

ThermoFisher
S C I E N T I F I C

**Come Discover the Best Kept Secret in Metabolomics.
Thermo Scientific Compound Discoverer Software.**

The world leader in serving science

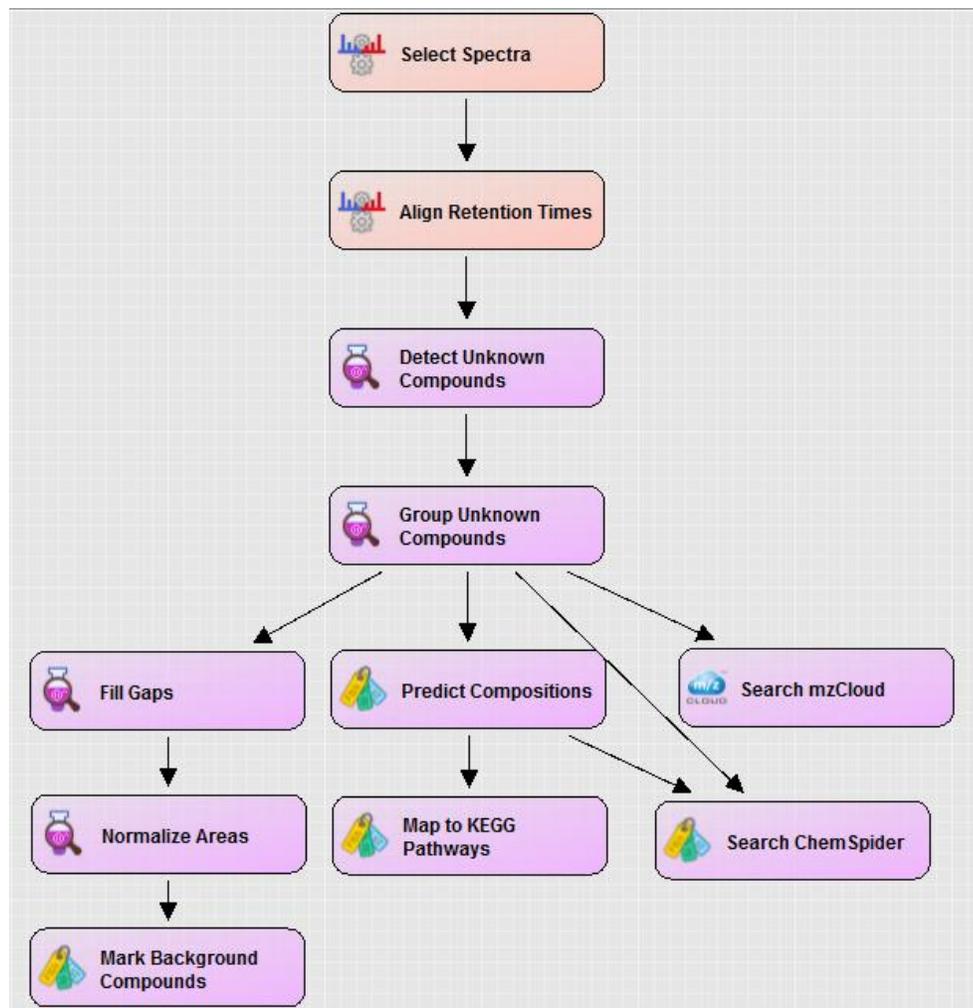
Thermo Scientific™ Compound Discoverer™ 2.1 Software

Complete small molecule structure identification in a **Next Generation** platform.



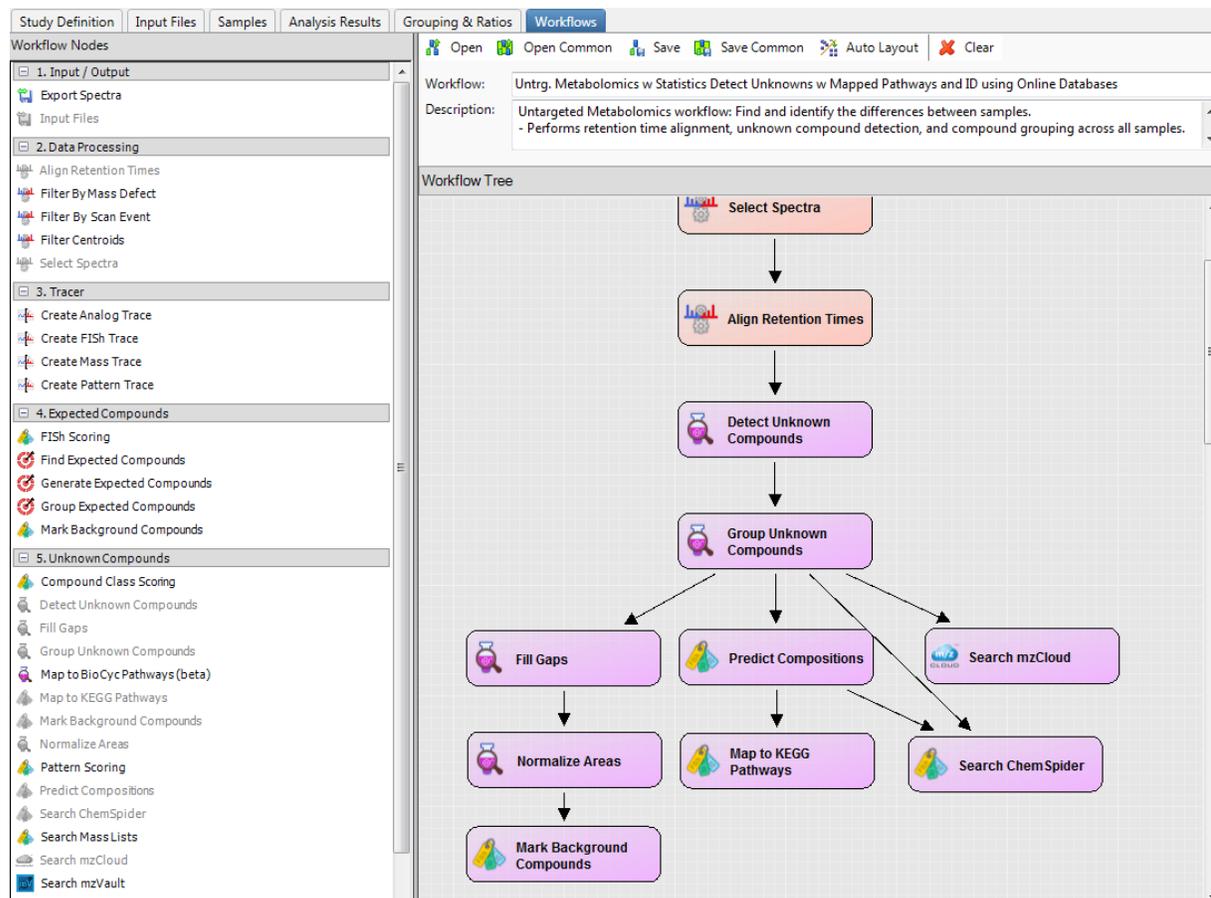
Compound Discoverer 2.1 offers flexible workflows for **Discovery Metabolomics**: Fundamental Research, Biomarker Discovery, Pharma, Environmental Research, Forensics, Foodomics, etc.

Data Processing Workflows



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

Data Processing Workflows



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

Enter a study name

In the Study Name box, type a descriptive name.

The application uses this name for both the study file (*.cdStudy) and the study folder where it stores the study file. This folder also stores the result files (*.cdResult) that data processing creates.

Select the top-level folder for your studies

1. Click the browse icon to the right of the Studies Folder box.
2. In the Select Folder dialog box, browse to an existing folder or create a new folder. Then, click **Select Folder**.

The application stores the study subfolders in this folder.

Note. Selecting a study template file (*.cdStudy) and adding a study description are optional

Select the processing workflow for this analysis

In the Workflow list, select a processing workflow.

This list displays the processing workflows in the Common Templates folder. A description of the workflow appears below the workflow list, if one is available.

For more information about this page, press the F1 key.

Study Name and Processing Workflow

Specify a unique name for this study and its folder, select the studies folder for storing all of your study folders, and select a processing workflow for the current analysis.

Study Name and Directory Structure

Study Name: New Study 1

Studies Folder: C:\Users\valf.tautenhahn\Desktop\ZDF demo

Study Template File: (Optional)

Description: (Optional)

Processing

Workflow: (empty workflow)

- WorkflowTemplates \ Degradants \ Degradants Expected w FISH Scoring and Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Degradants \ Degradants w Statistics Expected w FISH Scoring and Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ E and L \ E and L Expected with FISH Scoring
- WorkflowTemplates \ E and L \ E and L Unknown ID with Online and Local Database Searches
- WorkflowTemplates \ E and L \ E and L w Statistics Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Environmental \ Environmental Expected with FISH Scoring
- WorkflowTemplates \ Environmental \ Environmental Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Environmental \ Environmental w Statistics Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Food Research \ Food Research Expected with FISH Scoring
- WorkflowTemplates \ Food Research \ Food Research Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Food Research \ Food Research w Statistics Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Forensics \ Forensics Expected with FISH Scoring
- WorkflowTemplates \ Forensics \ Forensics Unknown ID w Compound Class Scoring, Online and Local Database Searches
- WorkflowTemplates \ Forensics \ Forensics w Statistics Unknown ID w Compound Class Scoring, Online and Local Database Searches
- WorkflowTemplates \ Impurities \ Impurities Expected w FISH Scoring and Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Impurities \ Impurities w Statistics Expected w FISH Scoring and Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Metabolism \ Metabolism Expected w FISH Scoring and Unknown w Pattern Scoring
- WorkflowTemplates \ Metabolism \ Metabolism w Statistics Expected w FISH Scoring
- WorkflowTemplates \ Metabolism \ Metabolism w Statistics Expected w FISH Scoring and Unknown w Pattern Scoring
- WorkflowTemplates \ Metabolomics \ max ID - Detect Unknowns with ID Using Online Database Searches Single Sample
- WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics Quick Detection Unknowns No ID

Workflow Templates for Metabolomics

Enter a study name
In the Study Name box, type a descriptive name.
The application uses this name for both the study file (*.cdStudy) and the study folder where it stores the study file. This folder also stores the result files (*.cdResult) that data processing creates.

Select the top-level folder for your studies
1. Click the browse icon to the right of the Studies Folder box.
2. In the Select Folder dialog box, browse to an existing folder or create a new folder. Then, click **Select Folder**.
The application stores the study subfolders in this folder.
Note. Selecting a study template file (*.cdStudy) and adding a study description are optional

Select the processing workflow for this analysis
In the Workflow list, select a processing workflow.
This list displays the processing workflows in the Common Templates folder. A description of the workflow appears below the workflow list, if one is available.
For more information about this page, press the F1 key.

Study Name and Processing Workflow
Specify a unique name for this study and its folder, select the studies folder for storing all of your study folders, and select a processing workflow for the current analysis.

