

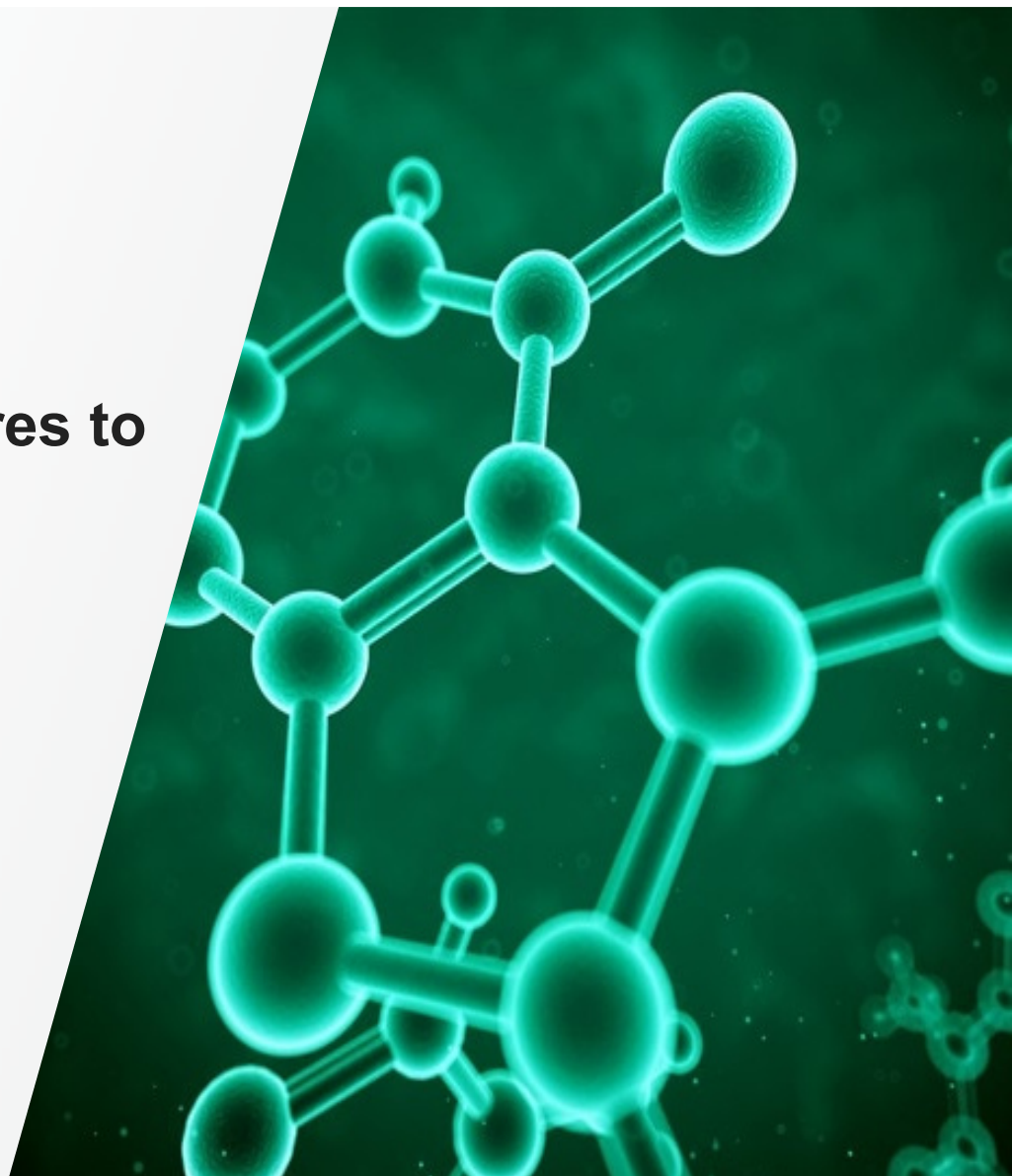
HRMS data elaboration: from features to compounds

Igor Fochi

Application Specialist

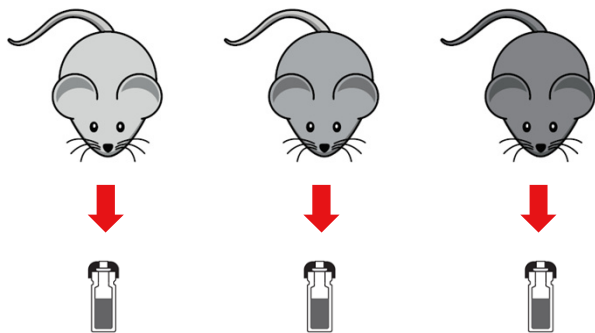
LSMS Support Team, Southern Europe

 The world leader in serving science

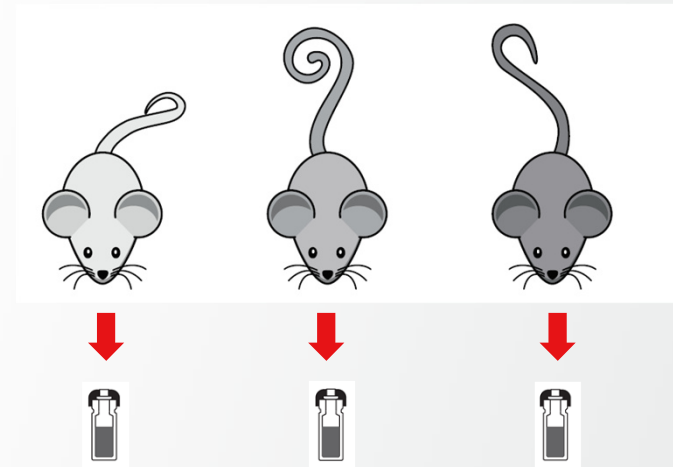


Untargeted Approach Scenario

Condition A



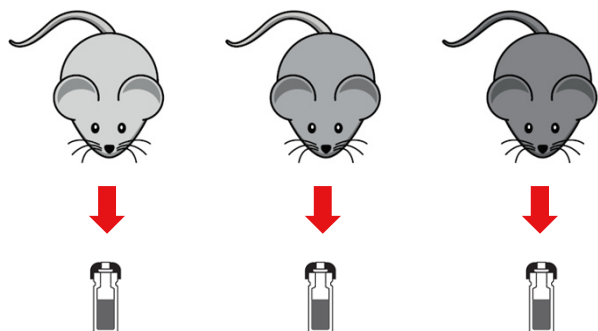
Condition B



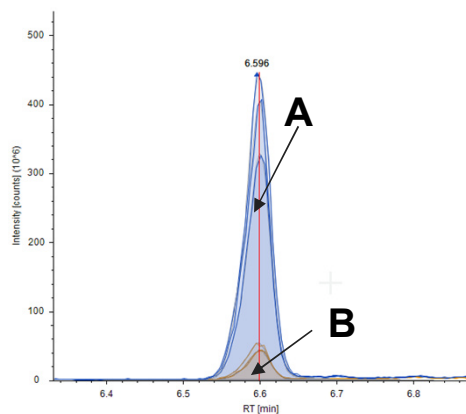
Find and identify the differences !

Untargeted Approach Scenario

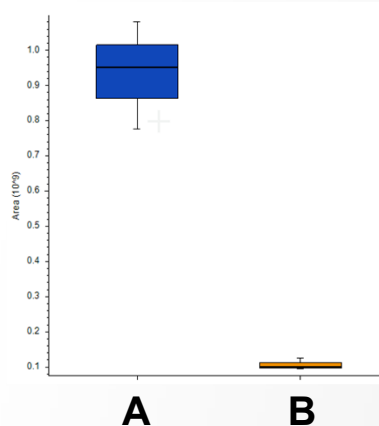
Condition A



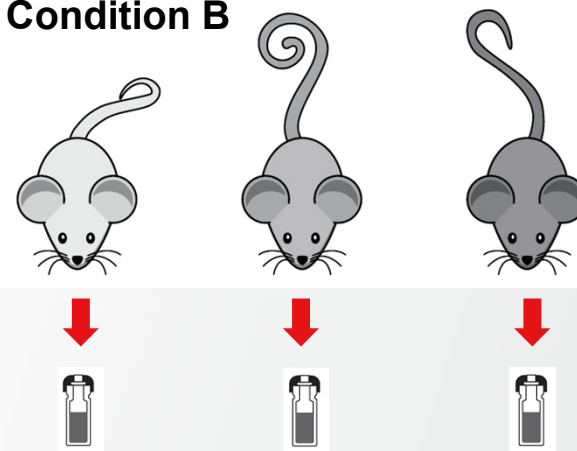
Compounds detected



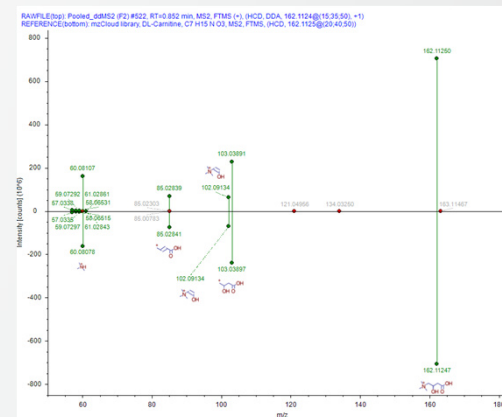
Statistics



Condition B



Identification

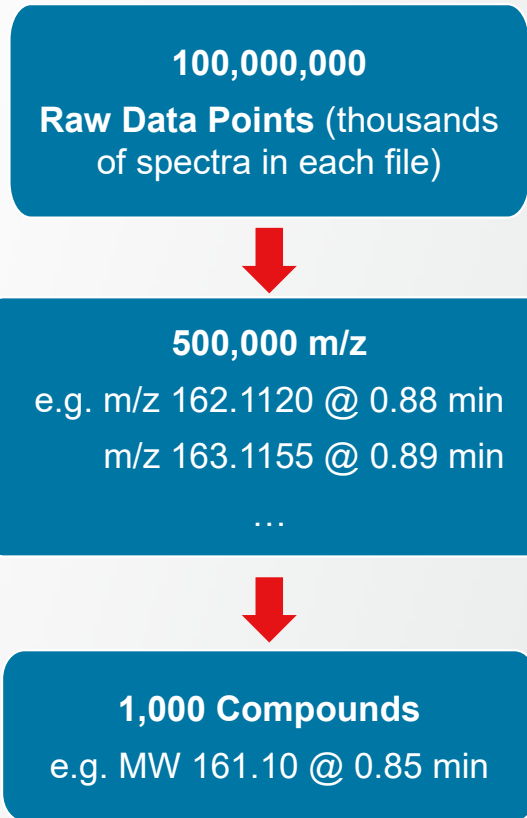
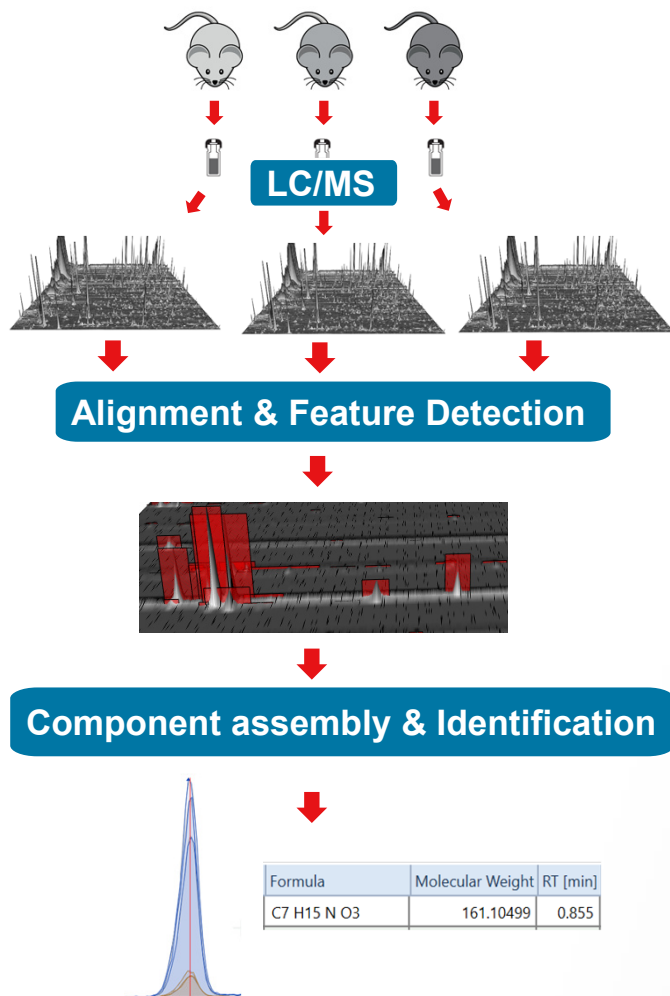


