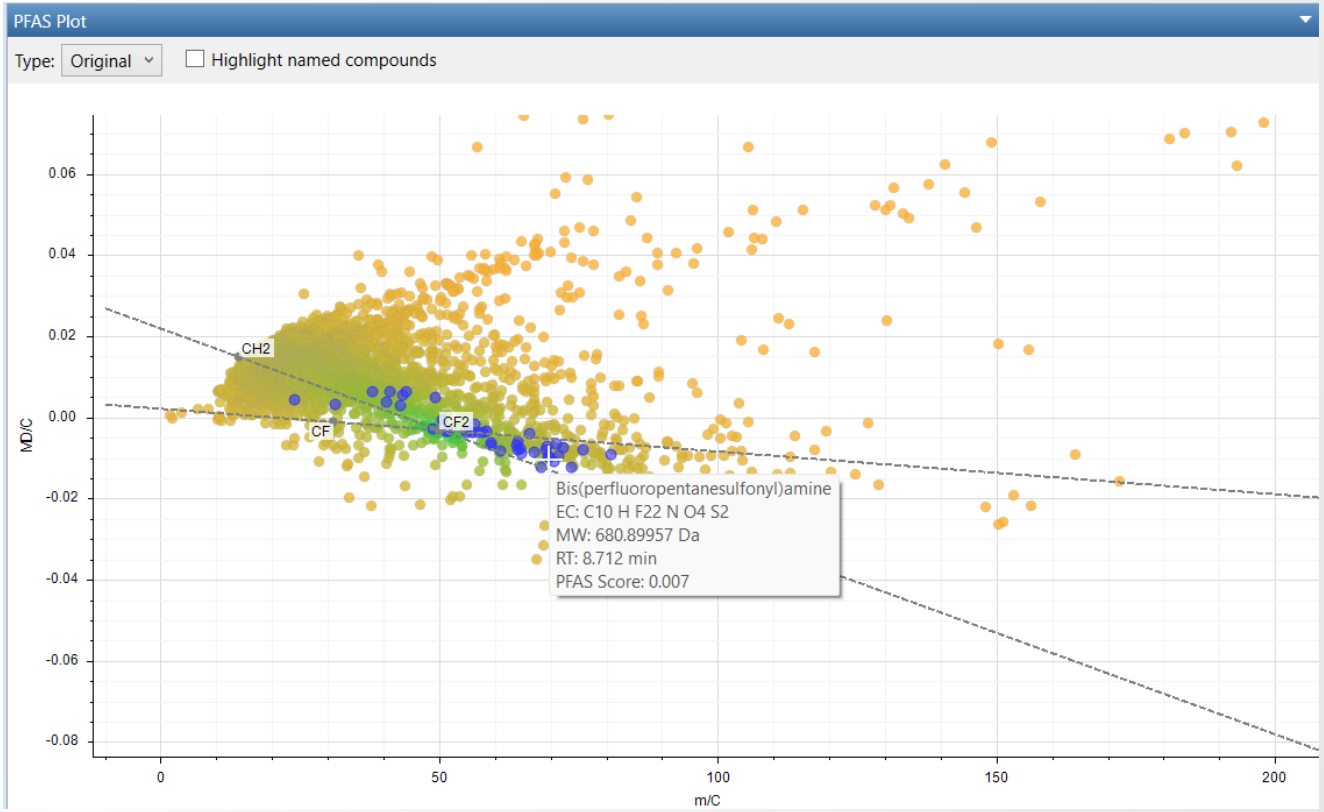
Compound Discoverer 3.5 software

PFAS scoring node and PFAS Plot



PFAS Score Matrix

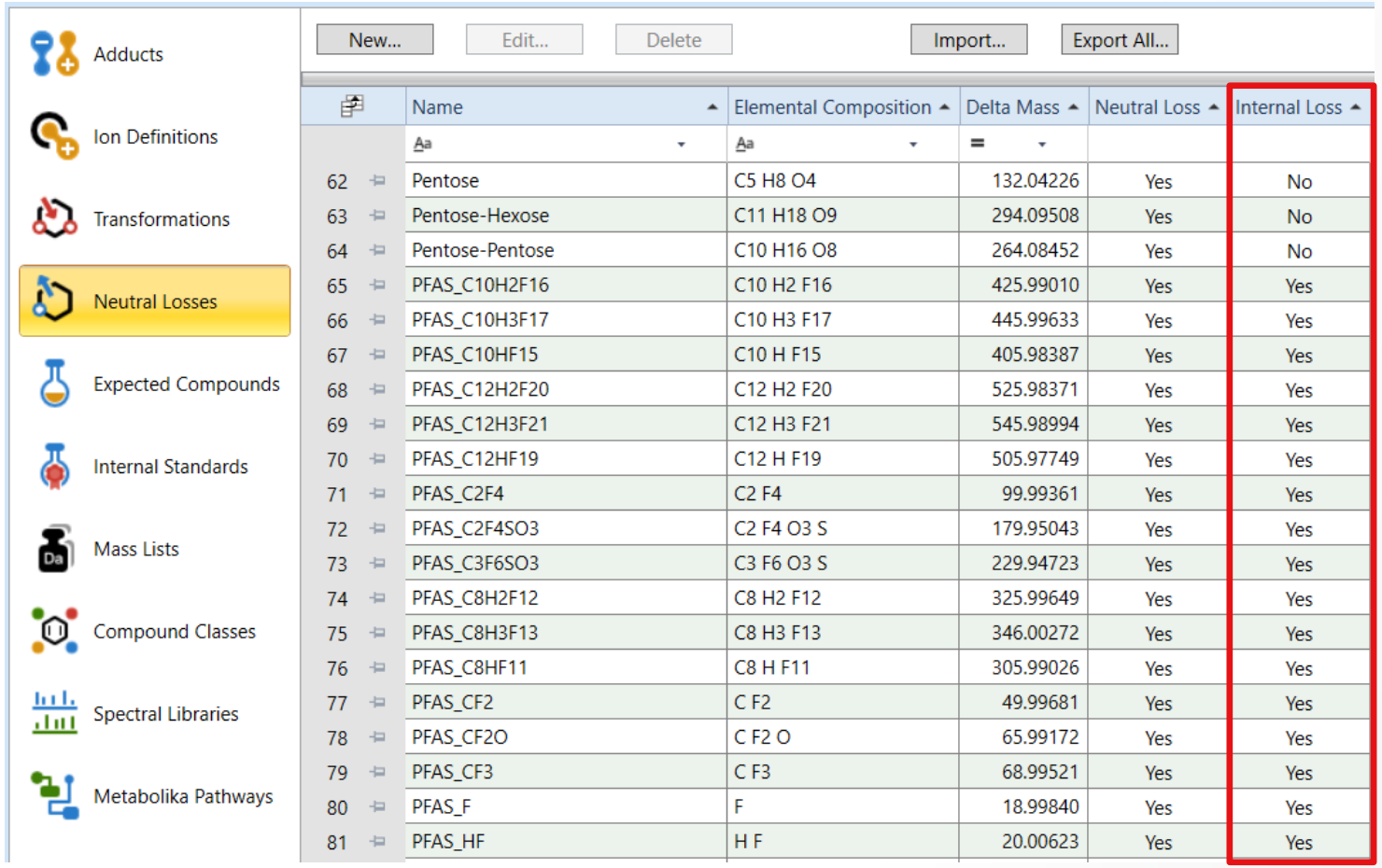
PFAS Score	Assigned F*	Assigned C	Estimated C	m/C	MD/C	m/Cm	MD/Cm	rCF2	Standard MD [0.80]	Kendrick MD [C F2]	Kendrick MD [C H2]
0.005	17	8	7.805	64.053	-0.008	14.056	0.002	0.005	-0.063	-0.031	0.379
0.005	13	13	12.792	41.283	0.006	-8.714	0.004	0.005	0.075	0.108	0.485
0.010	0	17	12.793	23.308	0.014	-26.689	0.003	0.01	0.181	0.2	-0.152
0.009	0	12	11.745	22.661	0.013	-27.336	0.002	0.009	0.155	0.172	-0.142
0.011	13	6	5.518	72.304	-0.007	22.308	0.008	0.011	-0.041	-0.015	0.514



Zweigle et al. *Efficient PFAS prioritization in non-target HRMS data: systematic evaluation of the novel MD/C-m/C approach*. 2023 link.springer.com/article/10.1007/s00216-023-04601-1

Compound Discoverer 3.5 software

Search Neutral Loss| Internal Loss Search

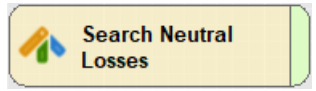