Study Name and Directory Structure

Study Name: New Study 1

Studies Folder: C:\Users\valf.tautenhahn\Desktop\ZDF demo

Study Template File: (Optional)

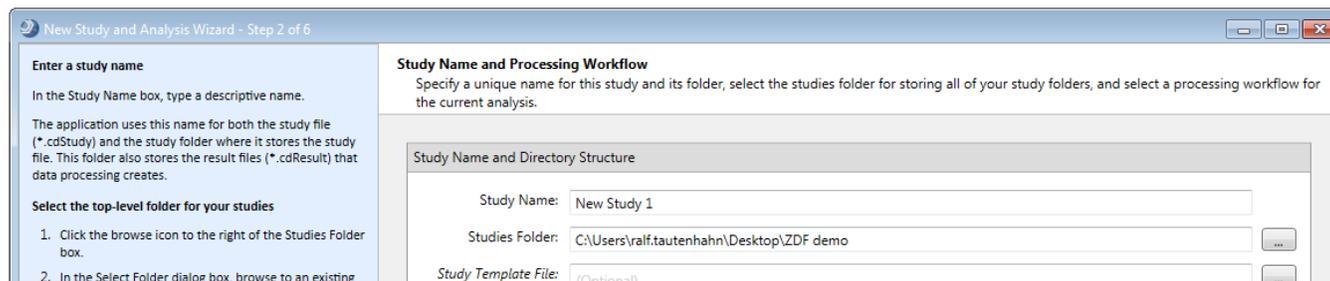
Description: (Optional)

Processing

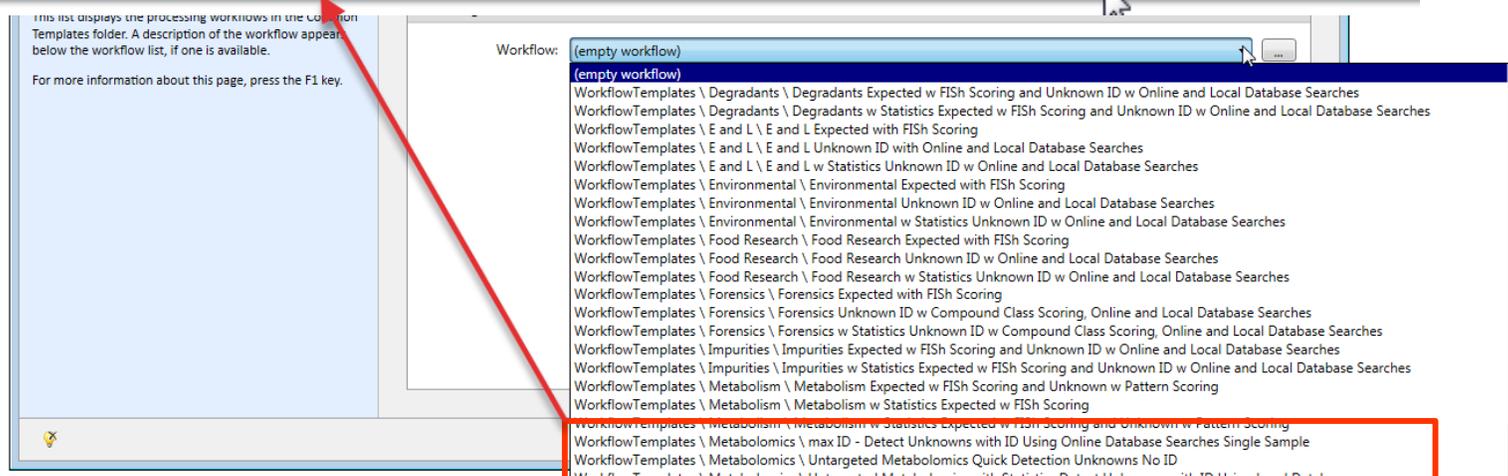
Workflow: (empty workflow)

- (empty workflow)
- WorkflowTemplates \ Degradants \ Degradants Expected w FISH Scoring and Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Degradants \ Degradants w Statistics Expected w FISH Scoring and Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ E and L \ E and L Expected with FISH Scoring
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- WorkflowTemplates \ E and L \ E and L w Statistics Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Environmental \ Environmental Expected with FISH Scoring
- WorkflowTemplates \ Environmental \ Environmental Unknown ID w Online and Local Database Searches
- WorkflowTemplates \ Environmental \ Environmental w Statistics Unknown ID w Online and Local Database Searches
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- WorkflowTemplates \ Forensics \ Forensics w Statistics Unknown ID w Compound Class Scoring, Online and Local Database Searches
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- WorkflowTemplates \ Metabolism \ Metabolism w Statistics Expected w FISH Scoring
- WorkflowTemplates \ Metabolism \ Metabolism w Statistics Expected w FISH Scoring and Unknown w Pattern Scoring
- WorkflowTemplates \ Metabolomics \ max ID - Detect Unknowns with ID Using Online Database Searches Single Sample
- WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics Quick Detection Unknowns No ID

Workflow Templates for Metabolomics



WorkflowTemplates \ Metabolomics \ max ID - Detect Unknowns with ID Using Online Database Searches Single Sample
WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics Quick Detection Unknowns No ID
WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics with Statistics Detect Unknowns with ID Using Local Databases
WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics with Statistics Detect Unknowns with Mapped Pathways and ID using Online Databases



Workflow Templates for Metabolomics

WorkflowTemplates \ Metabolomics \ max ID - Detect Unknowns with ID Using Online Database Se
WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics Quick Detection Unknowns No ID
WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics with Statistics Detect Unknowns w
WorkflowTemplates \ Metabolomics \ Untargeted Metabolomics with Statistics Detect Unknowns w

Max ID workflow. Detect and identify all compounds in a single sample (with ddMS2)- even compounds with very low abundances.

Quick compound detection. Detect compounds in a single sample or multiple samples.

Untargeted Metabolomics workflow: Find and identify the differences between samples (offline databases).

Untargeted Metabolomics workflow: Find and identify the differences between samples (online databases).

Workflow Details

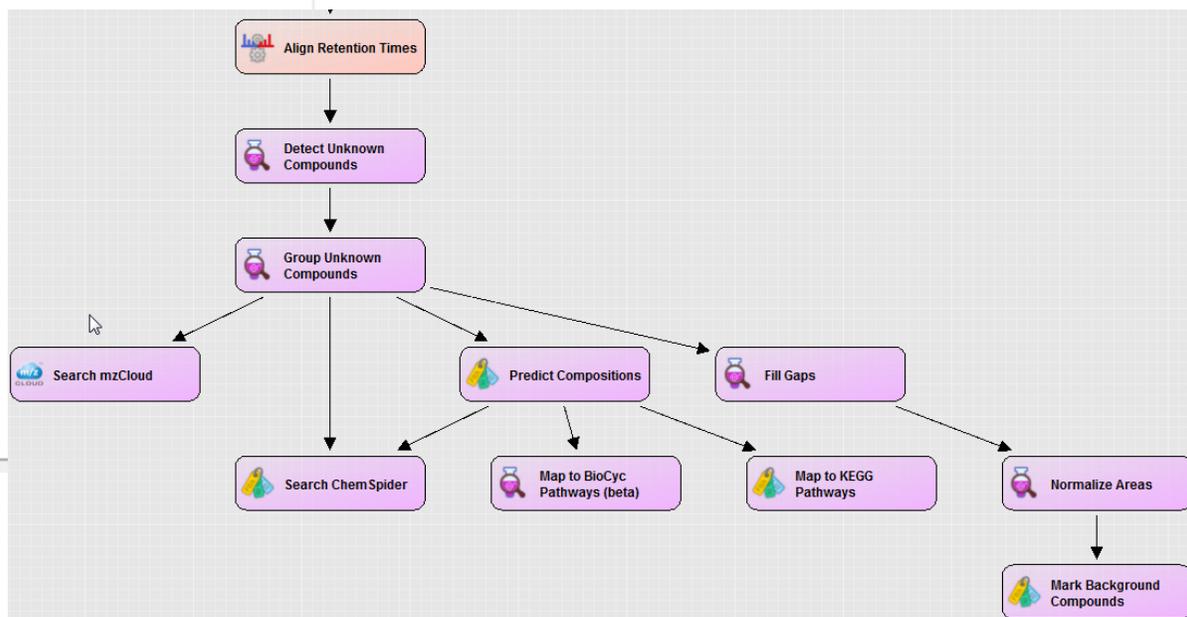
Processing

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

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 (exact mass or formula). Also performs similarity search for all compounds with ddMS2 data using mzCloud. Maps compounds to biological pathways using BioCyc and KEGG databases. 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.).



Sample Types in Compound Discoverer Software

| | | |
|-------|-------------------|----------|
| ⊕ S39 | Soy_8_Replicate_2 | Sample ▾ |
| ⊕ S40 | Soy_8_Replicate_3 | Sample ▾ |
| ⊕ S41 | Soy_9_Replicate_1 | Sample ▾ |
| ⊕ S42 | Soy_9_Replicate_2 | Sample ▾ |
| ⊕ S43 | Soy_9_Replicate_3 | Sample ▾ |



Sample: full scan data for peak detection, alignment, statistics (required)

Sample Types in Compound Discoverer Software

| | | | |
|-------|-------------------|--------|---|
| ⊕ S39 | Soy_8_Replicate_2 | Sample | ▼ |
| ⊕ S40 | Soy_8_Replicate_3 | Sample | ▼ |
| ⊕ S41 | Soy_9_Replicate_1 | Sample | ▼ |
| ⊕ S42 | Soy_9_Replicate_2 | Sample | ▼ |
| ⊕ S43 | Soy_9_Replicate_3 | Sample | ▼ |



Sample: full scan data for peak detection, alignment, statistics (required)

| | | | |
|------|---------------------|-------|---|
| ⊕ S1 | Blank_1_Replicate_1 | Blank | ▼ |
| ⊕ S2 | Blank_1_Replicate_2 | Blank | ▼ |
| ⊕ S3 | Blank_1_Replicate_3 | Blank | ▼ |



Blank: solvent or matrix blanks for background removal (optional)

Sample Types in Compound Discoverer Software

| | | | |
|-------|-------------------|--------|---|
| ⊕ S39 | Soy_8_Replicate_2 | Sample | ▼ |
| ⊕ S40 | Soy_8_Replicate_3 | Sample | ▼ |
| ⊕ S41 | Soy_9_Replicate_1 | Sample | ▼ |
| ⊕ S42 | Soy_9_Replicate_2 | Sample | ▼ |
| ⊕ S43 | Soy_9_Replicate_3 | Sample | ▼ |



Sample: full scan data for peak detection, alignment, statistics (required)

| | | | |
|------|---------------------|-------|---|
| ⊕ S1 | Blank_1_Replicate_1 | Blank | ▼ |
| ⊕ S2 | Blank_1_Replicate_2 | Blank | ▼ |
| ⊕ S3 | Blank_1_Replicate_3 | Blank | ▼ |



Blank: solvent or matrix blanks for background removal (optional)

| | | | |
|-------|------|----------------|---|
| ⊕ S5 | QC_1 | QualityControl | ▼ |
| ⊕ S6 | QC_2 | QualityControl | ▼ |
| ⊕ S7 | QC_3 | QualityControl | ▼ |
| ⊕ S8 | QC_4 | QualityControl | ▼ |
| ⊕ S9 | QC_5 | QualityControl | ▼ |
| ⊕ S10 | QC_6 | QualityControl | ▼ |



QualityControl: pooled samples for Normalization and QC (optional)

Sample Types in Compound Discoverer Software

| | | | |
|-------|-------------------|--------|---|
| ⊕ S39 | Soy_8_Replicate_2 | Sample | ▼ |
| ⊕ S40 | Soy_8_Replicate_3 | Sample | ▼ |
| ⊕ S41 | Soy_9_Replicate_1 | Sample | ▼ |
| ⊕ S42 | Soy_9_Replicate_2 | Sample | ▼ |
| ⊕ S43 | Soy_9_Replicate_3 | Sample | ▼ |



Sample: full scan data for peak detection, alignment, statistics (required)

| | | | |
|------|---------------------|-------|---|
| ⊕ S1 | Blank_1_Replicate_1 | Blank | ▼ |
| ⊕ S2 | Blank_1_Replicate_2 | Blank | ▼ |
| ⊕ S3 | Blank_1_Replicate_3 | Blank | ▼ |