Thermo Scientific™ Compound Discoverer™ Software

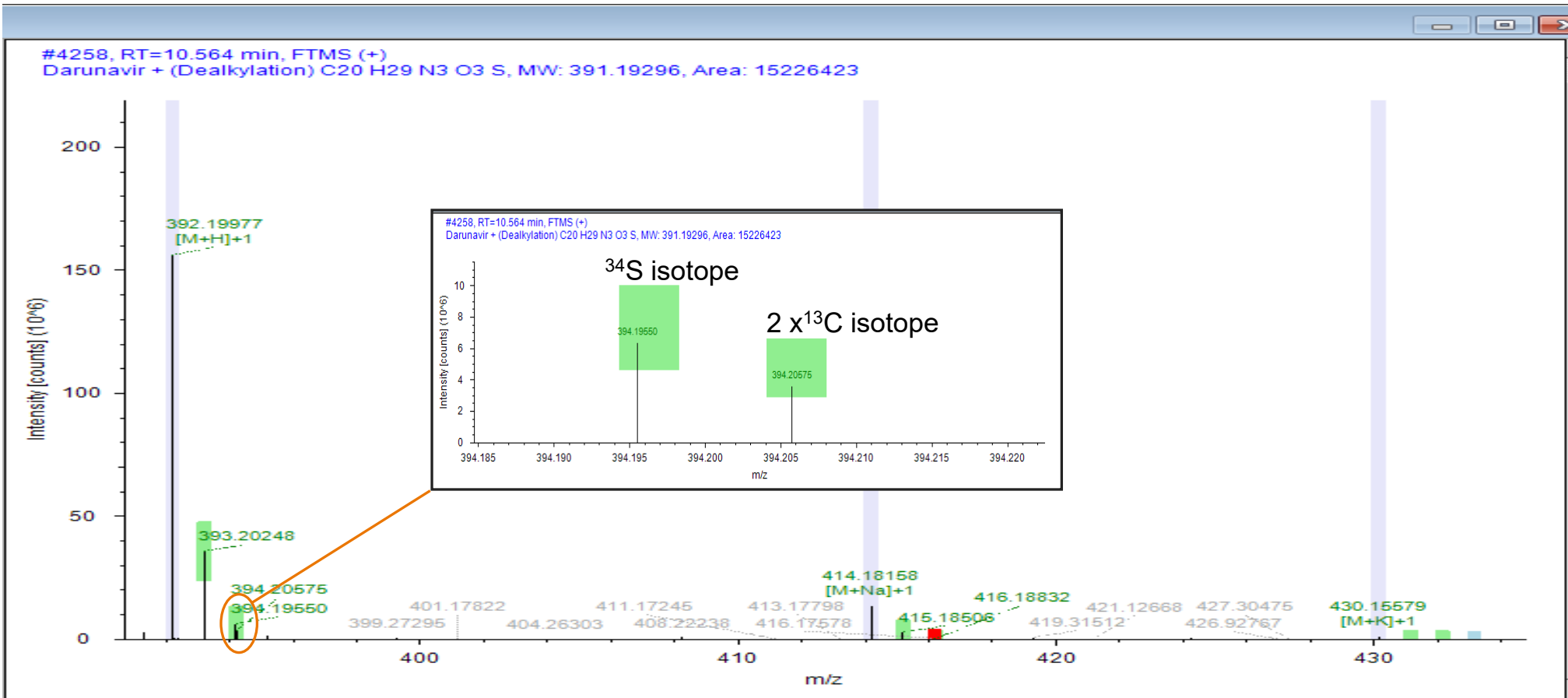
Metabolomics, Metabolites and Biomarkers Discovery,
Environmental research, Clinical and Forensics
research, Foodomics, ...



Data Reduction



Features



Workflow Details

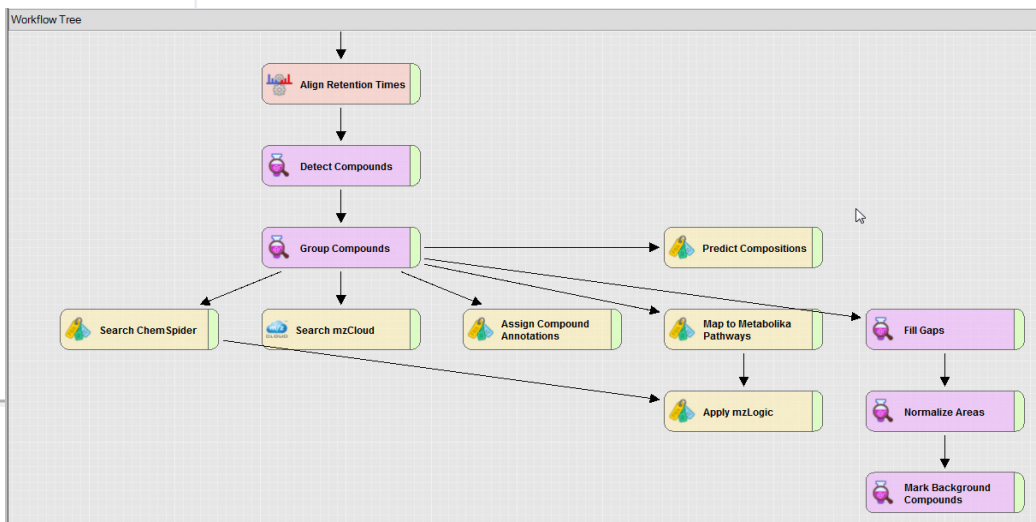
Processing

Workflow: WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics with Statistics Detect Unknowns with ID using Online Databases and mzLogic

Workflow Description:

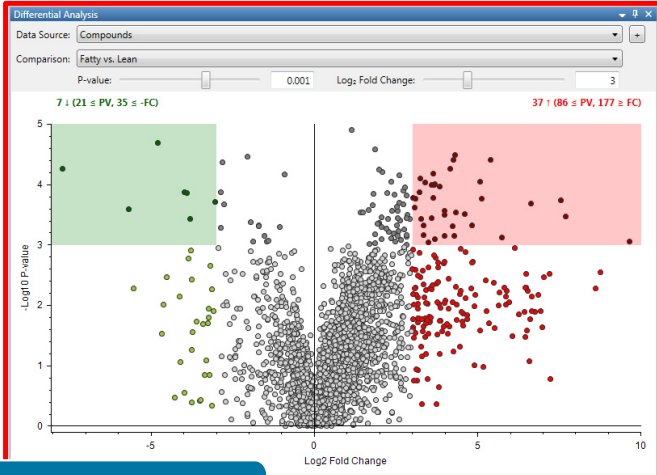
Untargeted Metabolomics workflow: Find and identify the differences between samples.

- Performs retention time alignment, unknown compound detection, and compound grouping across all samples. Predicts elemental compositions for all compounds, fills gaps across all samples, and hides chemical background (using Blank samples). Identifies compounds using mzCloud (ddMS2) and ChemSpider (formula or exact mass). Also performs similarity search for all compounds with ddMS2 data using mzCloud. Applies mzLogic algorithm to rank order ChemSpider results. Maps compounds to biological pathways using Metabolika. Applies QC-based batch normalization if QC samples are available. Calculates differential analysis (t-test or ANOVA), determines p-values, adjusted p-values, ratios, fold change, CV, etc.).

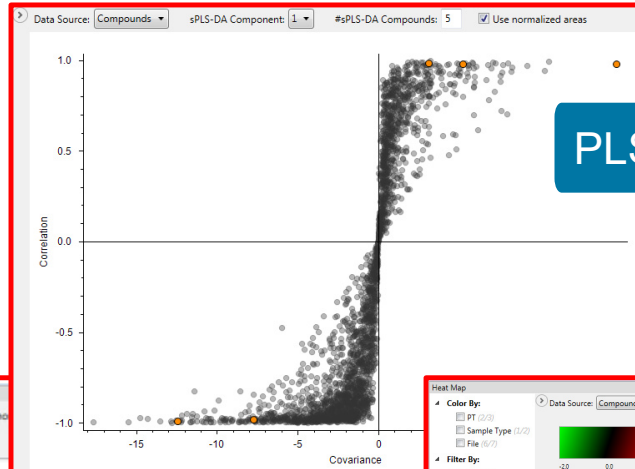


- Flexible data processing workflows
- Use drag & drop, “smart” connection
- Work with predefined workflows or create your own