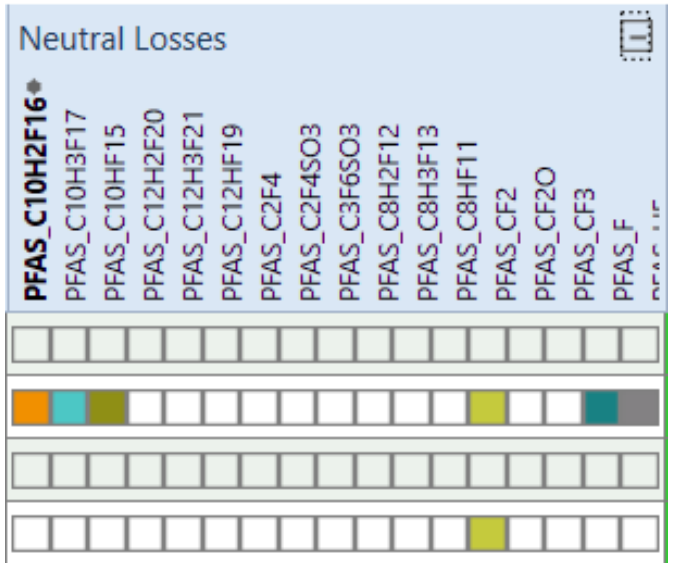
	Name	Elemental Composition	Delta Mass	Neutral Loss	Internal Loss
62	Pentose	C5 H8 O4	132.04226	Yes	No
63	Pentose-Hexose	C11 H18 O9	294.09508	Yes	No
64	Pentose-Pentose	C10 H16 O8	264.08452	Yes	No
65	PFAS_C10H2F16	C10 H2 F16	425.99010	Yes	Yes
66	PFAS_C10H3F17	C10 H3 F17	445.99633	Yes	Yes
67	PFAS_C10HF15	C10 H F15	405.98387	Yes	Yes
68	PFAS_C12H2F20	C12 H2 F20	525.98371	Yes	Yes
69	PFAS_C12H3F21	C12 H3 F21	545.98994	Yes	Yes
70	PFAS_C12HF19	C12 H F19	505.97749	Yes	Yes
71	PFAS_C2F4	C2 F4	99.99361	Yes	Yes
72	PFAS_C2F4SO3	C2 F4 O3 S	179.95043	Yes	Yes
73	PFAS_C3F6SO3	C3 F6 O3 S	229.94723	Yes	Yes
74	PFAS_C8H2F12	C8 H2 F12	325.99649	Yes	Yes
75	PFAS_C8H3F13	C8 H3 F13	346.00272	Yes	Yes
76	PFAS_C8HF11	C8 H F11	305.99026	Yes	Yes
77	PFAS_CF2	C F2	49.99681	Yes	Yes
78	PFAS_CF2O	C F2 O	65.99172	Yes	Yes
79	PFAS_CF3	C F3	68.99521	Yes	Yes
80	PFAS_F	F	18.99840	Yes	Yes
81	PFAS_HF	H F	20.00623	Yes	Yes