Blank: solvent or matrix blanks for background removal (optional)

| | | | |
|-------|------|----------------|---|
| ⊕ S5 | QC_1 | QualityControl | ▼ |
| ⊕ S6 | QC_2 | QualityControl | ▼ |
| ⊕ S7 | QC_3 | QualityControl | ▼ |
| ⊕ S8 | QC_4 | QualityControl | ▼ |
| ⊕ S9 | QC_5 | QualityControl | ▼ |
| ⊕ S10 | QC_6 | QualityControl | ▼ |



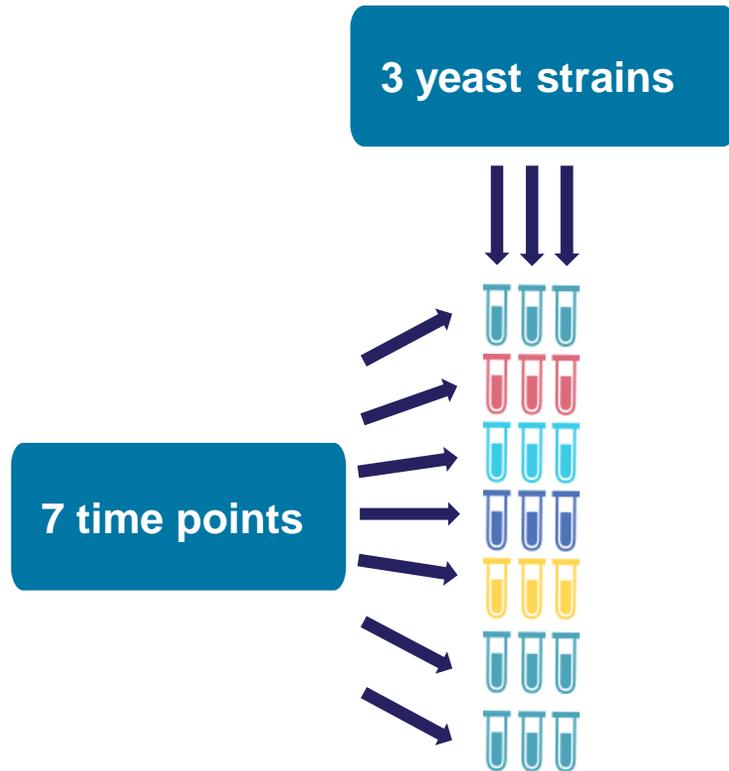
QualityControl: pooled samples for Normalization and QC (optional)

| | | | |
|--------|-----------|---------------------|---|
| ⊕ S119 | Soy_ID_L1 | Identification Only | ▼ |
| ⊕ S120 | Soy_ID_L2 | Identification Only | ▼ |
| ⊕ S121 | Soy_ID_L3 | Identification Only | ▼ |



Identification Only: one or more ddMS² for compound identification (optional)

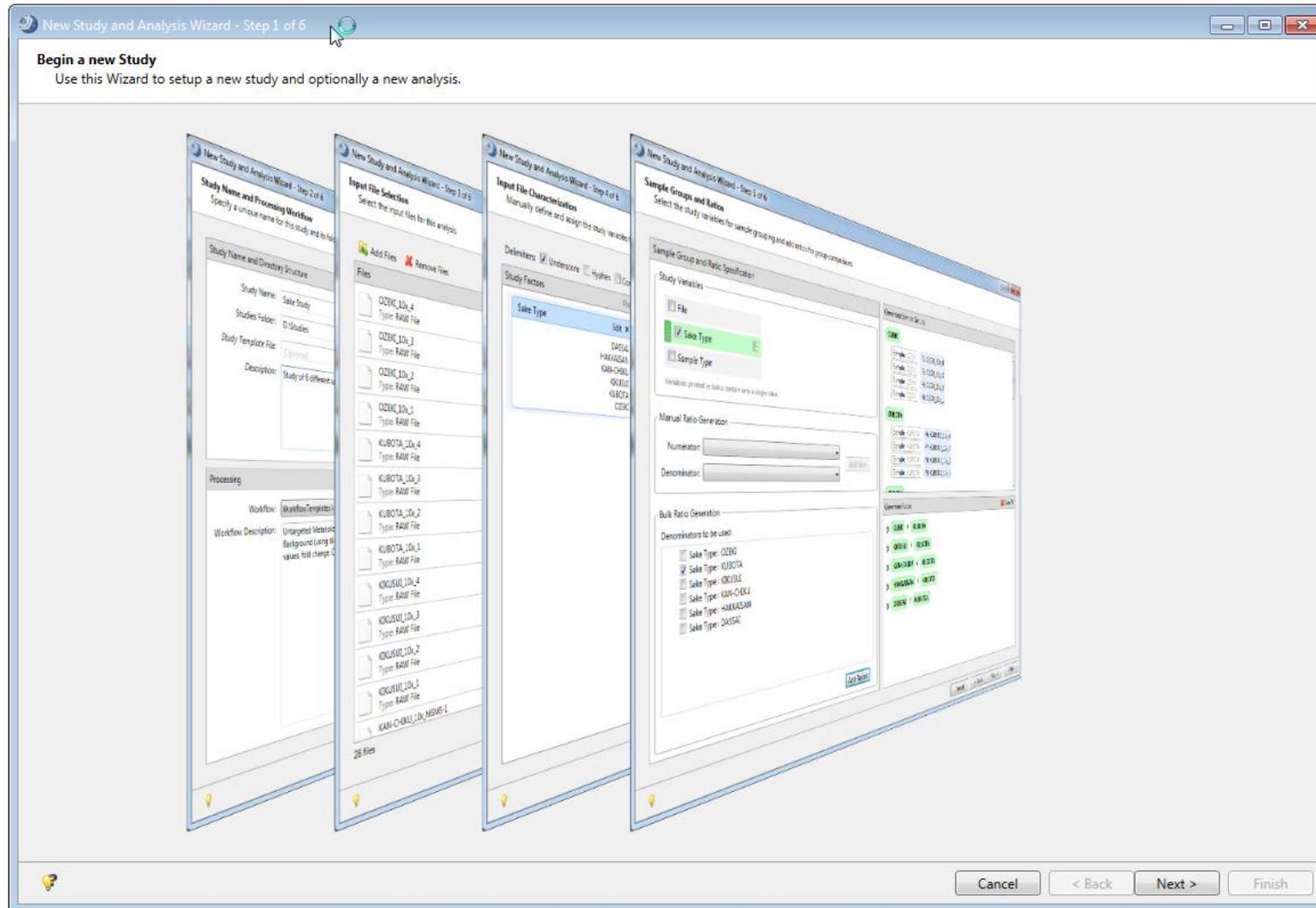
Study Factors in Compound Discoverer Software



Study factors (or study variables):
Information about your samples.

Study factors are used for statistics
and interactive visualizations.

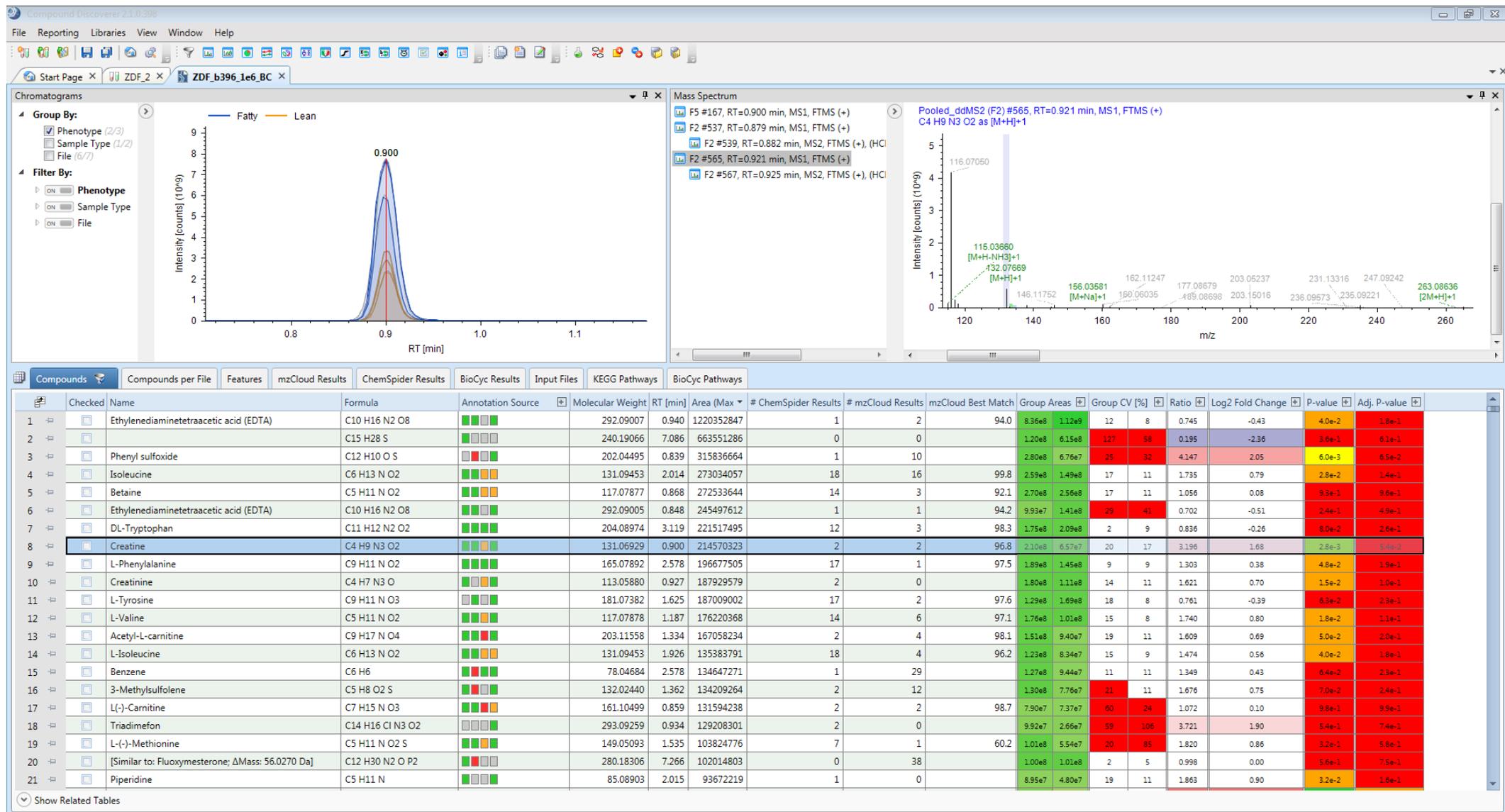
Create New Study Using the Wizard in Compound Discoverer Software