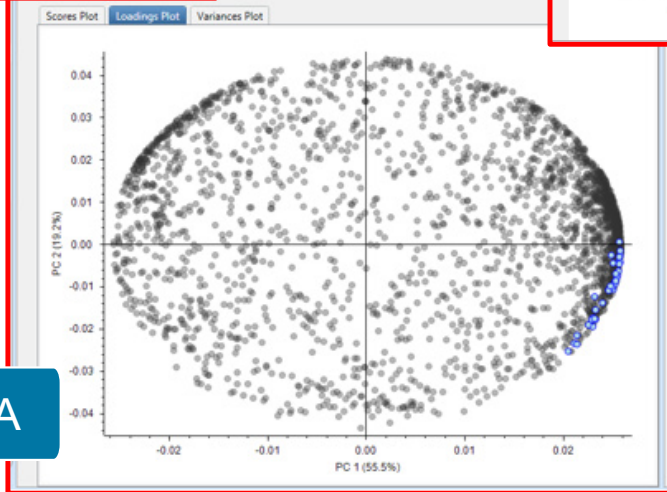
Statistics



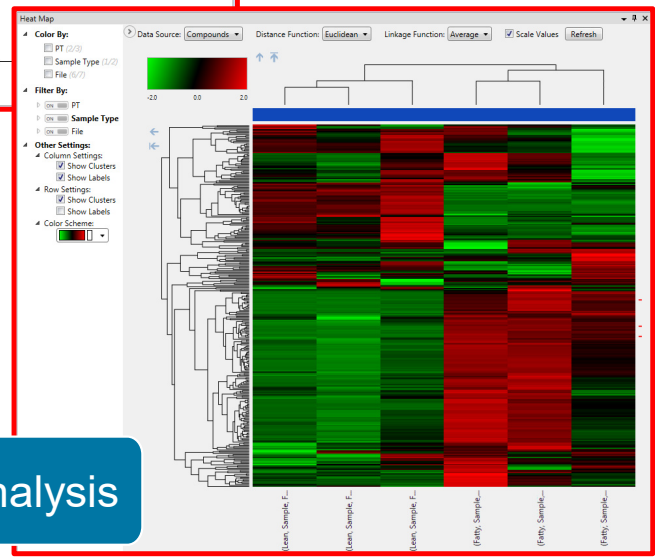
Volcano Plot



PLS-DA

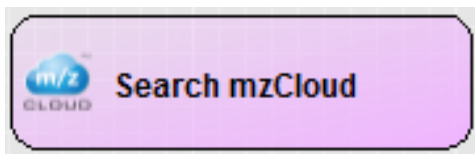


PCA

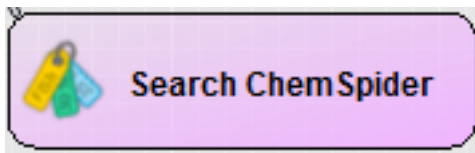


Cluster Analysis

Spectral Libraries and Compound Databases

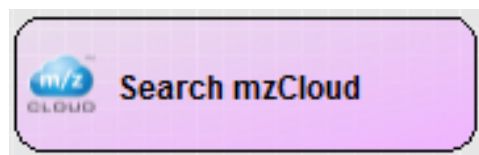


← Online spectral library
> 9 million spectra

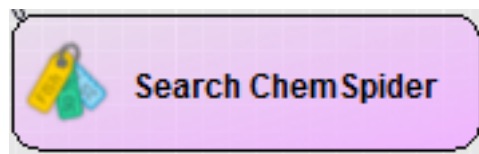


← Chemical structure database
> 110 million structures

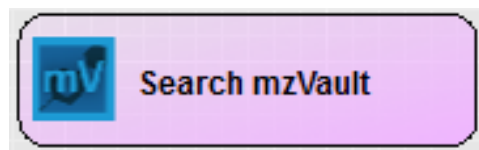
Spectral Libraries and Compound Databases



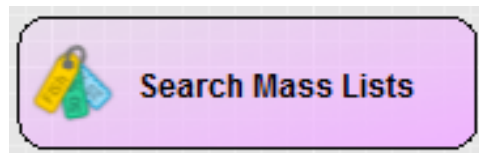
← Online spectral library
> 9 million spectra



← Chemical structure database
> 110 million structures



← Local msms spectral libraries



← Local databases

What is mzCloud?

ThermoFisher
SCIENTIFIC

mzCloud is a state of the art mass spectral database that assists analysts in identifying compounds in areas such as life sciences, metabolomics, pharmaceutical research, toxicology, forensic investigations, environmental analysis, food control and various industrial applications. mzCloud™ features a freely searchable collection of high resolution/accurate mass spectra using a new third generation spectra correlation algorithm.

Online access to the database is free of charge and no registration is required.

[read more...](#)

Enter
Database



New mzCloud App!



19,939 (+22)
compounds

27,539 (+22)
trees

9,058,715 (+27,724)
spectra

mzCloud™ - World's largest spectral library

ThermoFisher
SCIENTIFIC

- HRAM MS/MS and MSⁿ
- High quality curated data
- Wide chemical diversity
- Searchable web UI
- Integrated into TFS software

The screenshot displays the mzCloud web interface. On the left, a navigation menu includes 'Views', 'Reference Library', 'Search', and 'Tools'. The 'Reference Library' section lists several compounds with their IDs and monoisotopic masses, such as Glycitin (No: 6137, Monoiso. Mass: 446.12130) and Trilostane (No: 6143, Monoiso. Mass: 329.19909). The main content area shows a 'Spectral Tree' for Trilostane, a 'Recalibrated Spectrum' plot with peaks at m/z 112.03930, 147.11683, 201.16378, 303.1965, and 330.2064, and a 'Precursor Structure' section showing the chemical structure of Trilostane with a heuristic prediction (blue) and a quantum chemical prediction (brown). The 'Metadata' section provides citation links for the compound, tree, and spectrum. The 'Compound' section lists the names and systematic name of Trilostane.

Install mzCloud app
Desktop Application

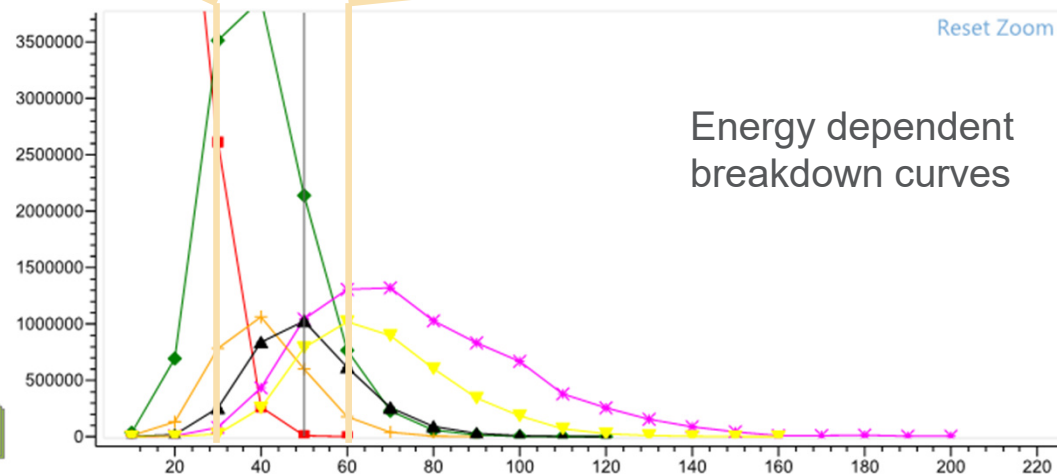
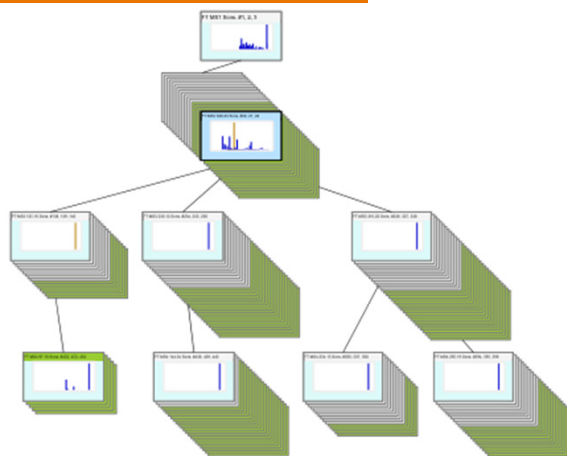
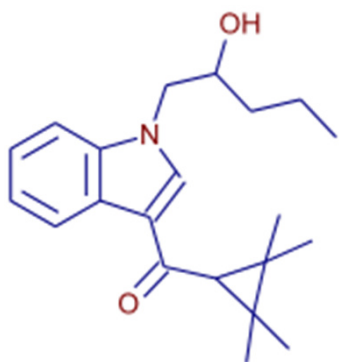
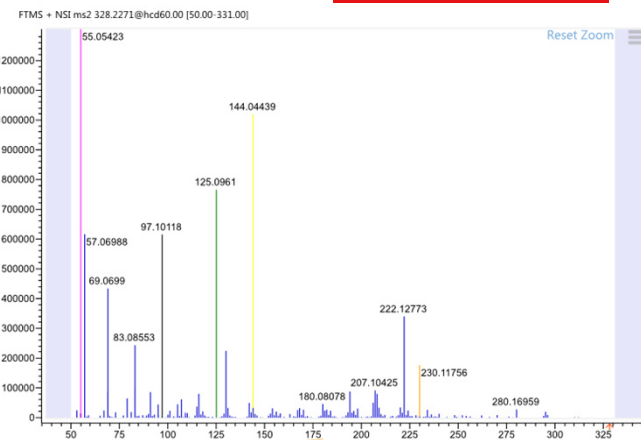
Terms and Conditions
© 2013 - 2016 HighChem LLC, Slovakia
mzCloud is a trademark of HighChem LLC, Slovakia
1.1.5.50139

record count 828

mzCloud™ - World's largest spectral library

ThermoFisher
SCIENTIFIC

- Spectral data at more than 10 collision energies
- Easily match spectra across different platforms
- Knowledge of energy dependent fragmentation