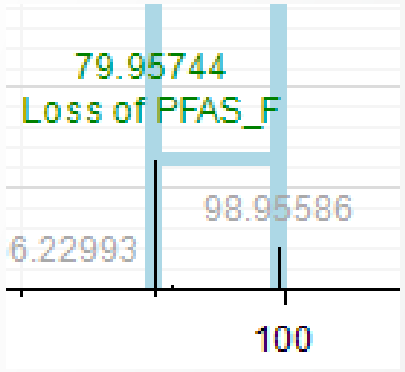
Loss (mass difference) can be defined as Neutral Loss (Precursor⇔Fragment) or Internal Loss (Fragment⇔Fragment) or both

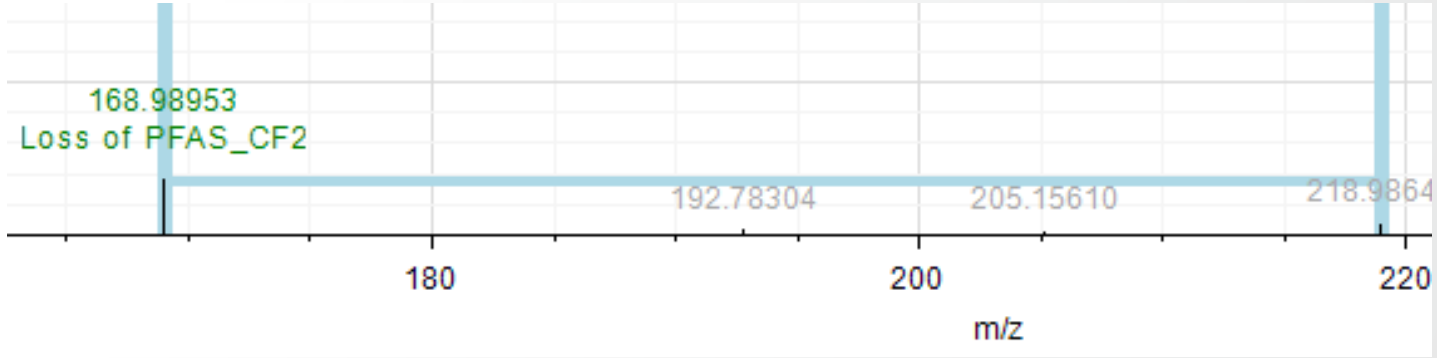
Compound Discoverer 3.5 software

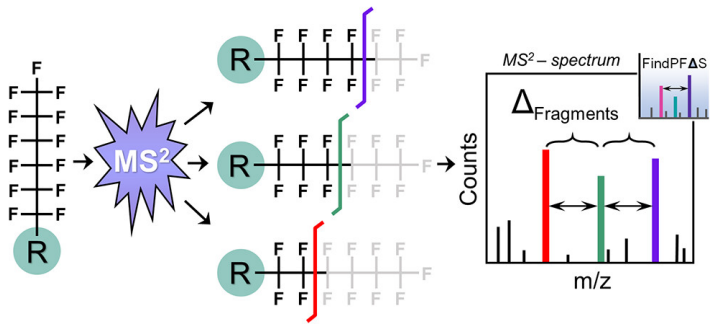
Internal Loss Search for NTA PFAS











Zweigle et al, FindPFΔS: Non-Target Screening for PFAS–Comprehensive Data Mining for MS2 Fragment Mass Differences, 2022, https://pubs.acs.org/doi/10.1021/acs.analchem.2c01521