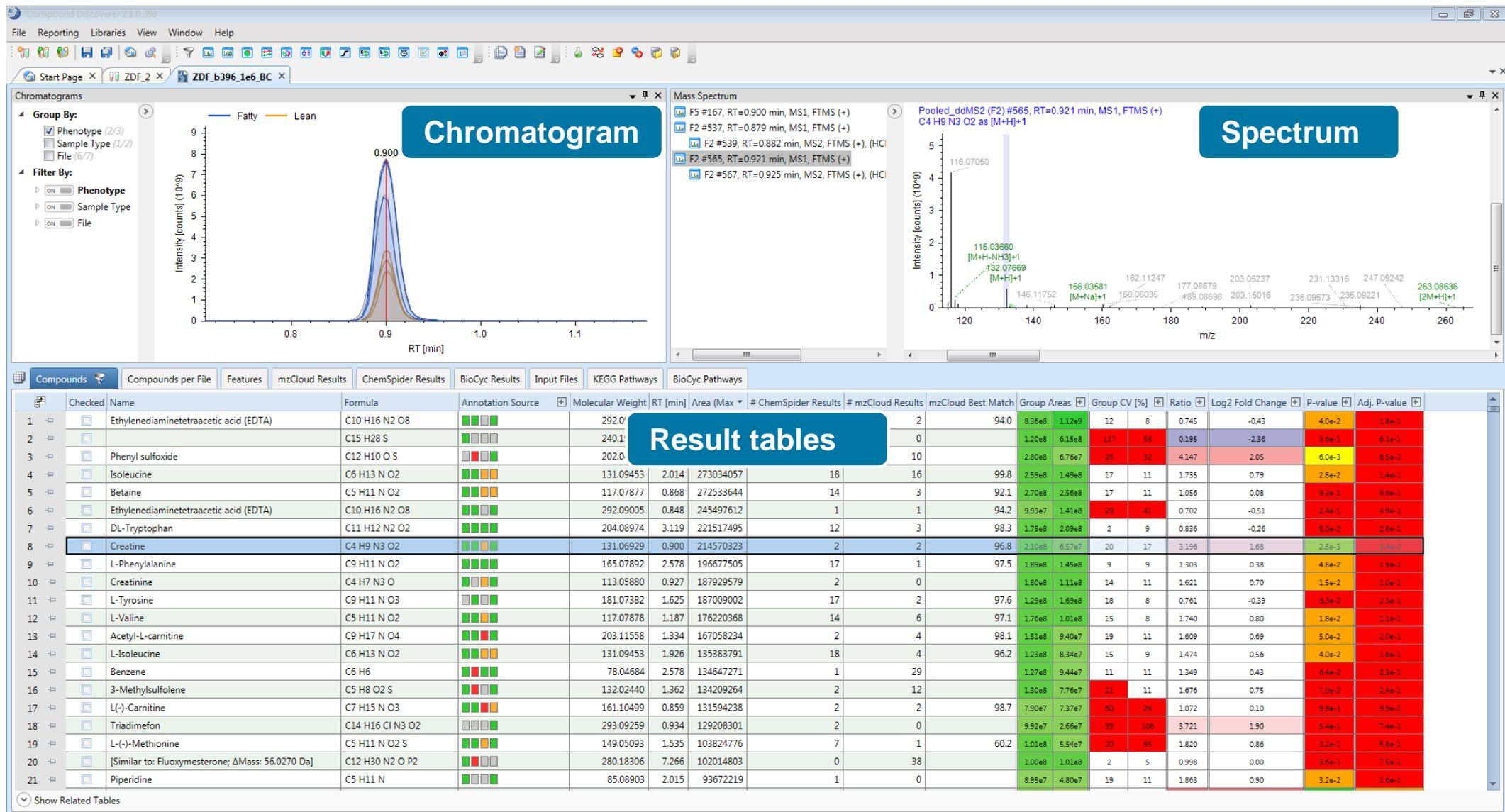
Create a new study in 4 steps

- Select samples
- Select workflow
- Define sample types (optional)
- Define study factors (optional)

Interpreting the Results



Interpreting the Results



Interpreting the Results

Compound Discoverer 2.1.0.398

File Reporting Libraries View Window Help

Start Page ZDF_2 ZDF_b396_1e6_BC

Chromatogram

Intensity [counts] (10⁶)

RT [min]

Group By: Phenotype (2/3), Sample Type (1/2), File (6/7)

Filter By: Phenotype, Sample Type, File

Spectrum

Intensity [counts] (10⁹)

m/z

RAWFILE (top): Pooled_d4MS2 (F2) #1638, RT=2.578 min, MS2, FTMS (+), (HCD, ...)

REFERENCE (bottom): mzCloud library, L-Phenylalanine, C...

Result tables

| 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"/> | Isoleucine | C6 H13 N O2 | | 131.0 | | | | 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 | | 117.0 | | | | 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 | | 292.0 | | | | 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 | 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 | 0.900 | 214570323 | 2 | 2 | 96.8 | 2.10e8 6.57e7 | 20 17 | 3.196 | 1.68 | 2.8e-3 | 5.4e-2 |
| <input checked="" type="checkbox"/> | L-Phenylalanine | C9 H11 N O2 | | 165.07892 | 2.578 | 196677505 | 17 | 1 | 97.5 | 1.89e8 1.45e8 | 9 9 | 1.303 | 0.38 | 4.8e-2 | 1.9e-1 |
| <input type="checkbox"/> | Creatinine | C4 H7 N3 O | | 113.05880 | 0.927 | 1875196677505.1928429 | 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 | 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 | 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 | | | | | | | | | | 19 11 | 1.609 | 0.69 | 5.0e-2 | 2.0e-1 |
| <input type="checkbox"/> | L-Isoleucine | | | | | | | | | | 15 9 | 1.474 | 0.56 | 4.0e-2 | 1.8e-1 |
| <input type="checkbox"/> | Benzene | | | | | | | | | | 11 11 | 1.349 | 0.43 | 6.4e-2 | 2.3e-1 |
| <input type="checkbox"/> | 3-Methylsulfolene | C5 H6 S | | 132.02440 | 1.362 | 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 | 98.7 | 7.90e7 7.37e7 | 60 24 | 1.072 | 0.10 | 3.8e-1 | 8.9e-1 |

Associated details for each compound in sub-tables

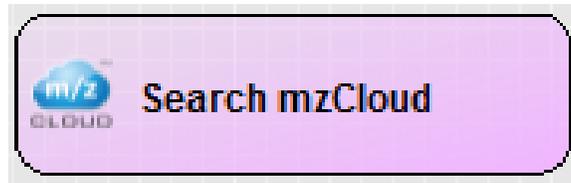
Hide Related Tables

Structure Proposals Compounds per File Predicted Compositions **mzCloud Results** ChemSpider Results BioCyc Results KEGG Pathways BioCyc Pathways

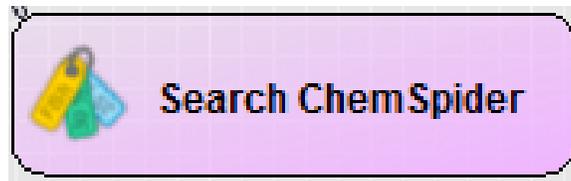
| Checked | Compound Match | Structure | Name | Formula | Molecular Weight | ΔMass [Da] | ΔMass [ppm] | Type | Scan # | Match | Best Match | Best Sim. Match | mzCloud ID | KEGG ID |
|--------------------------|-------------------------------------|-----------|-----------------|-------------|------------------|------------|-------------|----------|--------|-------|------------|-----------------|------------|---------|
| <input type="checkbox"/> | <input checked="" type="checkbox"/> | | L-Phenylalanine | C9 H11 N O2 | 165.07898 | 0.00006 | 0.38 | Identity | 1638 | 97.5 | 97.5 | 97.9 | g | C00079 |

Show Related Tables

Identifying Unknowns – Spectral Libraries and Compound Databases

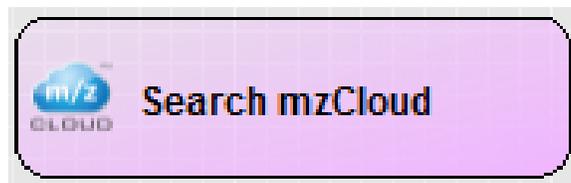


Online spectral library
> 2 million spectra

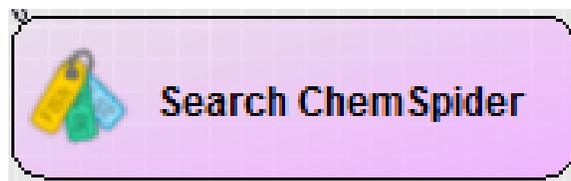


Chemical structure database with >480
data sources, 59 million structures

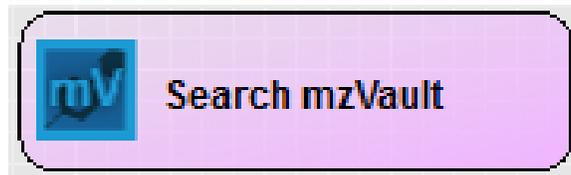
Identifying Unknowns – Spectral Libraries and Compound Databases



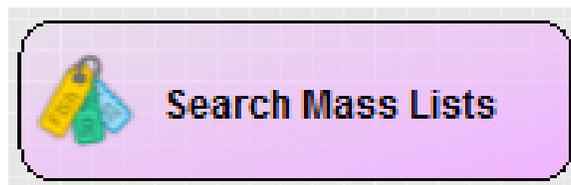
← Online spectral library
> 2 million spectra



← Chemical structure database with >480
data sources, 59 million structures



← Local spectral libraries



← Local databases

Identifying Unknowns: mzCloud

The screenshot displays the Compound Discoverer 2.1.0.398 interface. The top section shows a chromatogram with peaks labeled 'Fatty' (blue) and 'Lean' (orange), with a peak at 1.331 minutes. The middle section shows a mass spectrum with a peak at m/z 85.02844. The right section shows a 'Raw file' and a 'Reference (mzCloud)' mass spectrum. A blue arrow points from the reference spectrum to the 'Spectrum match' callout. Below the mass spectra is a table of compounds with columns for Name, Formula, Molecular Weight, RT [min], Area (Max), # ChemSpider Results, # mzCloud Results, and P-value. A blue arrow points from the 'Compound name and structure' callout to the 'Acetyl-L-carnitine' entry in the table. The bottom section shows the 'Structure Proposals' table with columns for Checked, Compound Match, Structure, Name, Formula, Molecular Weight, ΔMass [Da], ΔMass [ppm], Type, Scan #, Match %, Best Match %, Best Sim. Match %, mzCloud ID, and KEGG ID. The 'Acetyl-L-carnitine' entry is highlighted, and a blue arrow points from the 'Structure' column to the chemical structure image.

Chromatograms

Group By: Phenotype (2/3), Sample Type (1/2), File (6/7)

Filter By: Phenotype, Sample Type, File

Mass Spectrum

RAWFILE(top): Pooled_ddMS2 (F2) #792, RT=1.266 min, MS2, FTMS (+), (HCD, DDF, 204.1231@(15:35:50), +1)
 REFERENCE(bottom): mzCloud library, Acetyl-L-carnitine, C9 H17 N O4, MS2, FTMS, (HCD, 204.1230@(10:20:40))

Table 1: Compound Identification Results

| Checked | Name | Formula | Annotation Source | Molecular Weight | RT [min] | Area (Max) | # ChemSpider Results | # mzCloud Results | mzCloud ID | P-value | Adj. P-value |
|--------------------------|--|------------------|-------------------|------------------|----------|------------|----------------------|-------------------|------------|---------|--------------|
| <input type="checkbox"/> | Isoleucine | C6 H13 N O2 | Green | 131.09453 | 2.014 | 273034057 | 18 | 16 | | 2.8e-2 | 1.4e-1 |
| <input type="checkbox"/> | Betaine | C5 H11 N O2 | Green | 117.07877 | 0.868 | 272533644 | 14 | 3 | | 9.3e-1 | 9.6e-1 |
| <input type="checkbox"/> | Ethylenediaminetetraacetic acid (EDTA) | C10 H16 N2 O8 | Green | 292.09005 | 0.848 | 245497612 | 1 | 1 | | 2.4e-1 | 4.9e-1 |
| <input type="checkbox"/> | DL-Tryptophan | C11 H12 N2 O2 | Green | 204.08974 | 3.119 | 221517495 | 12 | 3 | | 8.0e-2 | 2.6e-1 |
| <input type="checkbox"/> | Creatine | C4 H9 N3 O2 | Green | 131.06929 | 0.900 | 214570323 | 2 | 2 | 90.8 | 2.10e8 | 6.57e7 |
| <input type="checkbox"/> | L-Phenylalanine | C9 H11 N O2 | Green | 165.07892 | 2.578 | 196677505 | 17 | 1 | 97.5 | 1.89e8 | 1.45e8 |
| <input type="checkbox"/> | Creatinine | C4 H7 N3 O | Green | 113.05880 | 0.927 | 187929579 | 2 | 0 | | 1.80e8 | 1.11e8 |
| <input type="checkbox"/> | L-Tyrosine | C9 H11 N O3 | Green | 181.07382 | 1.625 | 187009002 | 17 | 2 | 97.6 | 1.29e8 | 1.69e8 |
| <input type="checkbox"/> | L-Valine | C5 H11 N O2 | Green | | | | | | 97.1 | 1.76e8 | 1.01e8 |
| <input type="checkbox"/> | Acetyl-L-carnitine | C9 H17 N O4 | Green | | | | | | 98.1 | 1.51e8 | 9.40e7 |
| <input type="checkbox"/> | L-Isoleucine | C6 H13 N O2 | Green | | | | | | 96.2 | 1.23e8 | 8.34e7 |
| <input type="checkbox"/> | Benzene | C6 H6 | Green | | | | | | | 1.27e8 | 9.44e7 |
| <input type="checkbox"/> | 3-Methylsulfolene | C5 H8 O2 S | Green | | | | | | | 1.30e8 | 7.76e7 |
| <input type="checkbox"/> | L(-)-Carnitine | C7 H15 N O3 | Green | | | | | | 98.7 | 7.90e7 | 7.37e7 |
| <input type="checkbox"/> | Triadimefon | C14 H16 Cl N3 O2 | Green | | | | | | | 9.92e7 | 2.66e7 |