Interpreting the Results



Compound Discoverer 2.1.0.396

File Reporting Libraries View Window Help

Start Page ZDF_2 ZDF_b396_1e6_BC

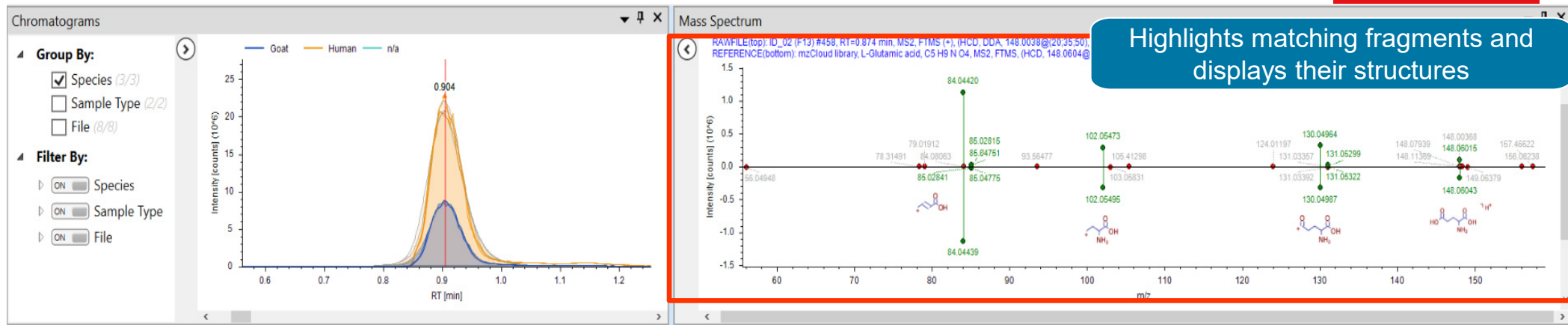
Chromatogram

Spectrum

Checked	Name	Formula	Annotation Source	Molecular Weight	RT [min]	Area (Max)	# ChemSpider Results	# mzCloud Results	mzCloud Best Match	Group Areas	Group CV [%]	Ratio	Log2 Fold Change	P-value	Adj. P-value		
<input type="checkbox"/>	Ethylendiaminetetraacetic acid (EDTA)	C10 H16 N2 O8	292.09007	292.09007				2	94.0	8.36e8	1.12e9	12	8	0.745	-0.43	4.0e-2	1.8e-1
<input type="checkbox"/>	Phenyl sulfoxide	C12 H10 O S	202.04495	202.04495				10		2.80e8	6.76e7	25	32	4.147	2.05	6.0e-3	8.5e-2
<input type="checkbox"/>	Isoleucine	C6 H13 N O2	131.09453	131.09453	2.014	273034057	18	16	99.8	2.59e8	1.49e8	17	11	1.735	0.79	2.8e-2	1.4e-1
<input type="checkbox"/>	Betaine	C5 H11 N O2	117.07877	117.07877	0.868	272533644	14	3	92.1	2.70e8	2.56e8	17	11	1.056	0.08	9.3e-1	9.6e-1
<input type="checkbox"/>	Ethylendiaminetetraacetic acid (EDTA)	C10 H16 N2 O8	292.09005	292.09005	0.848	245497612	1	1	94.2	9.93e7	1.41e8	29	41	0.702	-0.51	2.4e-1	4.9e-1
<input type="checkbox"/>	DL-Tryptophan	C11 H12 N2 O2	204.08974	204.08974	3.119	221517495	12	3	98.3	1.75e8	2.09e8	2	9	0.836	-0.26	8.0e-2	2.6e-1
<input type="checkbox"/>	Creatine	C4 H9 N3 O2	131.06929	131.06929	0.900	214570323	2	2	96.8	2.10e8	6.57e7	20	17	3.196	1.66	2.6e-1	9.0e-1
<input type="checkbox"/>	L-Phenylalanine	C9 H11 N O2	165.07892	165.07892	2.578	196677505	17	1	97.5	1.89e8	1.45e8	9	9	1.305	0.38	4.8e-2	1.9e-1
<input type="checkbox"/>	Creatinine	C4 H7 N3 O	113.05880	113.05880	0.927	187929579	2	0		1.80e8	1.11e8	14	11	1.621	0.70	1.5e-2	1.0e-1
<input type="checkbox"/>	L-Tyrosine	C9 H11 N O3	181.07382	181.07382	1.625	187009002	17	2	97.6	1.29e8	1.69e8	18	8	0.761	-0.39	6.3e-2	2.3e-1
<input type="checkbox"/>	L-Valine	C5 H11 N O2	117.07878	117.07878	1.187	176220368	14	6	97.1	1.76e8	1.01e8	15	8	1.740	0.80	1.8e-2	1.1e-1
<input type="checkbox"/>	Acetyl-L-carnitine	C9 H17 N O4	203.11558	1334	167058234	2	4	98.1	1.51e8	9.40e7	19	11	1.609	0.69	5.0e-2	2.0e-1	
<input type="checkbox"/>	L-Isoleucine	C6 H13 N O2	131.09453	131.09453	1.926	135383791	18	4	96.2	1.23e8	8.34e7	15	9	1.474	0.56	4.0e-2	1.8e-1
<input type="checkbox"/>	Benzene	C6 H6	78.04684	78.04684	2.578	134647271	1	29		1.27e8	9.44e7	11	11	1.349	0.43	6.4e-2	2.3e-1
<input type="checkbox"/>	3-Methylsulfolene	C5 H8 O2 S	132.02440	1362	134209264	2	12			1.30e8	7.76e7	21	11	1.676	0.75	7.0e-2	2.4e-1
<input type="checkbox"/>	L(-)-Carnitine	C7 H15 N O3	161.10499	0.859	131594238	2	2			7.90e7	7.37e7	60	34	1.072	0.10	9.8e-1	9.9e-1
<input type="checkbox"/>	Triadimefon	C14 H16 Cl N3 O2	293.09259	0.934	129208301	2	0			9.92e7	2.66e7	59	106	3.721	1.90	5.4e-1	7.4e-1
<input type="checkbox"/>	L(-)-Methionine	C5 H11 N O2 S	149.05093	1.535	103824776	7	1			1.01e8	5.54e7	20	85	1.820	0.86	3.2e-1	5.8e-1
<input type="checkbox"/>	[Similar to: Fluoxymesterone; ΔMass: 56.0270 Da]	C12 H30 N2 O P2	280.18306	7.266	102014803	0	38			1.00e8	1.01e8	2	5	0.998	0.00	5.6e-1	7.5e-1
<input type="checkbox"/>	Piperidine	C5 H11 N	85.08903	2.015	93672219	1	0			8.95e7	4.80e7	19	11	1.863	0.90	3.2e-2	1.6e-1

Show Related Tables

mzCloud search



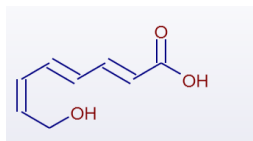
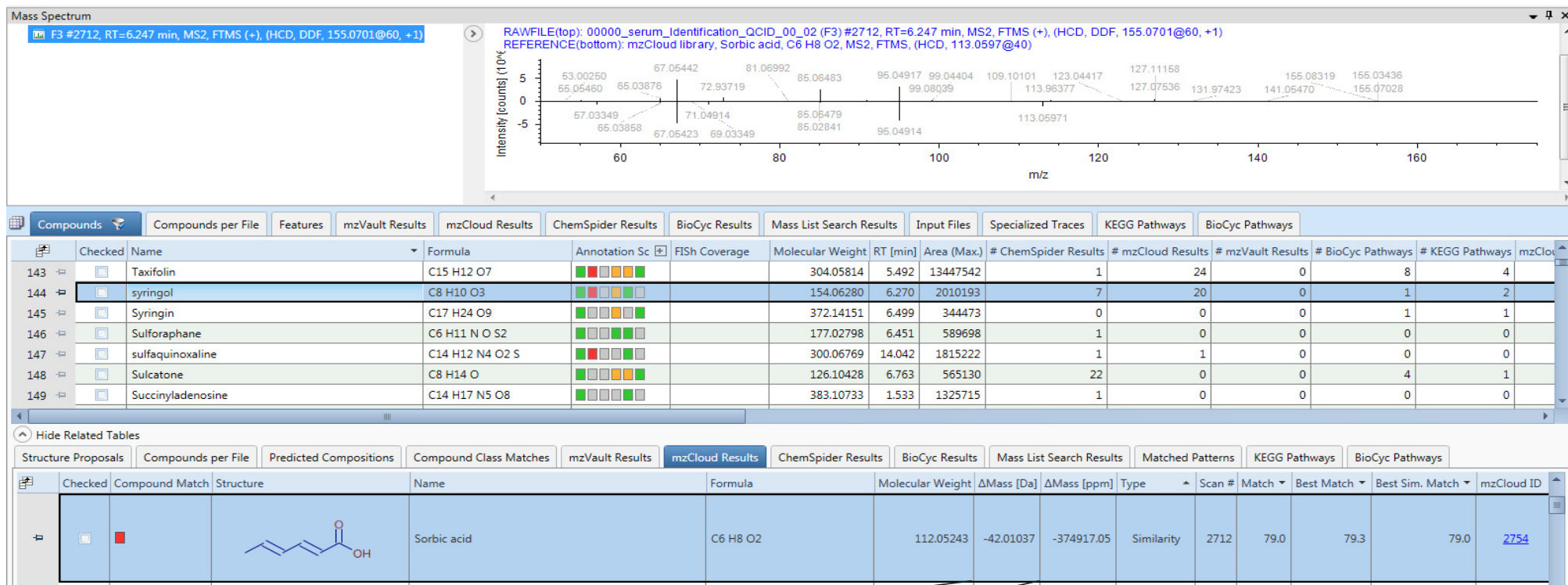
Checked	Name	Formula	Annotation Sc	Molecular Weight	RT [min]	Area (Max.)	# ChemSpider Results	# mzCloud Results	mzCloud Best Ma	MS2	Group Areas	Group CV [%]	Ratio
<input type="checkbox"/>	L-Glutamic acid	C5 H9 N O4	■■■■	147.05316	0.905	91075755	16	1	98.9	■	3.47e7 8.74e7	2 3	0.397
<input type="checkbox"/>	DL-Glutamine	C5 H10 N2 O3	■■■■	146.06920	0.879	31726336	9	6	98.9	■	7.51e6 3.10e7	9 4	0.242
<input type="checkbox"/>	Valsartan	C24 H29 N5 O3	■■■	435.22733	9.871	30309913	1	1	98.7	■	5.34e4 2.91e7	36 4	0.002

Hide Related Tables

Checked	Compound Match	Structure	Name	Formula	Molecular Weight	ΔMass [Da]	ΔMass [ppm]	Match	Best Match	Scan #	mzCloud ID	KEGG ID
<input type="checkbox"/>	■	<chem>NC(CC(=O)O)C(=O)O</chem>	L-Glutamic acid	C5 H9 N O4	147.05316	0.00001	0.04	98.9	98.9	458	Reference-470	C00025