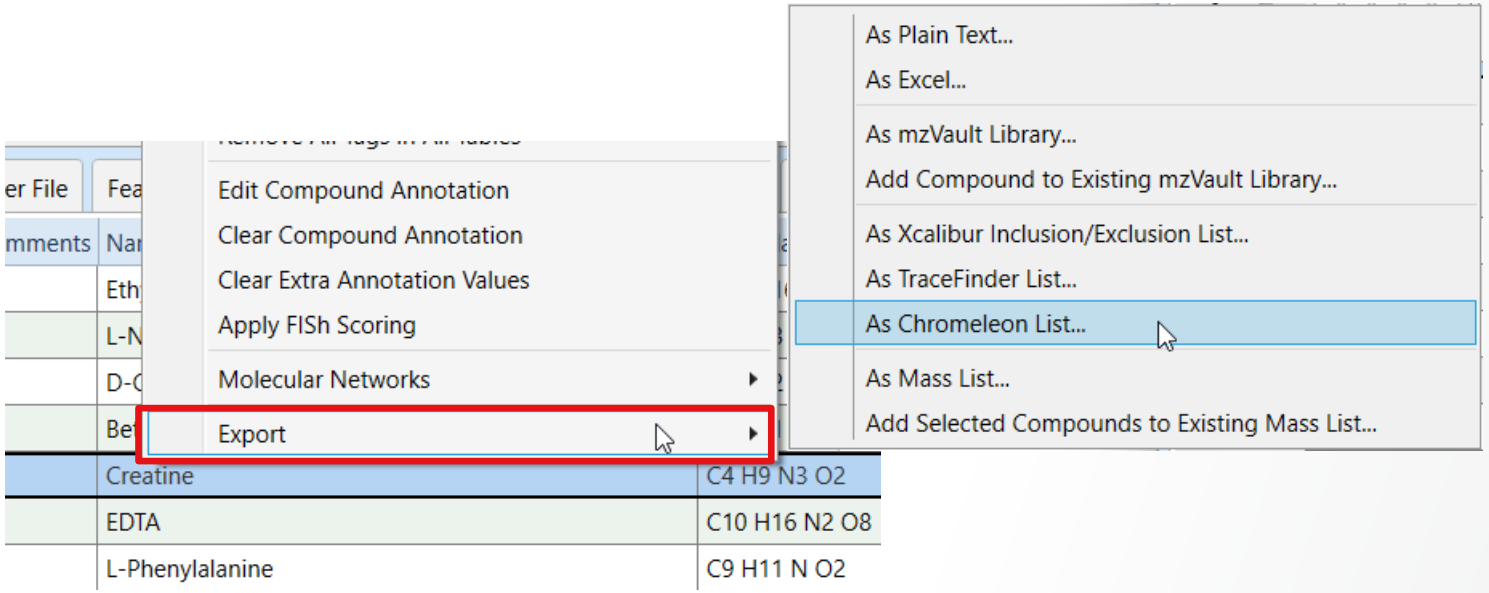
Compound Discoverer 3.5 software

Export to Chromeleon CDS

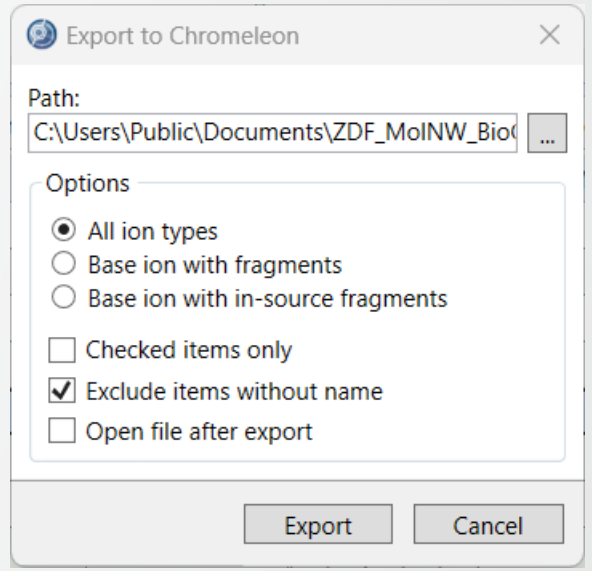
To export from Compound Discoverer software, right-click in

- *Compounds* or
- *GC/EI Compounds* table and select Export.

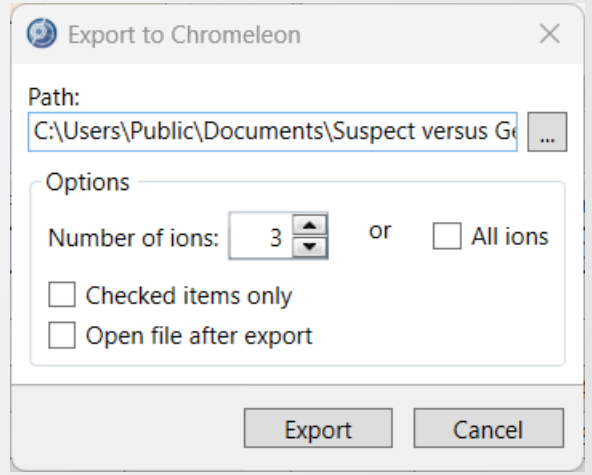
Import into Chromeleon 7.4 software using the Compound Data Import button on the Processing method toolbar, select Custom Definition, Custom Definition (CSV)



LC/MS



GC/EI



Compound Discoverer 3.5 software

New Formulas table (related table)

Compounds | Compounds per File | Features | Features per File | Formulas | mzCloud Results | ChemSpider Results | Input Files | Study Information | Statistical Methods | Metabolika Pathways

	Tags	Checked	Comments	Name	Formula	Annot. Source	# Annots.					Annot. ΔMass [Da]	Annot. ΔMass [ppm]	Calc. MW	m/z
1				Ethylenediaminetetraacetic acid (EDTA)	C10 H16 N2 O8		2	0	2	1	4	-0.00061	-2.07	292.09006	293.09735
2				L-Norleucine	C6 H13 N O2		1	2	8	20	20	-0.00009	-0.69	131.09454	132.10182
3				D-Glucose	C6 H12 O6		1	12	0	98	26	-0.00036	-2.00	180.06303	203.05225
4				Betaine	C5 H11 N O2		1	2	6	14	13	-0.00020	-1.75	117.07877	118.08605
5		☑		Creatine	C4 H9 N3 O2		1	0	3	2	5	-0.00018	-1.40	131.06929	132.07657

Hide Related Tables

Structure Proposals | Compounds per File | Predicted Compositions | Features | Similar Compounds | Formulas | mzCloud Results | Metabolika Results | ChemSpider Results | Mass List Search Results | Metabolika P

	Tags	Checked	Formula	Formula Results						Molecular Weight	RDBE	# C	# H	# N	# O	# P	# S	# F	H/C	N/C	O/C	P/C	S/C	F/C
				Compounds	Predicted Compositions	Metabolika Search	mzCloud Search	ChemSpider Search	MassList Search															
1			C4 H9 N3 O2	2	1	0	3	2	5	131.06948	2.0	4	9	3	2	0	0	0	2.25	0.75	0.50	0.00	0.00	0.00