Table 2: Structure Proposals

| Checked | Compound Match | Structure | Name | Formula | Molecular Weight | ΔMass [Da] | ΔMass [ppm] | Type | Scan # | Match % | Best Match % | Best Sim. Match % | mzCloud ID | KEGG ID |
|--------------------------|-------------------------------------|-----------|--------------------|-------------|------------------|------------|-------------|----------|--------|---------|--------------|-------------------|------------|---|
| <input type="checkbox"/> | <input checked="" type="checkbox"/> | | Acetyl-L-carnitine | C9 H17 N O4 | 203.11576 | 0.00017 | 0.85 | Identity | 792 | 98.1 | 98.1 | 90.8 | 879 | https://mzcloud.org/DataViewer.aspx#Reference879 |

mzCloud is a trademark of HighChem LLC.

Identifying Unknowns: ChemSpider

Compound Discoverer 2.1.0.398

File Reporting Libraries View Window Help

Start Page x ZDF_2 x ZDF_b396_1e6_BC x

Chromatograms

Group By: Phenotype (2/3) Sample Type (1/2) File (6/7)

Filter By: Phenotype Sample Type File

Intensity [counts] (10⁹)

RT [min]

Mass Spectrum

F4 #489, RT=2.579 min, MS1, FTMS (+)

F2 #1637, RT=2.576 min, MS1, FTMS (+)

F2 #1638, RT=2.578 min, MS2, FTMS (+), (H)

ZDF_Fatty_2 (F4) #489, RT=2.579 min, MS1, FTMS (+)

C9 H11 N O2 as [M+H]⁺+1

Intensity [counts] (10⁹)

m/z

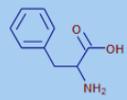
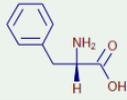
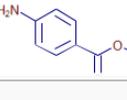
Compounds

| Checked | Name | 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"/> | Isoleucine | 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 | 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"/> | Ethylenediaminetetraacetic acid (EDTA) | 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 | 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 | 0.900 | 214570323 | 2 | 2 | 96.8 | 2.10e8 6.57e7 | 20 17 | 3.196 | 1.68 | 2.8e-3 | 5.4e-2 |
| <input type="checkbox"/> | L-Phenylalanine | C9 H11 N O2 | 165.07892 | 2.578 | 196677505 | 17 | 1 | 97.5 | 1.89e8 1.45e8 | 9 9 | 1.303 | 0.38 | 4.8e-2 | 1.0e-1 |
| <input type="checkbox"/> | Creatinine | C4 H7 N3 O | 113.05880 | 0.927 | 187929579 | 2 | 0 | 1.80e8 1.11e8 | 14 11 | 1.621 | 0.70 | 1.5e-2 | 1.0e-1 | |

ChemSpider results

Hide Related Tables

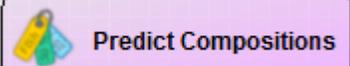
Structure Proposals

| Checked | Compound Match | Structure | Name | Formula | Molecular Weight | ΔMass [Da] | ΔMass [ppm] | CSID | # References |
|--------------------------|-------------------------------------|---|---------------------|-------------|------------------|------------|-------------|---|--------------|
| <input type="checkbox"/> | <input checked="" type="checkbox"/> |  | DL-Phenylalanine | C9 H11 N O2 | 165.07898 | 0.00006 | 0.39 | 969 | 13580 |
| <input type="checkbox"/> | <input type="checkbox"/> |  | L-(-)-Phenylalanine | C9 H11 N O2 | 165.07898 | 0.00006 | 0.39 | 5910 | 841 |
| <input type="checkbox"/> | <input type="checkbox"/> |  | Benzocaine | C9 H11 N O2 | 165.07898 | 0.00006 | 0.39 | 13854242 | 832 |

Show Related Tables

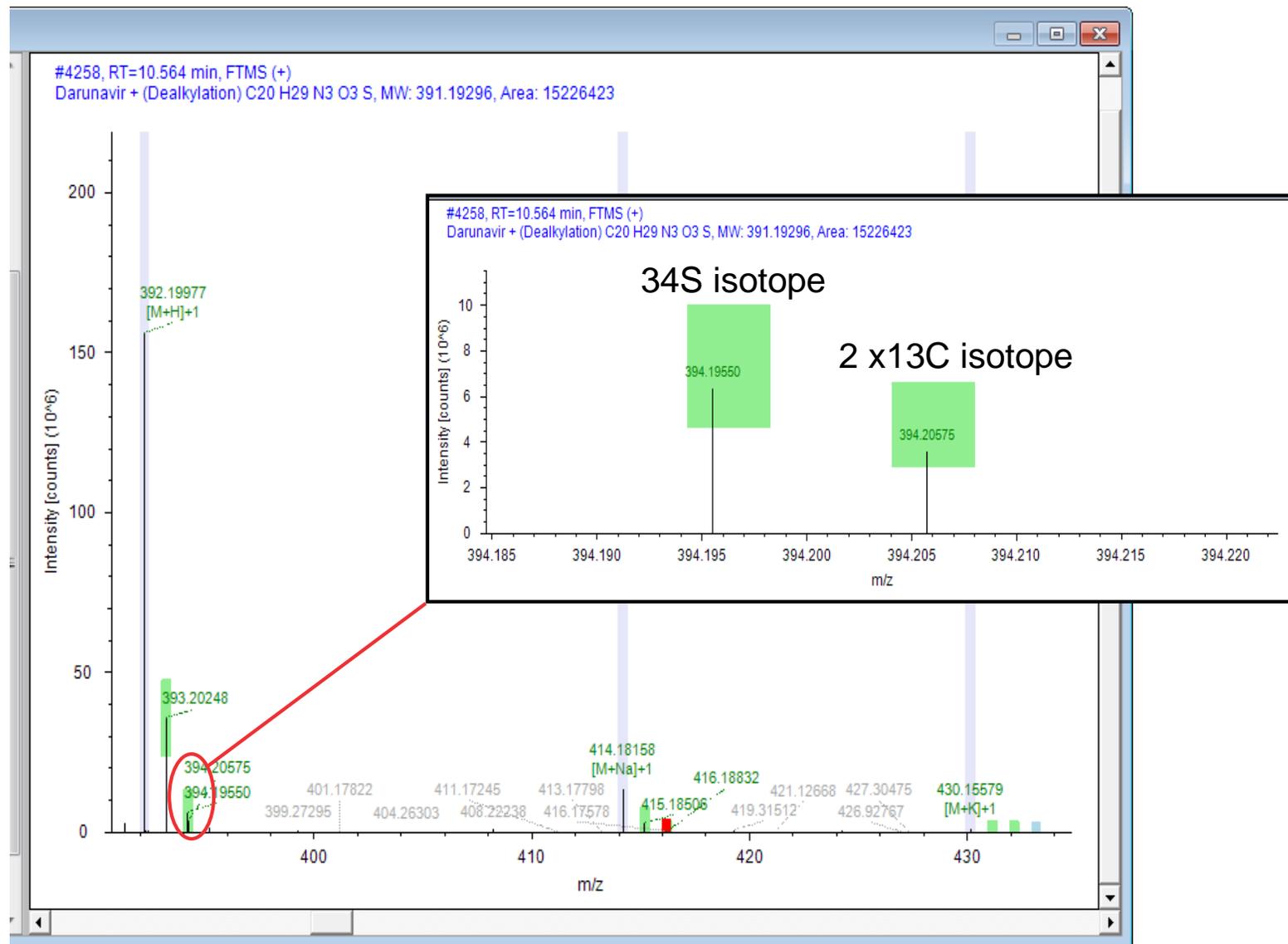
ChemSpider is a trademark of Royal Society of Chemistry.

Identifying Unknowns: Predict Elemental Composition Using Very High Resolution Data

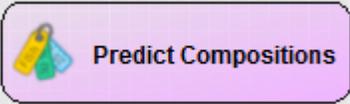


TrueComposition™
algorithm uses

- Exact mass
- Isotopic pattern
- *Fine* isotopic pattern
- MS² data

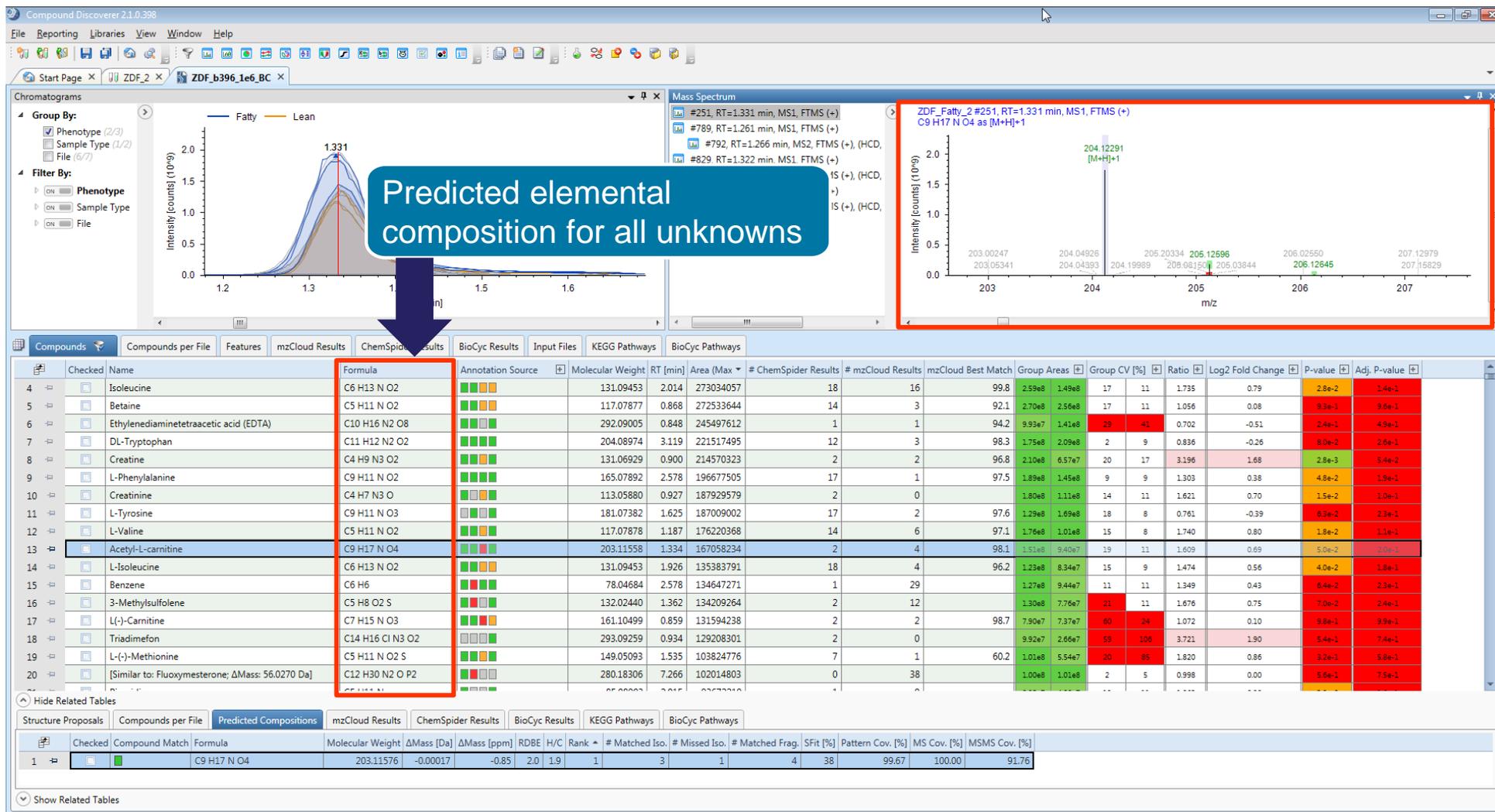


Identifying Unknowns: Predict Elemental Composition Using Very High Resolution Data



TrueComposition™ algorithm uses

- Exact mass
- Isotopic pattern
- *Fine* isotopic pattern
- MS² data



Identifying Unknowns: How to Interpret the Results from Multiple Sources?