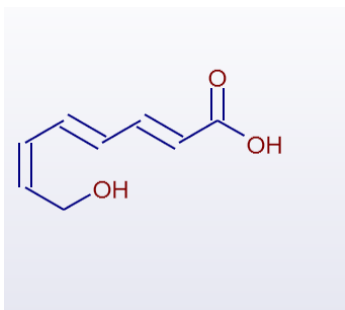
Similarity search: mzCloud

ThermoFisher
SCIENTIFIC

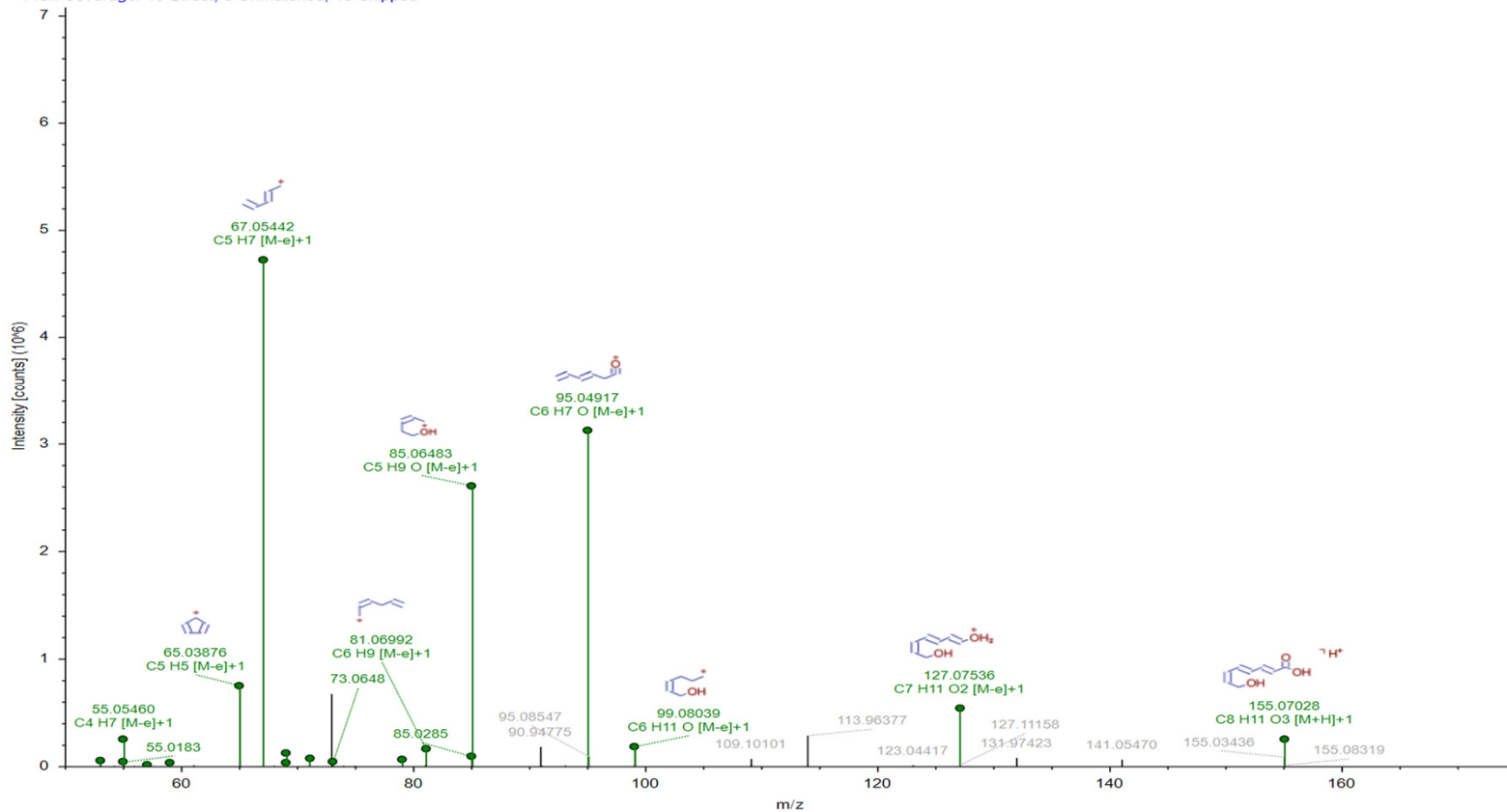


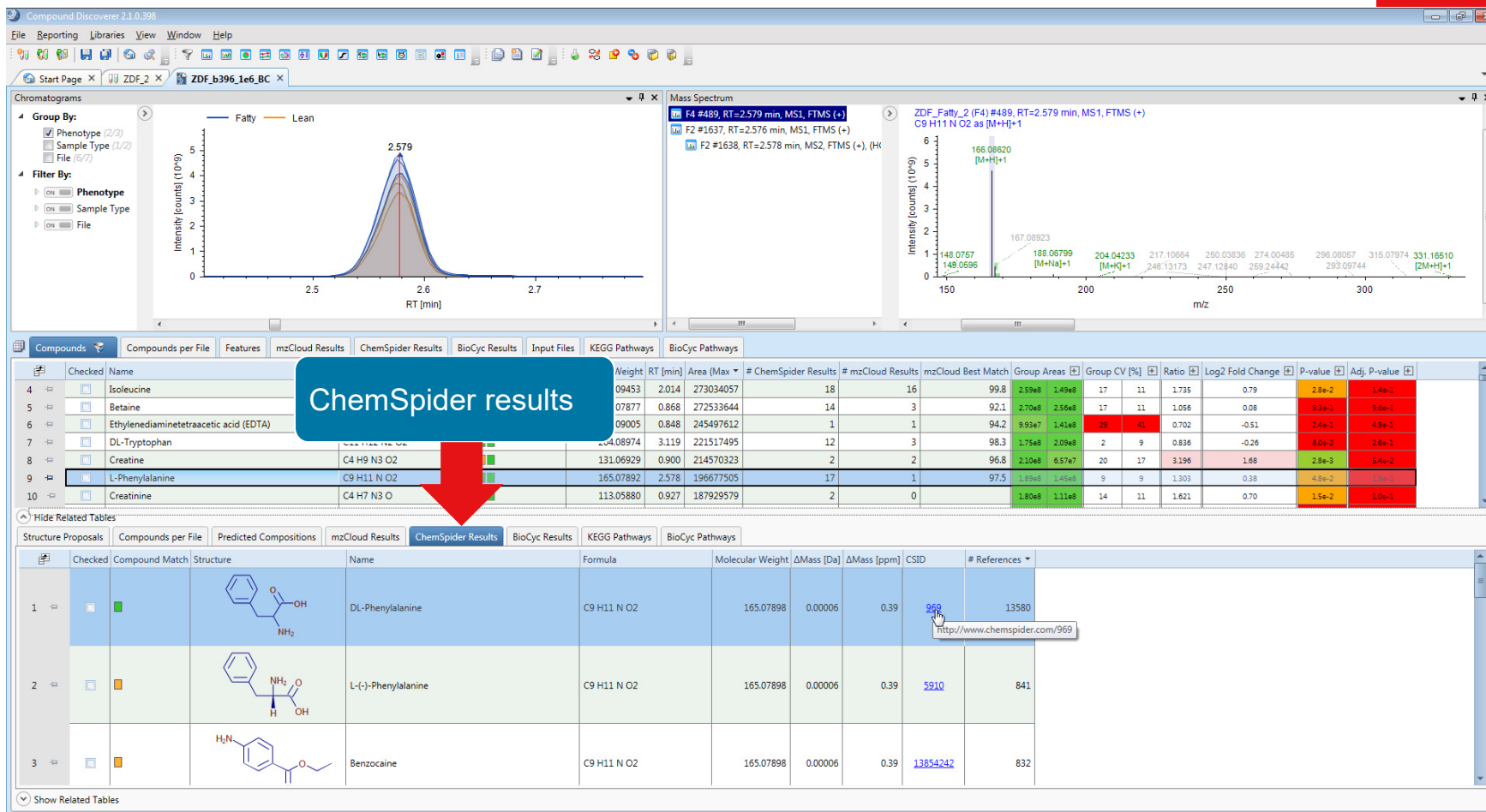
C2H2O

Methyl Hydroxy Sorbic Acid fragments explanation: FISh (Fragment Ion Search) scoring



00000_serum_Identification_QCID_00_02 (F3) #2712, RT=6.247 min, MS2, FTMS (+), (HCD, DDF, 155.0701@60, +1)
Sorbic acid +C2H2O, C8 H10 O3
FISh Coverage: 19 Direct, 8 Unmatched, 18 Skipped





FISh score for Structure Proposals

ThermoFisher
SCIENTIFIC

FISh annotation can be calculated as a batch

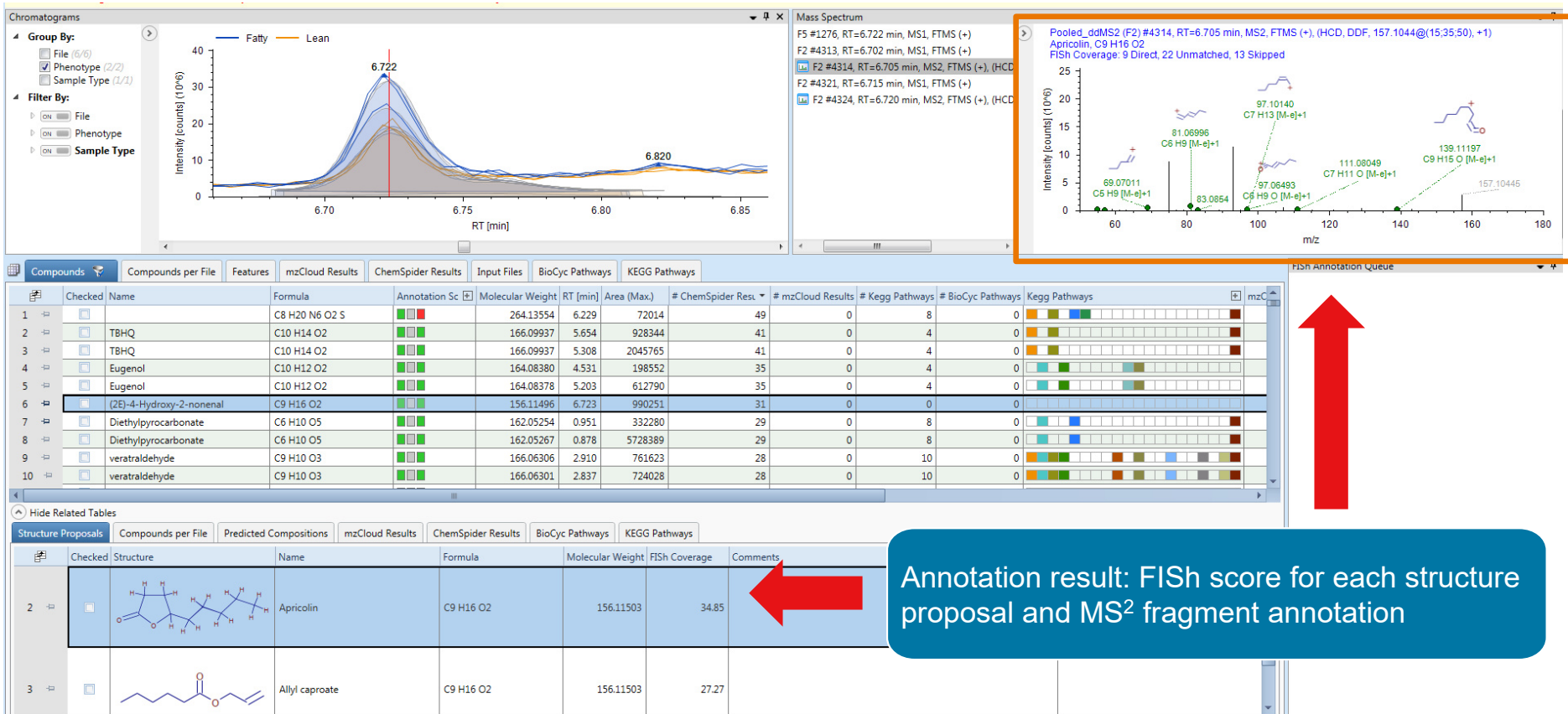
Checked	Name	Formula	Annotation Sc	Molecular Weight	RT [min]	Area (Max.)	# ChemSpider Res.	# mzCloud Results	# Kegg Pathways	Kegg Pathways	mzCloud Best Match	Gr
25	3-Phenyl-1-propanol	C9 H12 O	■■■■	136.08876	5.212	888554	21	0	0			6
26	mephensin	C10 H14 O3	■■■■	182.09400	3.713	5141144	21	0	3			6
27	Phenoxyethanol	C8 H10 O2	■■■■	138.06809	4.296	672557	20	0	7			6
28	Aminolevulinic acid	C5 H9 N O3	■■■■	131.05802	0.844	3435255	20	0	12			9
29	1,3,3-Trimethyl-2-oxabicyclo[2.2.2]o	C10 H18 O3	■■■■	186.12541	5.795	400666	20	0	2			3
30	Phenoxyethanol	C8 H10 O2	■■■■	138.06807	2.919	479742	20	0	7			3
31	2-Methyl-5-propionylfuran	C8 H10 O2	■■■■	138.06804	4.675	1198708	20	1	7			55.1
32	cis-4-Hydroxy-D-proline	C5 H9 N O3	■■■■	131.05806	0.939	8039552	20	1	12			50.7
33	cis-4-Hydroxy-D-proline	C5 H9 N O3	■■■■	131.05809	0.988	4139749	20	1	12			50.7

Checked	Compound Match	CSID	Formula	Molecular Weight	Name	ΔMass [Da]	Structure	ΔMass [ppm]	# References
20	■	28533156	C8 H10 O2	138.06808	(2E,4E,6E)-7-Hydroxy-4-methyl-2,4,6-heptatrienal	0.00005		0.35	2

FISh Annotation Queue

- Name: Tyrosol
MW [Da]: 138.06808
Queued Since: 65 ms
State: Processing
- Name: veratrol
MW [Da]: 138.06808
Queued Since: 74 ms
State: Waiting
- Name: p-ANISYL ALCOHOL
MW [Da]: 138.06808
Queued Since: 83 ms
State: Waiting
- Name: 1,4-Dimethoxybenzer
MW [Da]: 138.06808
Queued Since: 95 ms
State: Waiting
- Name: 1,3-Dimethoxybenzer
MW [Da]: 138.06808