Compound Discoverer 3.5 software

Formulas table is also available as Main table

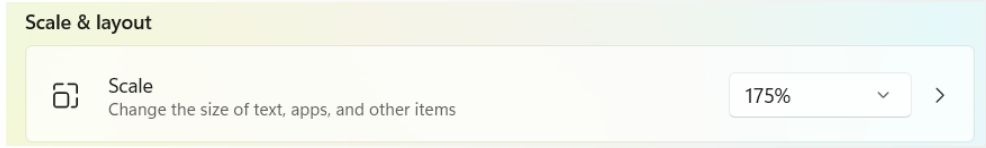
Compounds | Compounds per File | Features | Features per File | Formulas | mzCloud Results | ChemSpider Results | Input Files | Study Information | Statistical Methods | Metabolika Pathways

	Tags	Checked	Formula	Formula Results: Compounds	Predicted Compositions	Metabolika Search	mzCloud Search	ChemSpider Search	MassList Search	Molecular Weight	RDBE	# C	# H	# N	# O	# P	# S	# F	H/C	N/C	O/C	P/C	S/C	F/C
4			C H Cl N3 O8 P	1	1	0	0	0	0	248.91898	3.0	1	1	3	8	1	0	0	1.00	3.00	8.00	1.00	0.00	0.00
5			C H Cl N4 O2 S	1	1	0	0	0	0	167.95087	3.0	1	1	4	2	0	1	0	1.00	4.00	2.00	0.00	1.00	0.00
6			C H Cl2 N2 O2 P S	1	1	0	0	0	0	205.88734	2.0	1	1	2	2	1	1	0	1.00	2.00	2.00	1.00	1.00	0.00
7			C H Cl2 N2 O3 P S	1	1	0	0	0	0	221.88225	2.0	1	1	2	3	1	1	0	1.00	2.00	3.00	1.00	1.00	0.00
8			C H Cl2 N2 O14 P S	1	1	0	0	0	0	397.82632	2.0	1	1	2	14	1	1	0	1.00	2.00	14.00	1.00	1.00	0.00
9			C H Cl2 N3 O11	1	1	0	0	0	0	300.89881	2.0	1	1	3	11	0	0	0	1.00	3.00	11.00	0.00	0.00	0.00
10			C H Cl2 N8 O2 P3	2	2	0	0	0	0	319.88124	6.0	1	1	8	2	3	0	0	1.00	8.00	2.00	3.00	0.00	0.00
11			C H Cl3 N4 O S3	1	1	0	0	0	0	285.83781	2.0	1	1	4	1	0	3	0	1.00	4.00	1.00	0.00	3.00	0.00
12			C H Cl3 N6 O4 P2 S2	1	1	0	0	0	0	391.80415	4.0	1	1	6	4	2	2	0	1.00	6.00	4.00	2.00	2.00	0.00
13			C H Cl3 N6 O7 S	1	1	0	0	0	0	345.86930	3.0	1	1	6	7	0	1	0	1.00	6.00	7.00	0.00	1.00	0.00
14			C H Cl3 N9 P	1	1	0	0	0	0	274.91581	5.0	1	1	9	0	1	0	0	1.00	9.00	0.00	1.00	0.00	0.00
15			C H N2 O4 P S	1	1	0	0	0	0	167.93946	3.0	1	1	2	4	1	1	0	1.00	2.00	4.00	1.00	1.00	0.00
16			C H N3 O5	1	1	0	0	0	0	134.99162	3.0	1	1	3	5	0	0	0	1.00	3.00	5.00	0.00	0.00	0.00
17			C H N6 O3 P3	1	1	0	0	0	0	237.93230	6.0	1	1	6	3	3	0	0	1.00	6.00	3.00	3.00	0.00	0.00
18			C H N6 O7 P3 S3	1	1	0	0	0	0	397.82817	6.0	1	1	6	7	3	3	0	1.00	6.00	7.00	3.00	3.00	0.00
19			C H N6 P3	1	1	0	0	0	0	189.94755	6.0	1	1	6	0	3	0	0	1.00	6.00	0.00	3.00	0.00	0.00