Annotation Source

Annotation Source

- How was this compound identified?
- Is there consensus between the Annotation Sources?

| Checked | Name | Formula | Molecular Weight | RT [min] | Area (Max) | ChemSpider |
|--------------------------|--|--|------------------|----------|------------|------------|
| <input type="checkbox"/> | Isoleucine | C ₆ H ₁₃ N O ₂ | 131.09453 | 2.014 | 273034057 | |
| <input type="checkbox"/> | Betaine | C ₅ H ₁₁ N O ₂ | 117.07878 | 0.868 | 272533644 | |
| <input type="checkbox"/> | Ethylenediaminetetraacetic acid (EDTA) | C ₁₀ H ₁₆ N ₂ O ₈ | 292.09005 | 0.848 | 245497612 | |
| <input type="checkbox"/> | DL-Tryptophan | C ₁₁ H ₁₂ N ₂ O ₂ | 204.08974 | 3.119 | 221517495 | |
| <input type="checkbox"/> | Creatine | C ₄ H ₉ N ₃ O ₂ | 131.06929 | 0.900 | 214570323 | |
| <input type="checkbox"/> | L-Phenylalanine | C ₉ H ₁₁ N O ₂ | 165.07892 | 2.578 | 196677505 | |
| <input type="checkbox"/> | Creatinine | C ₄ H ₇ N ₃ O | 113.05880 | 0.927 | 187929579 | |
| <input type="checkbox"/> | L-Tyrosine | C ₉ H ₁₁ N O ₃ | 181.07382 | 1.625 | 187009002 | |
| <input type="checkbox"/> | L-Valine | C ₅ H ₁₁ N O ₂ | 117.07878 | 1.187 | 176220368 | |
| <input type="checkbox"/> | Acetyl-L-carnitine | C ₉ H ₁₇ N O ₄ | 203.11558 | 1.334 | 167058234 | |
| <input type="checkbox"/> | L-Isoleucine | C ₆ H ₁₃ N O ₂ | 131.09453 | 1.926 | 135383791 | |
| <input type="checkbox"/> | Benzene | C ₆ H ₆ | 78.04684 | 2.578 | 134647271 | |
| <input type="checkbox"/> | 3-Methylsulfolene | C ₅ H ₈ O ₂ S | 132.02440 | 1.362 | 134209264 | |
| <input type="checkbox"/> | L(-)-Carnitine | C ₇ H ₁₅ N O ₃ | 161.10499 | 0.859 | 131594238 | |
| <input type="checkbox"/> | Triadimefon | C ₁₄ H ₁₆ Cl N ₃ O ₂ | 293.09259 | 0.934 | 129208301 | |
| <input type="checkbox"/> | L(-)-Methionine | C ₅ H ₁₁ N O ₂ S | 149.05093 | 1.535 | 103824776 | |
| <input type="checkbox"/> | [Similar to: Fluoxymesterone; ΔMass: 56.0270 Da] | C ₁₂ H ₃₀ N ₂ O P ₂ | 280.18306 | 7.266 | 102014803 | |

Identifying Unknowns: How to Interpret the Results from Multiple Sources?

Assign compound name and formula based on multiple data sources



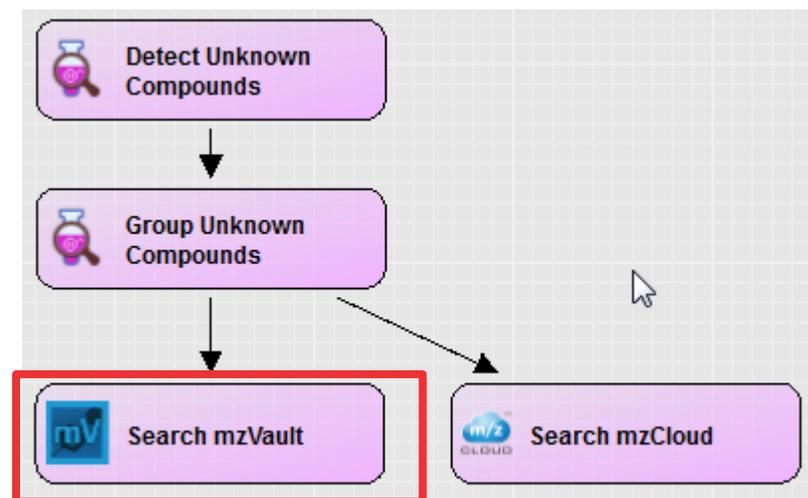
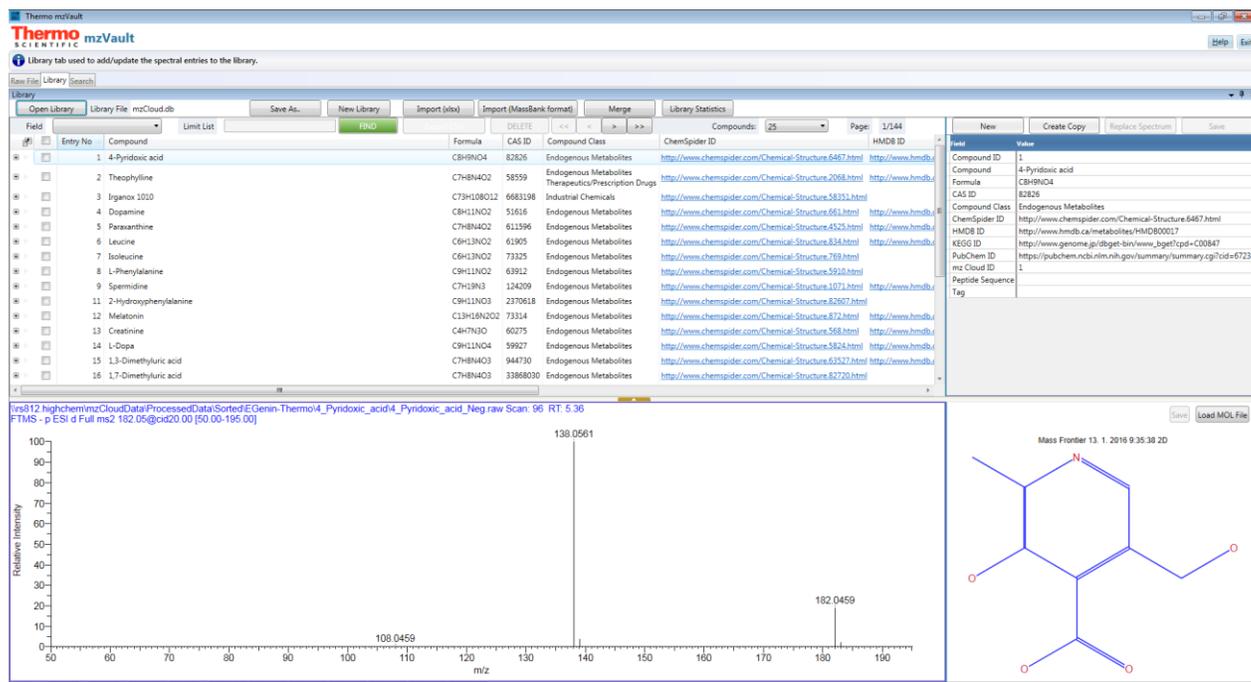
| | |
|---------------------|------------------------|
| 1. General Settings | |
| Mass Tolerance | 5 ppm |
| 2. Data Sources | |
| Data Source #1 | mzCloud Search |
| Data Source #2 | Predicted Compositions |
| Data Source #3 | MassList Match |
| Data Source #4 | ChemSpider Search |

Users can define priorities

| | Checked | Name | Formula | Annotation Source |
|----|--------------------------|--|-----------------|-------------------|
| 2 | <input type="checkbox"/> | L(-)-Carnitine | C7 H15 N O3 | |
| 3 | <input type="checkbox"/> | Acetyl-L-carnitine | C9 H17 N O4 | |
| 4 | <input type="checkbox"/> | DL-Tryptophan | C11 H12 N2 O2 | |
| 5 | <input type="checkbox"/> | L-Tyrosine | C9 H11 N O3 | |
| 6 | <input type="checkbox"/> | DL-Glutamine | C5 H10 N2 O3 | |
| 7 | <input type="checkbox"/> | L-Phenylalanine | C9 H11 N O2 | |
| 8 | <input type="checkbox"/> | L-Valine | C5 H11 N O2 | |
| 9 | <input type="checkbox"/> | Creatine | C4 H9 N3 O2 | |
| 10 | <input type="checkbox"/> | L-Histidine | C6 H9 N3 O2 | |
| | | | C10 H19 N O4 | |
| | | | C6 H13 N O2 | |
| | | | C10 H14 N5 O7 P | |
| 14 | <input type="checkbox"/> | DL-Arginine | C6 H14 N4 O2 | |
| 15 | <input type="checkbox"/> | PEG n6 | C12 H26 O7 | |
| 16 | <input type="checkbox"/> | Hexanoylcarnitine | C13 H25 N O4 | |
| 17 | <input type="checkbox"/> | Ethylenediaminetetraacetic acid (EDTA) | C10 H16 N2 O8 | |

Identifying Unknowns: Local Spectral Libraries (mzVault)

- **mzVault** – support for local spectral libraries
 - Compound Discoverer 2.1 comes with a local version of the mzCloud™ database
 - Custom spectral libraries can be created and edited using the mzVault application



Identifying Unknowns: Similarity Search Using mzCloud

Chromatograms

Group By: Phenotype (2/3) Sample Type (1/2) File (6/7)

Filter By: Phenotype

- n/a (0/1)
- Lean (3/3)
- Fatty (3/3)

Sample Type

File

Mass Spectrum

F2 #2687, RT=4.212 min, MS2, FTMS (+)

RAWFILE(top): Pooled_ddMS2 (F2) #2687, RT=4.212 min, MS2, FTMS (+), (HCD, DDF, 344.2279@(15:35:50), +1)