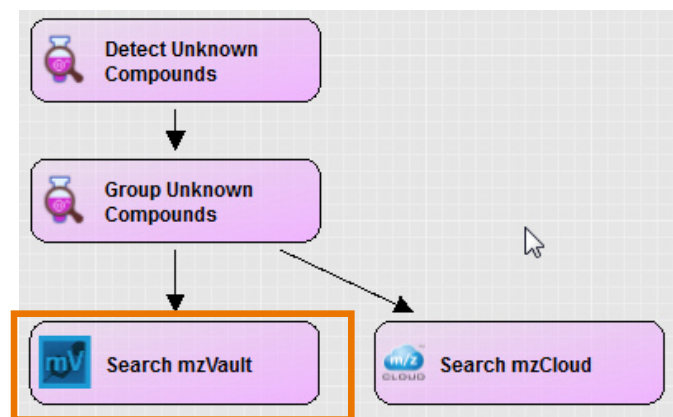
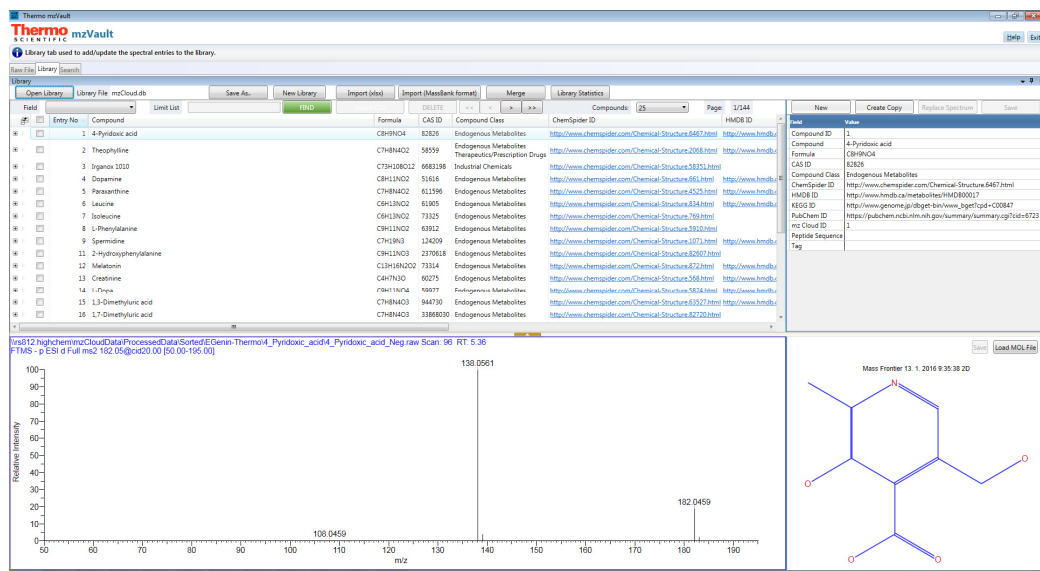
FISh Annotation for Structure Proposals



Annotation result: FISh score for each structure proposal and MS² fragment annotation

Local Spectral Libraries (mzVault)

- **mzVault** – support for local spectral libraries
 - Compound Discoverer software comes with a local version of the mzCloud™ database
 - Custom spectral libraries can be created and edited using mzVault application



Export to mzVault

The screenshot shows a software interface with a table of compounds. The table has columns for 'Checked', 'Name', 'Formula', 'Annotation Sc', 'Molecular Weight', and 'RT'. Five rows are visible, each with a checked box in the 'Checked' column and a name (X1 to X5) in the 'Name' column. A context menu is open over the table, showing various options. The 'Export' option at the bottom is highlighted, and a sub-menu is open, showing options like 'As Plain Text...', 'As Excel...', and 'To Existing mzVault Library...'. The 'To Existing mzVault Library...' option is highlighted with a red box.

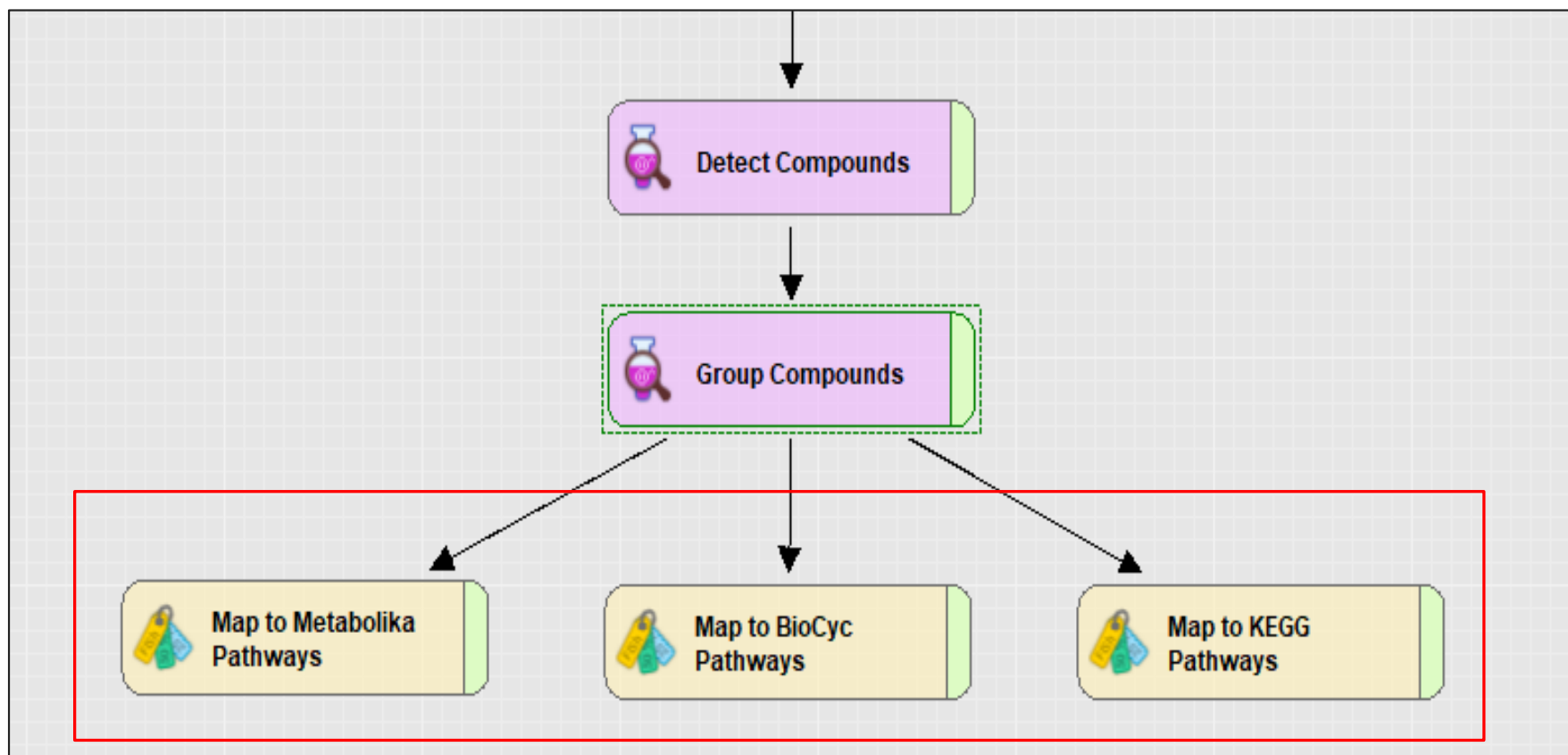
	Checked	Name	Formula	Annotation Sc	Molecular Weight	RT
1	<input checked="" type="checkbox"/>	X1	C6 H17 N2 O P S2	■ ■ ■ ■ ■	228.05104	
2	<input checked="" type="checkbox"/>	X2	C6 H14 O			
3	<input checked="" type="checkbox"/>	X3	C6 H9 N1			
4	<input checked="" type="checkbox"/>	X4	C3 H6 N4			
5	<input checked="" type="checkbox"/>	X5	C6 H14 O			

Context Menu Options:

- Copy With Headers (Ctrl+C)
- Copy
- Clear Selection
- Cell Selection Mode
- Enable Column Fixing
- Collapse All Column Headers
- Expand All Column Headers
- Check Selected
- Check All
- Uncheck Selected
- Uncheck All
- Remove All Checkmarks in All Tables
- Edit Compound Annotation
- Clear Compound Annotation
- Apply FISH Scoring
- Export
 - As Plain Text...
 - As Excel...
 - As Xcalibur Inclusion/Exclusion List...
 - As TraceFinder List...
 - To Existing mzVault Library...
 - To New mzVault Library...

Create a spectral library of known unknowns

Metabolomics Database



Metabolika Pathways

Start Page X Lists & Libraries X

New... Edit... Delete Import... Export... Replace...

Filename	Description	File Size	Uploaded
Aa	Aa	=	=
Superpathway of cholesterol biosynthesis		1,894.15 KB	8/1/2018 2:51 PM
Superpathway of fatty acids biosynthesis (E. coli)		1,760.51 KB	8/1/2018 2:52 PM
Superpathway of chorismate metabolism		1,743.23 KB	8/1/2018 2:51 PM
Methanobacterium thermoautotrophicum biosynthetic metabolism			
Superpathway of histidine, purine, and pyrimidine biosynthesis			
Superpathway of flavones and derivatives biosynthesis			
Superpathway of C28 brassinosteroid biosynthesis			
Superpathway of fatty acid biosynthesis II (plant)		1,497.32 KB	8/1/2018 2:52 PM
Superpathway of gibberellin biosynthesis		1,352.65 KB	8/1/2018 2:52 PM
Plant sterol biosynthesis		1,342.6 KB	8/1/2018 2:51 PM
Superpathway of aromatic compound degradation via 2-oxopent-4-enoate		1,309.42 KB	8/1/2018 2:51 PM
Superpathway of L-lysine degradation		1,194.29 KB	8/1/2018 2:52 PM
Adenosylcobalamin biosynthesis II (aerobic)		1,189.46 KB	8/1/2018 2:51 PM
Superpathway of cholesterol degradation II (cholesterol dehydrogenase)		1,164.05 KB	8/1/2018 2:51 PM
Adenosylcobalamin biosynthesis I (anaerobic)		1,139.54 KB	8/1/2018 2:51 PM
Superpathway of diterpene resin acids biosynthesis		1,132.49 KB	8/1/2018 2:52 PM
Superpathway of steroid hormone biosynthesis		1,103.3 KB	8/1/2018 2:52 PM
Superpathway of ergosterol biosynthesis I		1,085.19 KB	8/1/2018 2:52 PM
Superpathway of aerobic toluene degradation		1,079.15 KB	8/1/2018 2:51 PM
Superpathway of pentose and pentitol degradation		1,034.06 KB	8/1/2018 2:52 PM
Superpathway of trichothecene biosynthesis		1,030.72 KB	8/1/2018 2:52 PM
Superpathway of aromatic compound degradation via 3-oxoadipate		998.74 KB	8/1/2018 2:51 PM
Superpathway of bacteriochlorophyll a biosynthesis		995.34 KB	8/1/2018 2:51 PM