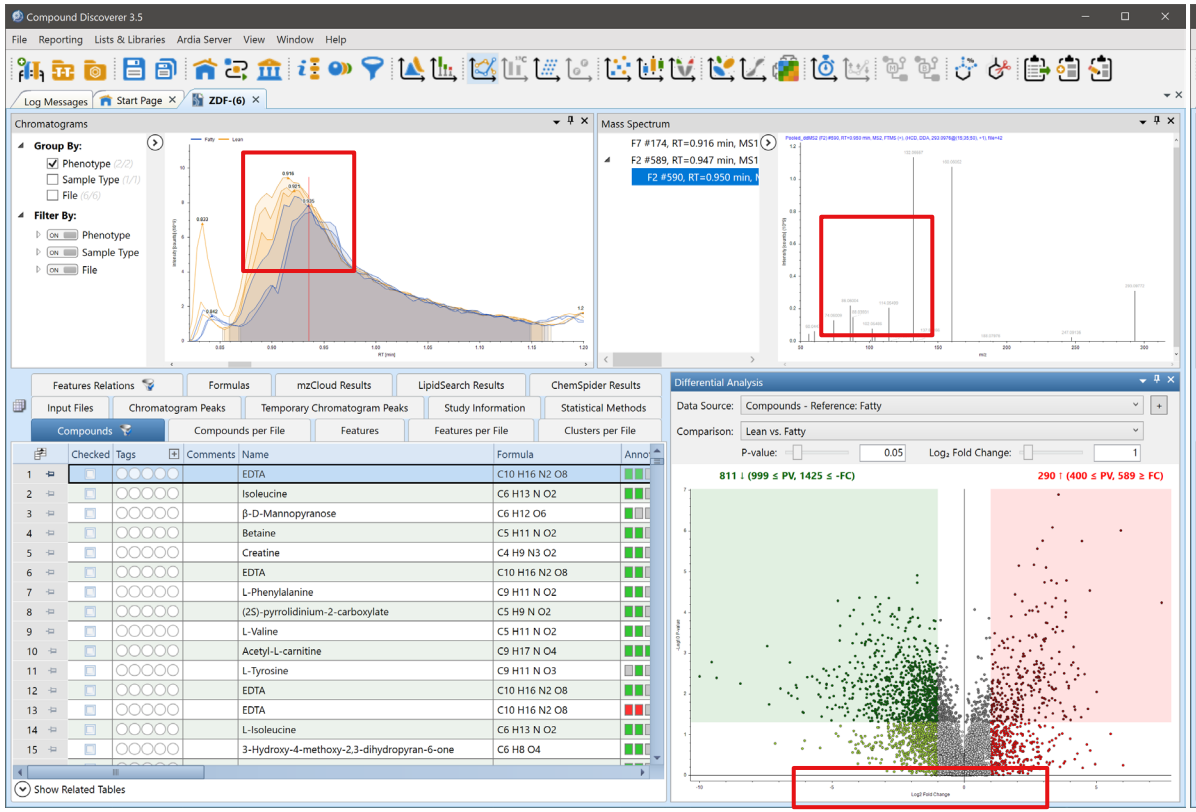
Show Related Tables

Compound Discoverer 3.5 software

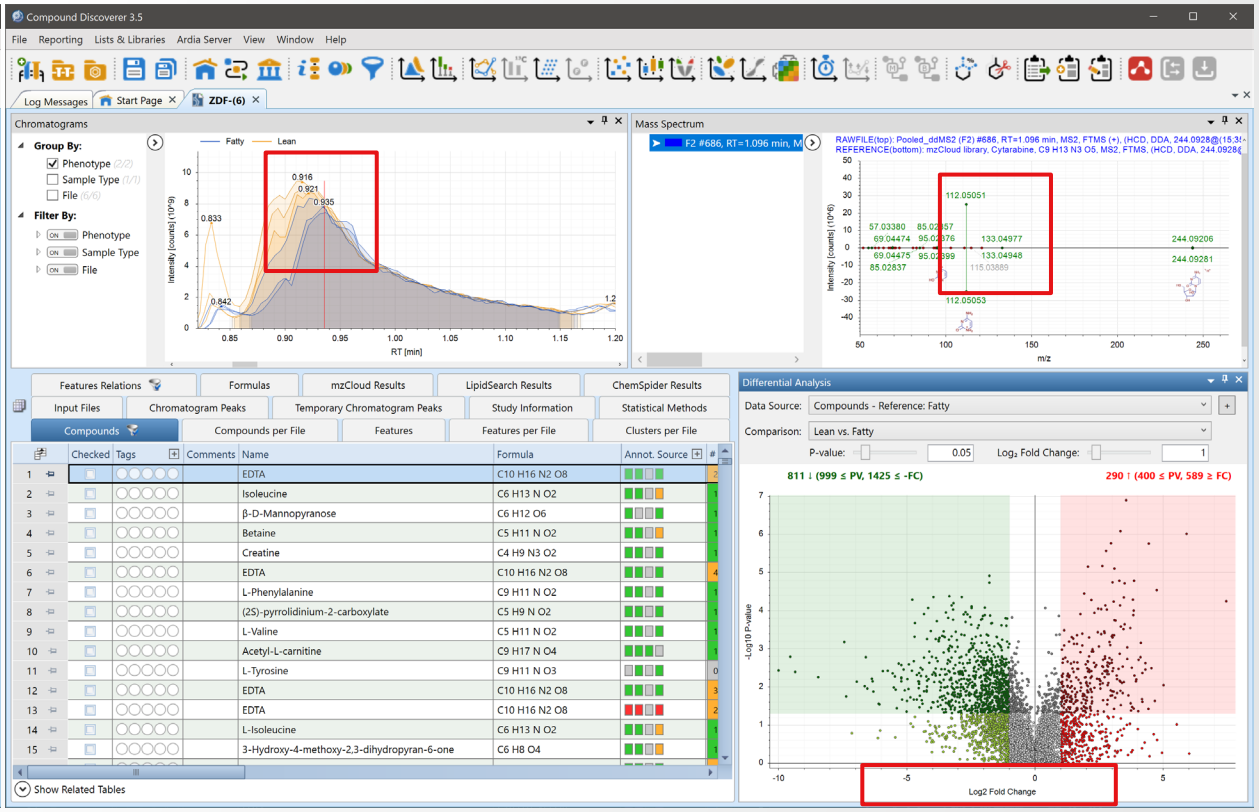
User interface now scales the font size used in most charts and views