REFERENCE(bottom): mzCloud library, PEG n7, C14 H30 O8, MS2, FTMS, (HCD, 327.2013@30)

| Name | Formula | Predicted Comp. Search | mzCloud Search | BioCyc Search | ChemSpider Search | Molecular Weight | RT [min] | mzCloud Best Sim. Match |
|--|---------------|---|---|---------------|-------------------|------------------|----------|-------------------------|
| [Similar to: PEG n7; ΔMass: -17.0262 Da] | C15 H29 N5 O4 | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 343.22026 | 4.226 | 93.5 |
| UNII:212QJ... | | | | | | | | |
| gaboxadol | C6 H8 N2 O2 | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 140.05842 | 1.071 | 1745565 |
| gaboxadol | C6 H8 N2 O2 | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 140.05841 | 1.024 | 1430747 |
| [Similar to: PEG n7; ΔMass: -17.0262 Da] | C15 H29 N5 O4 | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 343.22026 | 4.226 | 1171594 |
| [Similar to: N1-[3-(Trifluoromethyl)phenyl]-2-[[5-methyl-4-phenyl-1,3-oxazol | C9 H6 O | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 130.04175 | 2.578 | 2272923 |
| p-Cresol | C7 H8 O | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 108.05745 | 3.401 | 838321 |
| gaboxadol | C6 H8 N2 O2 | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 140.05841 | 1.141 | 1989592 |
| (2R,3S)-3-Hydroxy-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylic acid | C9 H15 N O3 | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 185.10520 | 1.823 | 491465 |
| .alpha.-Amino adipic acid | C6 H11 N O4 | ■ ■ ■ ■ | ■ ■ ■ ■ | | | 161.06866 | 0.904 | 666656 |

Hide Related Tables

Structure Proposals | Compounds per File | Predicted Compositions | **mzCloud Results** | ChemSpider Results | BioCyc Results | KEGG Pathways | BioCyc Pathways

| Checked | Compound Match | Structure | Name | Formula | Molecular Weight | ΔMass [Da] | ΔMass [ppm] | Type | Scan # | Match | Best Match | Best Sim. Match | mzCloud ID | KEGG ID |
|-------------------------------------|------------------------------------|-----------|--------|------------|------------------|------------|-------------|------------|--------|-------|------------|-----------------|----------------------|---------|
| <input checked="" type="checkbox"/> | ■ | | PEG n7 | C14 H30 O8 | 326.19407 | -17.02619 | -52196.52 | Similarity | 2687 | 93.5 | 92.0 | 93.5 | 1821 | |

Mass Frontier Annotation (FISH) for Structure Proposals

Chromatograms

Group By: File (6/6), Phenotype (2/2), Sample Type (1/1)

Filter By: File, Phenotype, Sample Type

Intensity [counts] (10⁶) vs RT [min]

Mass Spectrum

F4 #988, RT=5.204 min, MS1, FTMS (+)
F2 #3333, RT=5.202 min, MS1, FTMS (+)
F2 #3335, RT=5.206 min, MS2, FTMS (+)

ZDF_Fatty_2 (F4) #988, RT=5.204 min, MS1, FTMS (+)
C10 H14 O3 as [M+H]⁺+1

Intensity [counts] (10⁶) vs m/z

| Checked | Name | Formula | Annotation Sc | Molecular Weight | RT [min] | Area (Max.) | # ChemSpider Res | # mzCloud Results | # Kegg Pathways | # BioCyc Pathways | Kegg Pathways |
|--------------------------|--------------------------------------|--------------|--------------------------|------------------|----------|-------------|------------------|-------------------|-----------------|-------------------|---------------|
| <input type="checkbox"/> | mephesisin | C10 H14 O3 | <input type="checkbox"/> | 182.09426 | 5.204 | 978898 | 2 | | | | |
| <input type="checkbox"/> | 3-Phenyl-1-propanol | C9 H12 O | <input type="checkbox"/> | 136.08876 | 5.202 | 883561 | 2 | | | | |
| <input type="checkbox"/> | Aminolevulinic acid | C5 H9 N O3 | <input type="checkbox"/> | 131.05802 | 0.833 | 3670342 | 2 | | | | |
| <input type="checkbox"/> | 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]o | C10 H18 O3 | <input type="checkbox"/> | 186.12541 | 5.784 | 400556 | 2 | | | | |
| <input type="checkbox"/> | Phenoxyethanol | C8 H10 O | <input type="checkbox"/> | | | | 2 | | | | |
| <input type="checkbox"/> | Adipic acid | C6 H10 O4 | <input type="checkbox"/> | 146.05781 | 3.006 | 776507 | 1 | | | | |
| <input type="checkbox"/> | 2,4,5-Trimethoxybenzaldehyde | C10 H12 O3 | <input type="checkbox"/> | 184.07802 | 6.112 | 341345 | 1 | | | | |
| <input type="checkbox"/> | 3,4-Dihydroxyphenylpropionic acid | C9 H10 O5 | <input type="checkbox"/> | 182.06602 | 6.978 | 283874 | 1 | | | | |
| <input type="checkbox"/> | phenacetin | C10 H13 N O2 | <input type="checkbox"/> | | | | 1 | | | | |
| <input type="checkbox"/> | Adipic acid | C6 H10 O4 | <input type="checkbox"/> | 146.05786 | 6.112 | 341345 | 1 | | | | |
| <input type="checkbox"/> | Adipic acid | C6 H10 O4 | <input type="checkbox"/> | 146.05786 | 6.112 | 341345 | 1 | | | | |
| <input type="checkbox"/> | Cinnamyl alcohol | C9 H10 O | <input type="checkbox"/> | 134.07306 | 6.978 | 283874 | 1 | | | | |

How to prioritize multiple hits from ChemSpider?

Use as Compound Annotation

- Add to Structure Proposals
- Add to Structure Proposals and Apply FISH Annotations
- Export

| Checked | Compound Match | CSID | Formula | Molecular Weight | Name | References |
|--------------------------|--------------------------|--------------------------|------------|------------------|--|------------|
| <input type="checkbox"/> | <input type="checkbox"/> | 30791273 | C10 H14 O3 | 182.09430 | (1R,2S,5S)-2-[(1Z)-1-Hydroxy-3-oxo-1-propen-2-yl]-5-methylcyclopentanecarbaldehyde | 0.00004 |
| <input type="checkbox"/> | <input type="checkbox"/> | 30791566 | C10 H14 O3 | 182.09430 | (1S,2S,4S,5S,7R)-5-Hydroxy-5,8,8-trimethyl-3-oxatricyclo[5.1.0.0~2,4~]octan-6-one | 0.00004 |

Mass Frontier Annotation (FISh) for Structure Proposals

Mass Frontier annotation can be calculated as a batch

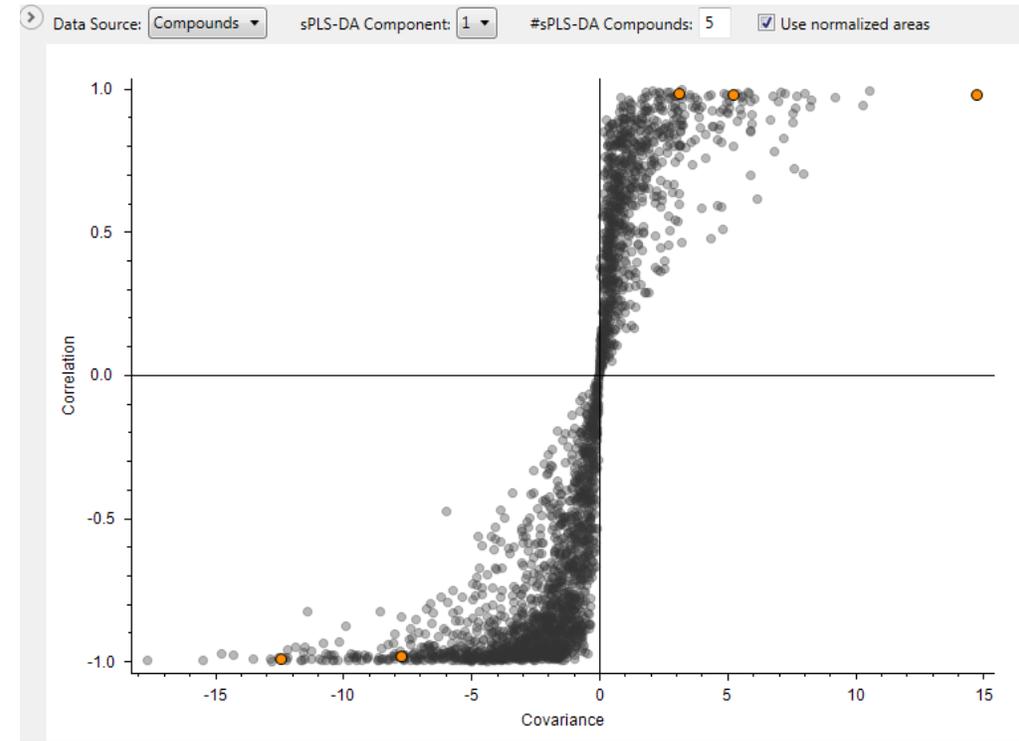
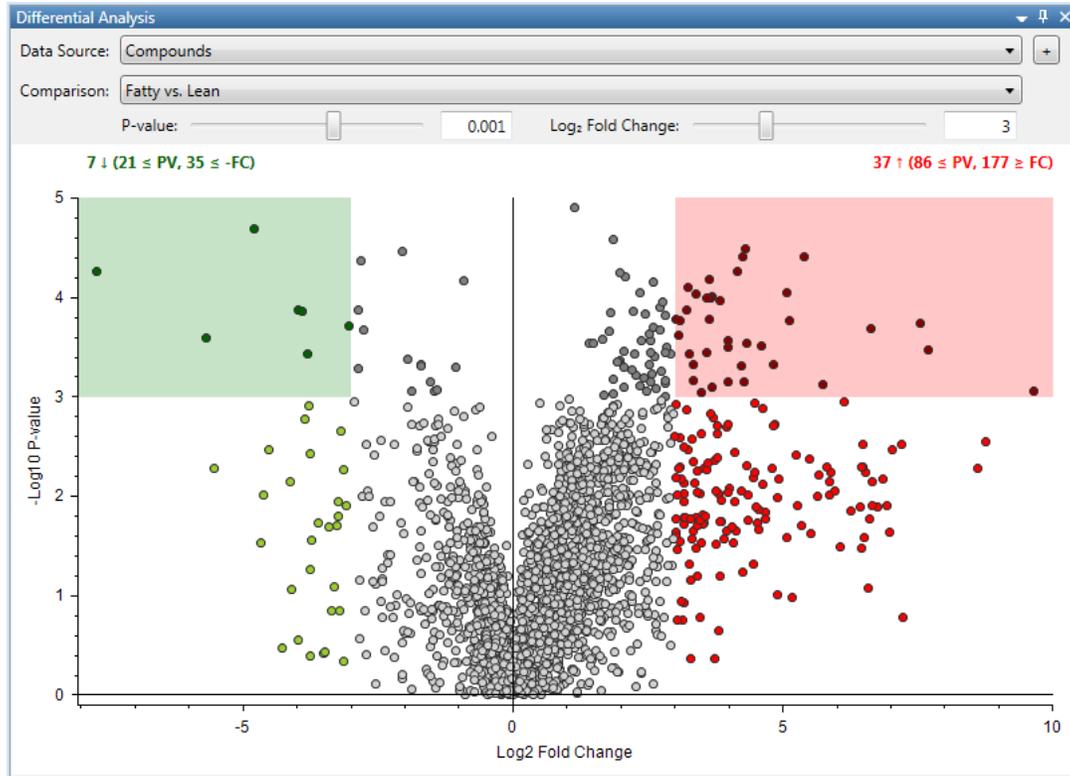
| Checked | Name | Formula | Annotation Sc | Molecular Weight | RT [min] | Area (Max.) | # ChemSpider Res. | # mzCloud Results | # Kegg Pathways | Kegg Pathways | mzCloud Best Match | Gr |
|-------------------------------------|--------------------------------------|------------|---------------|------------------|----------|-------------|-------------------|-------------------|-----------------|---------------|--------------------|------|
| <input type="checkbox"/> | 3-Phenyl-1-propanol | C9 H12 O | ■■■ | 136.08876 | 5.212 | 888554 | 21 | 0 | 0 | | | 8. |
| <input type="checkbox"/> | mephenesin | C10 H14 O3 | ■■■ | 182.09400 | 3.713 | 5141144 | 21 | 0 | 3 | | | 6. |
| <input type="checkbox"/> | Phenoxyethanol | C8 H10 O2 | ■■■ | 138.06809 | 4.296 | 672557 | 20 | 0 | 7 | | | 6. |
| <input type="checkbox"/> | Aminolevulinic acid | C5 H9 N O3 | ■■■ | 131.05802 | 0.844 | 3435255 | 20 | 0 | 12 | | | 9. |
| <input type="checkbox"/> | 1,3,3-Trimethyl-2-oxabicyclo[2.2.2]o | C10 H18 O3 | ■■■ | 186.12541 | 5.795 | 400666 | 20 | 0 | 2 | | | 3. |
| <input type="checkbox"/> | Phenoxyethanol | C8 H10 O2 | ■■■ | 138.06807 | 2.919 | 479742 | 20 | 0 | 7 | | | 3. |
| <input checked="" type="checkbox"/> | 2-Methyl-5-propionylfuran | C8 H10 O2 | ■■■ | 138.06804 | 4.675 | 1198708 | 20 | 1 | 7 | | | 55.1 |
| <input type="checkbox"/> | cis-4-Hydroxy-D-proline | C5 H9 N O3 | ■■■ | 131.05806 | 0.939 | 8039552 | 20 | 1 | 12 | | | 50.7 |
| <input type="checkbox"/> | 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 |
|--------------------------|-------------------------------------|--------------------------|-----------|------------------|--|------------|-----------|-------------|--------------|
| <input type="checkbox"/> | <input checked="" type="checkbox"/> | 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