Metabolika™ : set of 378 metabolic pathways, directly integrated into CD

Metabolika Pathways - Editor

ThermoFisher
SCIENTIFIC

Expected Compounds

Transformations

Adducts

Ion Definitions

Mass Lists

Spectral Libraries

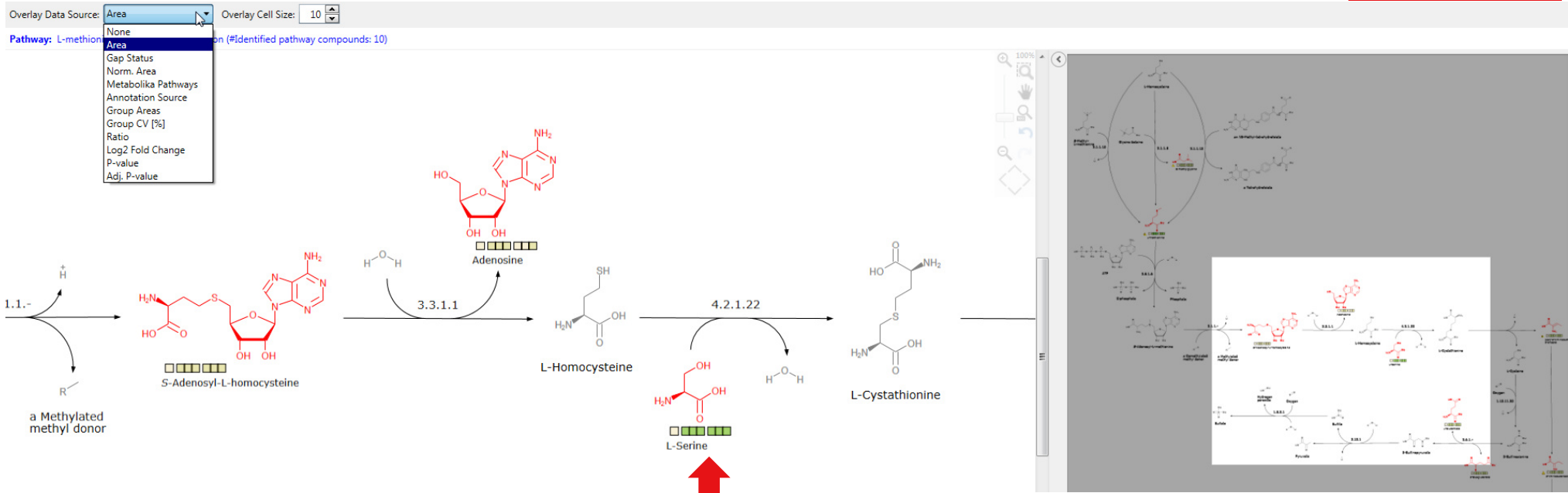
Metabolika Pathways

Compound Classes

Filename	Description	File Size	Uploaded	Updated	Context	State
Superpathway of cholesterol biosynthesis						
Superpathway of fatty acids biosynthesis (E. coli)						
Superpathway of chorismate metabolism						
Methanobacterium thermoautotrophicum biosynt						
Superpathway of histidine, purine, and pyrimidine						
Superpathway of flavones and derivatives biosynt						
Superpathway of C28 brassinosteroid biosynthesis						
Superpathway of fatty acid biosynthesis II (plant)						
Superpathway of gibberellin biosynthesis						
Plant sterol biosynthesis						
Superpathway of aromatic compound degradatio						
Superpathway of L-lysine degradation						
Adenosylcobalamin biosynthesis II (aerobic)						
Superpathway of cholesterol degradation II (chole						
Adenosylcobalamin biosynthesis I (anaerobic)						
Superpathway of diterpene resin acids biosynthes						
Superpathway of steroid hormone biosynthesis						
Superpathway of ergosterol biosynthesis I						
Superpathway of aerobic toluene degradation						
Superpathway of pentose and pentitol degradatio						
Superpathway of trichothecene biosynthesis						
Superpathway of aromatic compound degradatio						
Superpathway of bacteriochlorophyll a biosynthes						
Superpathway of purine nucleotides de novo bios						
Superpathway of aflatoxin biosynthesis						
Superpathway of cholesterol degradation I (chole						
Superpathway of inositol phosphate compounds						909
Anaerobic aromatic compound degradation (Thauera aromatica)						904
Superpathway of mycolyl-arabinogalactan-peptidoglycan complex biosynthesis		896.11 KB	6/1/2018 2:52 PM	5/4/2018 12:40 PM		Available

Built-in pathway editor

Metabolika Pathways



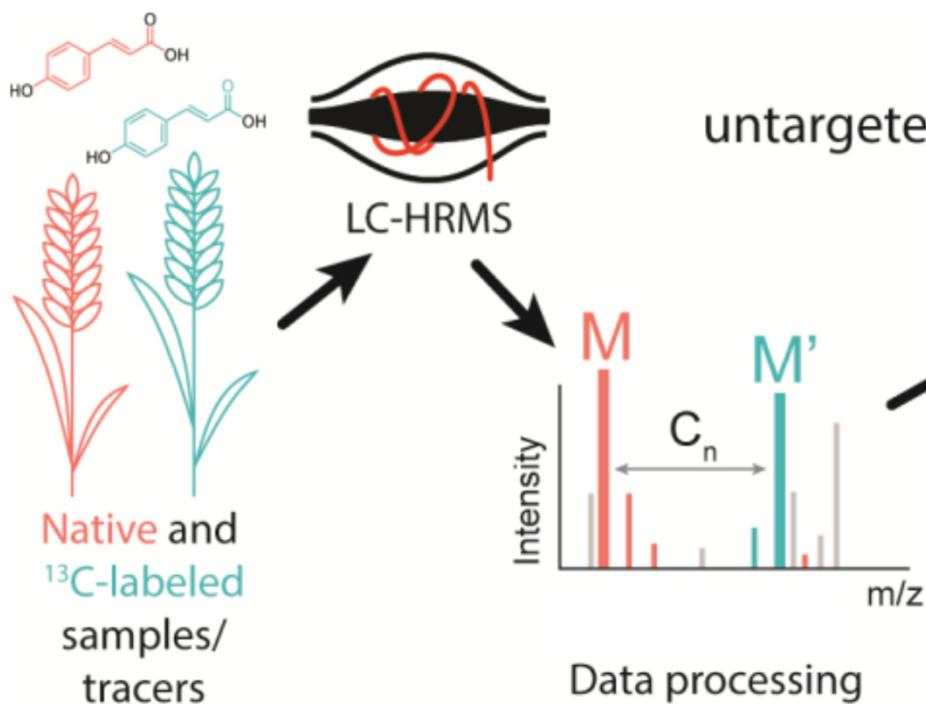
Interactive, customizable pathway maps

Statistical data can be overlaid onto the pathway

Stable Isotope Labeling



Stable Isotope Labeling



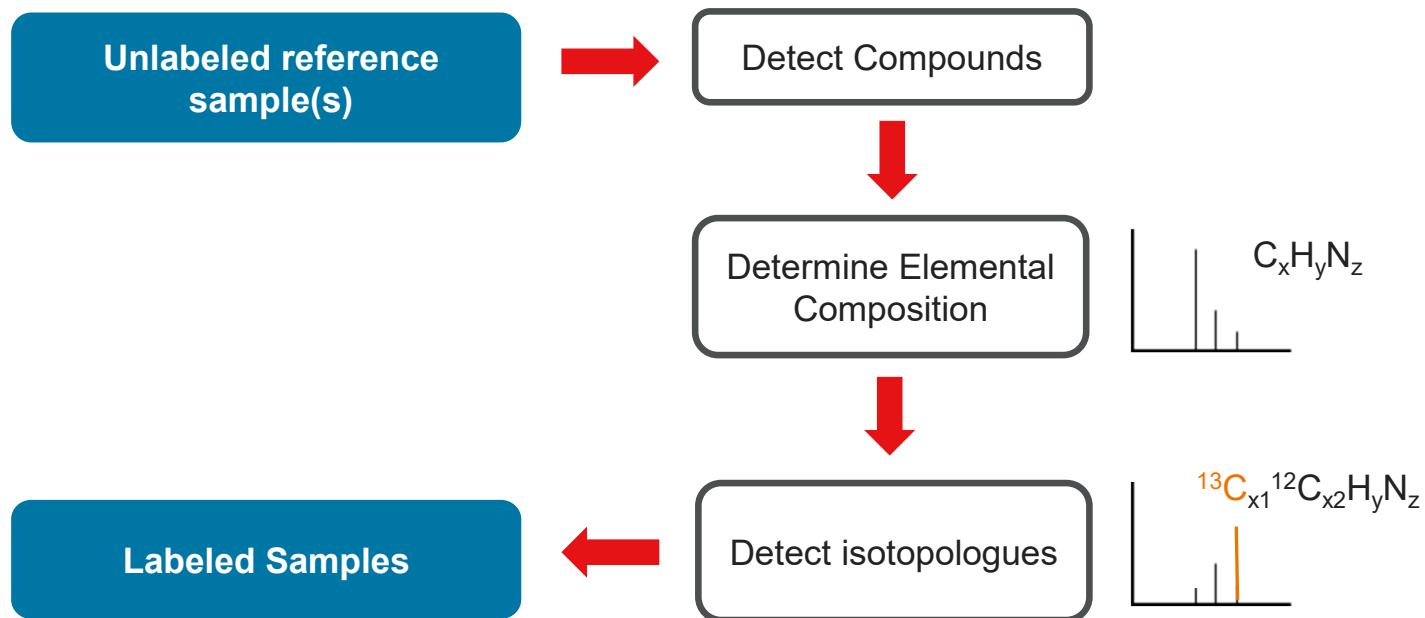
SIL assisted
untargeted metabolomics

Compounds	Compounds per File	Features	Labeled Features	Labeled Compounds per File	Mass List Search Results	Input Files	
Checked	Name	Formula	Annotation	Molecular Weight	RT [min]	Area (Max.)	Rel. Exchange [%]
<input checked="" type="checkbox"/>	Uridine	C9 H12 N2 O6	■ ■	244.06922	7.146	362256836	0 0 39 67 52 0
<input checked="" type="checkbox"/>	Proline	C5 H9 N O2	■ ■	115.06337	11.773	70424932	0 0 3 3 3 0
<input checked="" type="checkbox"/>	Malate	C4 H6 O5	■ ■	134.02156	24.962	56234422	0 0 8 9 9 0
<input checked="" type="checkbox"/>	Glutamine	C5 H10 N2 O3	■ ■	146.06924	13.956	48610589	0 0 0 0 0 0
<input checked="" type="checkbox"/>	Citrate/Isocitrate	C6 H8 O7	■ ■	192.02713	31.567	43732087	0 0 3 5 4 0
<input checked="" type="checkbox"/>	Lactate	C3 H6 O3	■ ■	90.03163	14.231	14127499	0 0 66 55 69 0
<input checked="" type="checkbox"/>	NAD	C21 H27 N7 O14 P2	■ ■	663.11102	20.138	5792721	0 0 40 39 39 0
<input checked="" type="checkbox"/>	Alanine	C3 H7 N O2	■ ■	89.04760	12.561	5698362	0 0 45 48 44 0
<input checked="" type="checkbox"/>	α-Ketoglutarate	C5 H6 O5	■ ■	146.02173	25.941	6177872	1 0 3 3 3 1
<input checked="" type="checkbox"/>	Hexose-6-phosphate	C6 H13 O9 P	■ ■	260.02978	25.877	3922810	0 0 11 11 11 0
<input checked="" type="checkbox"/>	Serine	C3 H7 N O3	■ ■	105.04258	14.386	3159629	0 0 13 10 10 0
<input checked="" type="checkbox"/>	Glycine	C2 H5 N O2	■ ■	75.03207	13.587	4393736	0 0 6 6 6 0