Windows 11
System > Display



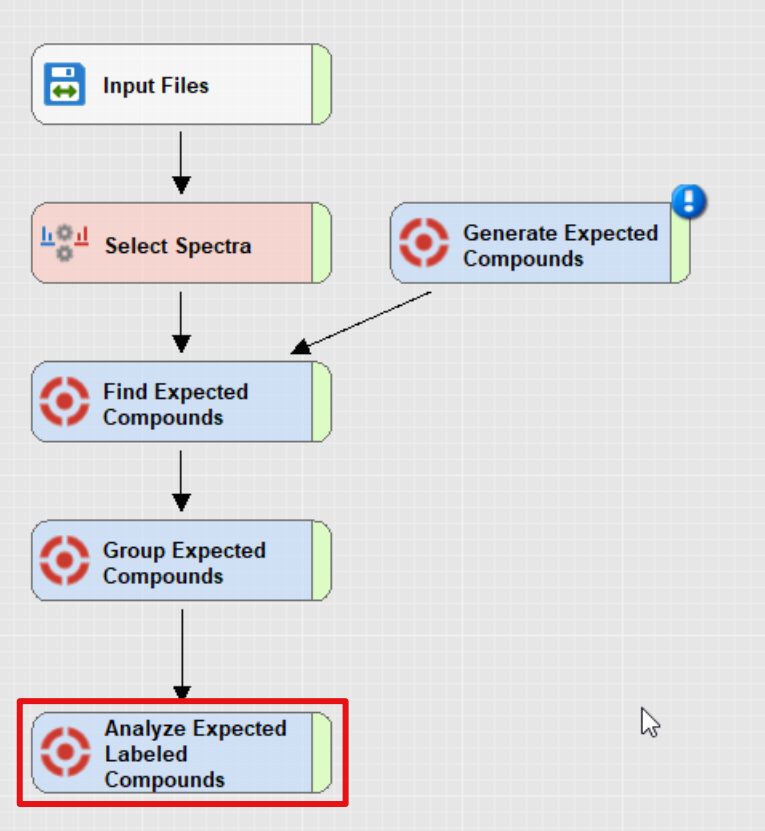
before



after

Compound Discoverer 3.5 software

Targeted Stable Isotope Labeling

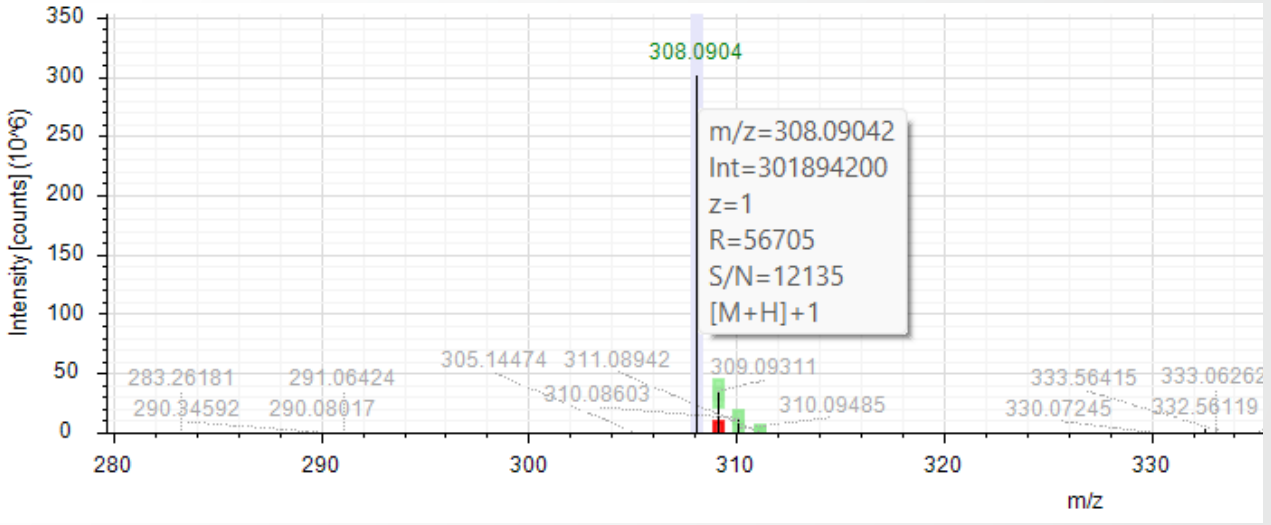


- Compound Discoverer software supports targeted and untargeted stable isotope labeling
- New workflow template for *targeted* stable isotope labeling in version 3.5
- Specify targets via Expected Compounds
- Requires unlabeled reference sample

Compound Discoverer 3.5 software

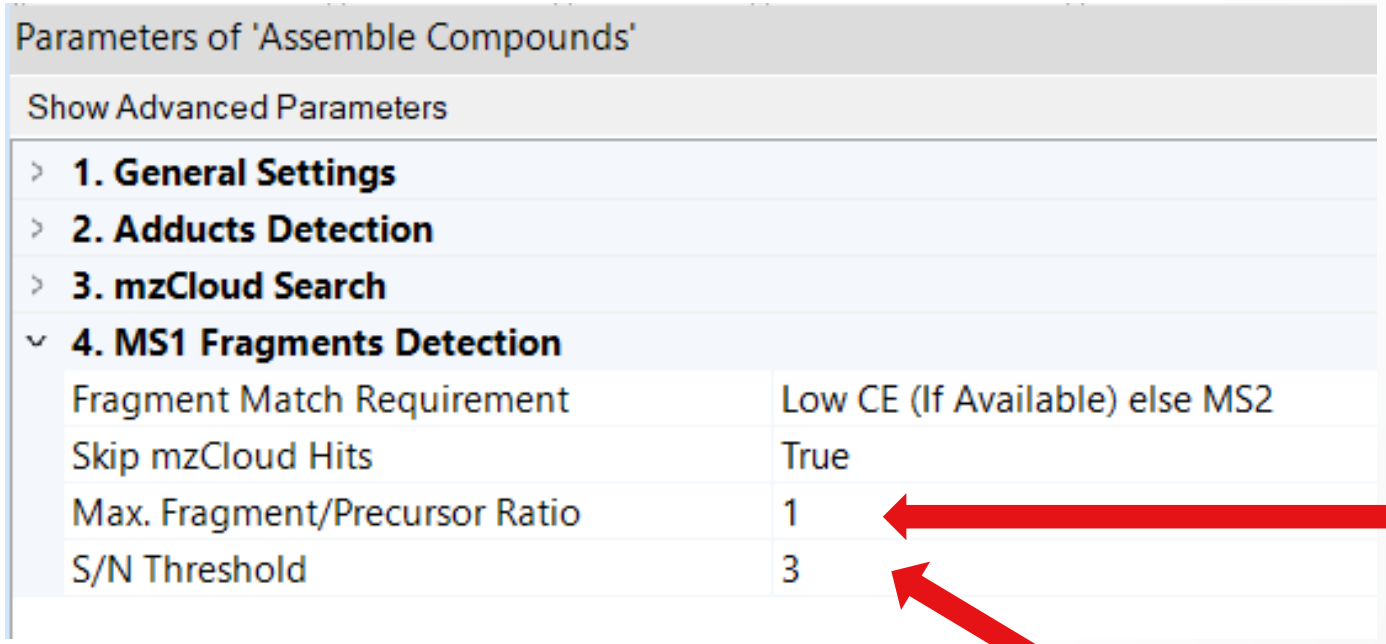
S/N and Intensity

- Mass Spectrum View shows charge state, resolution, and signal to noise ratio in the tooltip for each peak.
- *Intensity(Max)* column is now available in the Compounds & Expected Compounds table.
- *Max S/N column* is now available in the Compounds & Expected Compounds table.
- *Sample/Background Ratio* column is now available when the Mark Background node is used.



Compound Discoverer 3.5 software

Assemble Compounds: additional parameters to improve specificity for annotation of MS^1 fragments



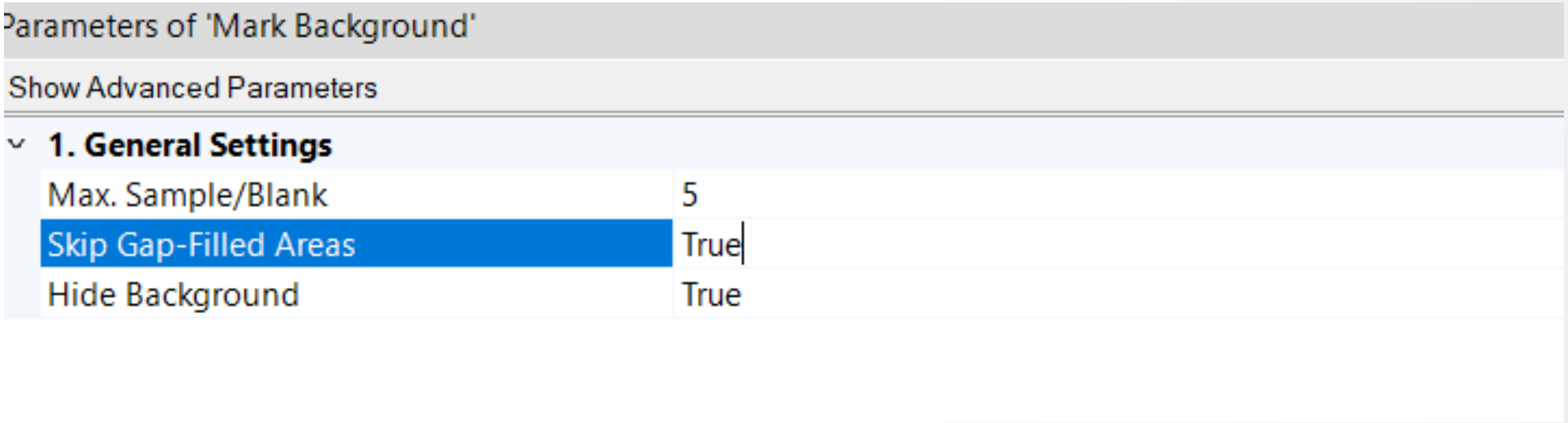
Maximum fragment/precursor intensity ratio.

- Default value=1: do not consider a peak in the full scan as a potential MS^1 fragment if the intensity of the presumed fragment is greater than the intensity of its precursor.
- With values greater than 1, the software still considers such a peak as a potential fragment if its intensity is higher than that of its presumed precursor (up to and including the set ratio value).

S/N threshold. Default=3: do not consider a peak X in the full scan as a potential MS^1 fragment if the S/N threshold of the corresponding fragment X in the MS^2 scan is less than 3.

Compound Discoverer 3.5 software

Mark Background: no longer uses data based on Gap Filling for increased sensitivity



Compound Discoverer 3.5 software

#Annotations column in the Compounds table

#Annotations: Result counts for all annotation sources

Name	Formula	Annot. Source: Predicted Compositions, Metabolika Search, mzCloud Search, ChemSpider Search	# Annots.: Predicted Compositions	Metabolika Search	mzCloud Search	ChemSpider Search	Annot. ΔMass [Da]
Gamma-glutamylcysteinylglycine	C10 H17 N3 O6 S		3	1	3	2	-0.00053
L-Glutamic acid	C5 H9 N O4		1	9	3	19	-0.00024
L-Glutathione Oxidized Hexhydrate	C20 H32 N6 O12 S2		0	0	3	0	-0.00073
N-Acetylputrescine	C6 H14 N2 O		1	0	1	2	-0.00021
Betaine	C5 H11 N O2		1	2	6	14	-0.00024
N-Acetylputrescine	C6 H14 N2 O		1	0	1	2	-0.00022
Adenosine	C10 H13 N5 O4		0	0	3	0	-0.00052

Questions