Detect labeled compounds

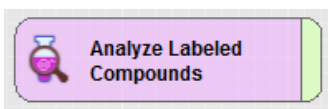
modified from Bueschl et. al. Analytical Chemistry 2017

Untargeted detection of labeled compounds



Untargeted Analysis: CD automatically detects labeled compounds (isotopologues) based on formulas of unlabeled compounds found in reference file(s)

Untargeted detection of labeled compounds



Study Definition		Input Files		Samples
Error	Sample	File	Sample Identifier	Sample Type
<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
	S1	F1	20150226_HeLa_24_NH2_NEG_12C_Glc_1_07	Sample
	S2	F2	20150226_HeLa_24_NH2_NEG_12C_Glc_3_13	Sample
	S6	F6	20150226_HeLa_24hr_NH2_NEG_12C_Glc_2_11	Sample
	S3	F3	20150226_HeLa_24_NH2_NEG_13C_Glc_1_06	Labeled
	S4	F4	20150226_HeLa_24_NH2_NEG_13C_Glc_2_09	Labeled
	S5	F5	20150226_HeLa_24_NH2_NEG_13C_Glc_3_14	Labeled

Unlabeled reference samples

Labeled Samples

Parameters of 'Analyze Labeled Compounds'

Show Advanced Parameters

1. Label Settings	
Label Element	[13]C
Max. Exchange	25
Source Efficiency [%]	100
2. Pattern Analysis	
Mass Tolerance [ppm]	5 ppm
Intensity Tolerance [%]	30
Intensity Threshold [%]	0.1
SN Threshold	3
3. General Settings	
Hide Unprocessed	True

Label is the only user-entered parameter required for automatic isotopologues detection.

Stable Isotope Labeling - Details

	Checked	Name	Formula	Annotation +	Molecular Weight	RT [min]	Area (Max.)	20150226_HeLa_24_NH2_NEG_12C_G	20150226_HeLa_24_NH2_NEG_12C_G	20150226_HeLa_24hr_NH2_NEG_12C_G	20150226_HeLa_24_NH2_NEG_13C_G	20150226_HeLa_24_NH2_NEG_13C_G	20150226_HeLa_24_NH2_NEG_13C_G
3	<input checked="" type="checkbox"/>	Lactate	C3 H6 O3	■ ■ ■ ■	90.03163	14.174	13540685	0	0	0	67	54	70
4	<input checked="" type="checkbox"/>	Alanine	C3 H7 N O2	■ ■ ■ ■	89.04760	12.577	5415885	0	0	0	45	48	44
5	<input checked="" type="checkbox"/>	Hexose-6-phosphate	C6 H13 O9 P	■ ■ ■ ■	260.02978	25.819	3930432	0	0	0	95	83	81

Total exchange rate for this compound in each sample


Hide Related Tables

Structure Proposals Compounds per File Predicted Compositions **Labeled Compounds per File**

	Checked	Molecular Weight	RT [min]	Max. # MI	Area	Max. Exchange	Avg. Exchange	Rel. Exchange [%]	Status	Exchange Rate [%]	Study File ID
1	<input type="checkbox"/>	260.02978	25.840	2	3930432	6	0.0	0	■	100 0 0 0 0 0 0	F1
2	<input type="checkbox"/>	260.02978	25.850	1	1498841	6	0.0	0	■	100 0 0 0 0 0 0	F2
3	<input type="checkbox"/>	260.02978	25.839	2	1043633	6	0.0	0	■	100 0 0 0 0 0 0	F6
4	<input type="checkbox"/>	260.02978	25.831	6	755352	6	5.0	83	■	15 0 0 2 1 4 77	F4
5	<input type="checkbox"/>	260.02978	25.835	5	497729	6	4.9	81	■	17 0 0 2 1 4 76	F5
6	<input type="checkbox"/>	260.02978	25.835	6	436343	6	5.7	95	■	3 0 0 3 0 4 90	F3

Exchange rates for each isotopologue in each sample

Expected Compound Generator

 **Generate Expected Compounds**

Parameters of 'Generate Expected Compounds'

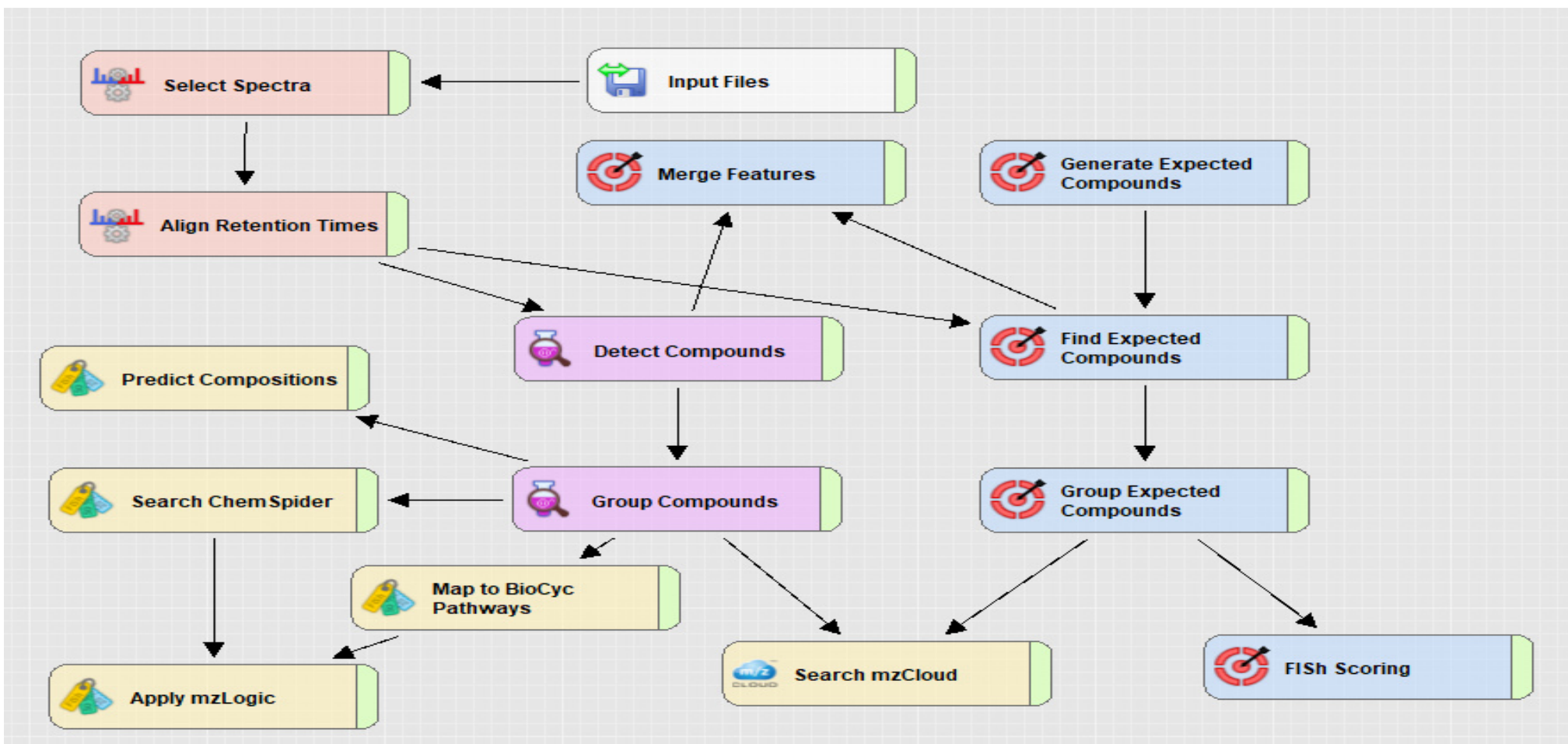
Show Advanced Parameters

- 1. **Compound Selection**
Compound: Omeprazole (C17 H19 N3 O3 S)
- 2. **Dealkylation**
Apply Dealkylation: True
Apply Dearylation: True
Max. # Steps: 2
Min. Mass [Da]: 150
- 3. **Transformations**
Phase I: Dehydration (H2 O ->); Desaturation (H2 ->); Hydrat
Phase II: Acetylation (H -> C2 H3 O); Arginine Conjugation (H
Others:
Max. # Phase II: 1
Max. # All Steps: 2
- 4. **Ionization**
Ions: [M+H]+1; [M-H]-1

Generate Expected Compounds

- dealkylation / dearylation
- Combinatorial common transformation list


Customizable Workflow For Identifying Both Expected and Unexpected



THANK YOU FOR YOUR ATTENTION

ThermoFisher
SCIENTIFIC

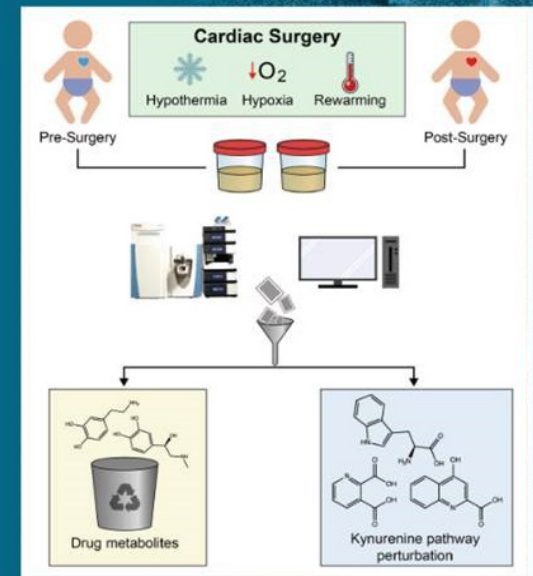
Urinary metabolomics reveals kynurenine pathway perturbation in newborns with transposition of great arteries after surgical repair

Manuela Simonato^{1,2}  · Igor Fochi³ · Luca Vedovelli² · Sonia Giambelluca⁴ · Cristiana Carollo¹ · Massimo Padalino⁵ · Virgilio P. Carnielli⁶ · Paola Cogo⁷

1. Anesthesiology and Intensive Care Unit, Department of Medicine-DIMED, University of Padova, Padua, Italy
2. PCare Laboratory, Fondazione Istituto di Ricerca Pediatrica, Padua, Italy
3. Thermo Fisher Scientific, Milan, Italy
4. Women and Child Health Department, University of Padova, Padua, Italy
5. Pediatric and Congenital Cardiac Surgical Unit, Department of Cardiac, Thoracic and Vascular Sciences, Padova University, Padua, Italy
6. Division of Neonatology, Department of Clinical Sciences, Polytechnic University of Marche and Azienda-Ospedaliero Universitaria Ospedali Riuniti, Ancona, Italy
7. Division of Pediatrics, Department of Medicine, Udine University, Udine, Italy

METABOLOMICS

Volume 15 • Number 12
December 2019



 Springer

11306 • ISSN 1573-3882
15(12) (2019)