Compound Discoverer Software: Statistics



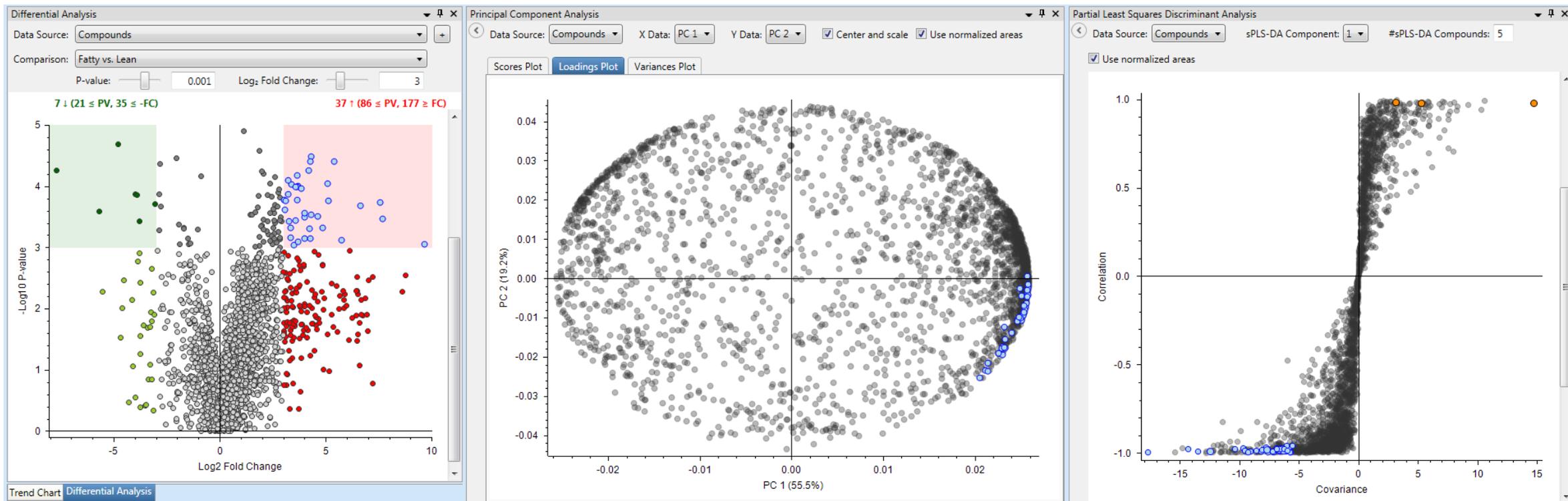
Differential Analysis, volcano plots,
ANOVA, PCA, PLS-DA ...

Compound Discoverer Software: Statistics



- Volcano plots, PCA, PLS-DA, ... are interactive
- Results are always directly linked to raw data.

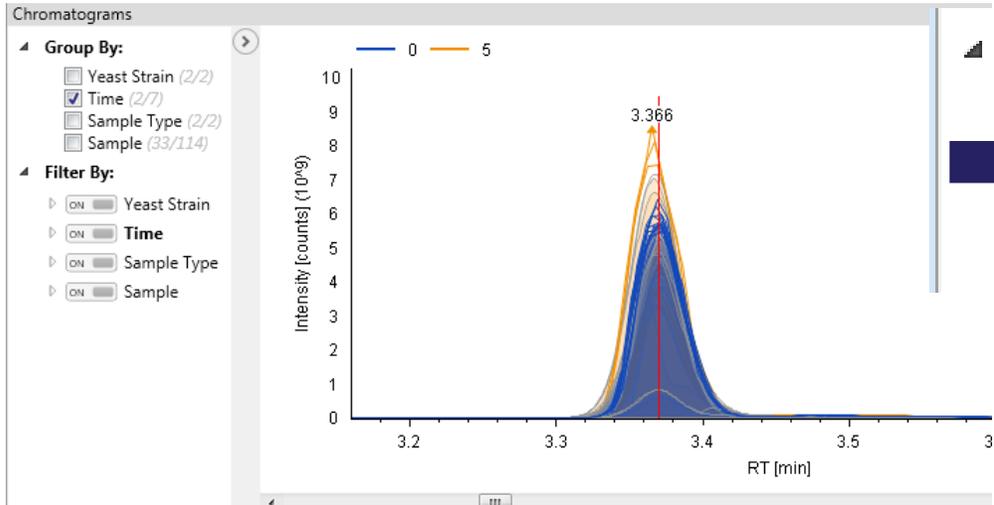
Compound Discoverer Software: Statistics



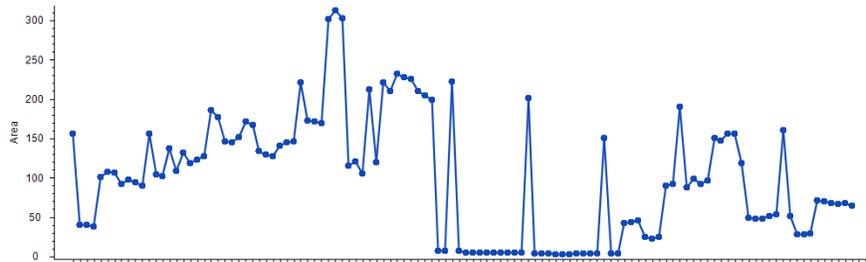
| Checked | Name | Formula | Annotat <input type="checkbox"/> | Molecular Weight | RT [min] |
|-------------------------------------|-----------------|---|----------------------------------|------------------|----------|
| <input type="checkbox"/> | DL-Tryptophan | C ₁₁ H ₁₂ N ₂ O ₂ | ■■■■■ | 204.08974 | 3.119 |
| <input checked="" type="checkbox"/> | Creatine | C ₄ H ₉ N ₃ O ₂ | ■■■●■ | 131.06929 | 0.900 |
| <input checked="" type="checkbox"/> | L-Phenylalanine | C ₉ H ₁₁ N O ₂ | ■■■■■ | 165.07892 | 2.578 |
| <input checked="" type="checkbox"/> | Creatinine | C ₄ H ₇ N ₃ O | ■■■●■ | 113.05880 | 0.927 |
| <input type="checkbox"/> | L-Tyrosine | C ₉ H ₁₁ N O ₃ | ■●■■■ | 181.07382 | 1.625 |

- Use tracking feature to navigate through complex datasets
- Interpret results from univariate and multivariate analysis

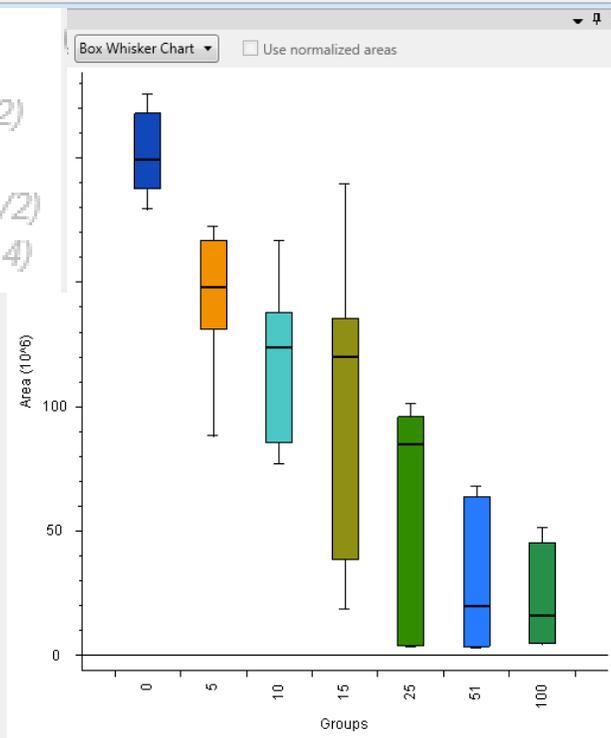
Utilize Study Factors for Statistics and Interactive Visualizations



Tryptophan



Relative abundance in 114 samples
(7 time points, 2 yeast strains x biol. replicates)



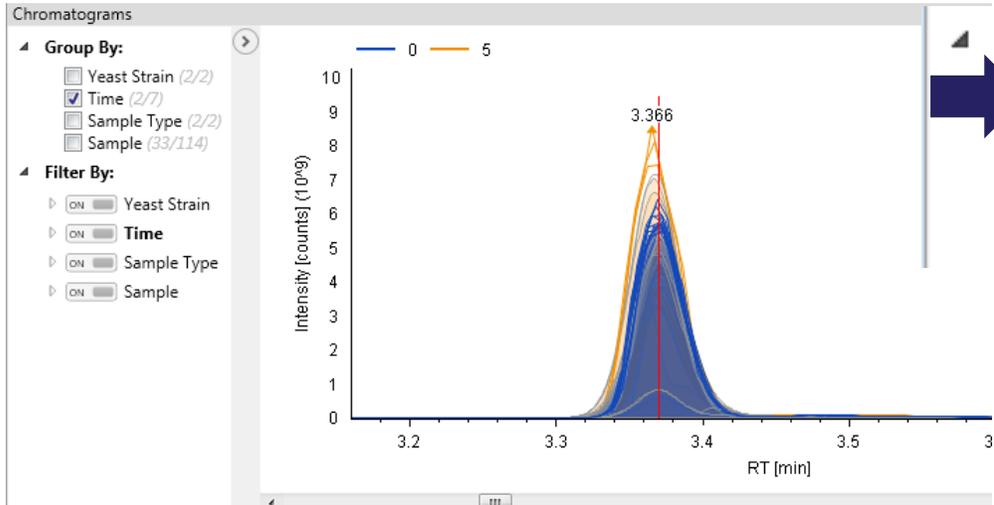
2 yeast strains



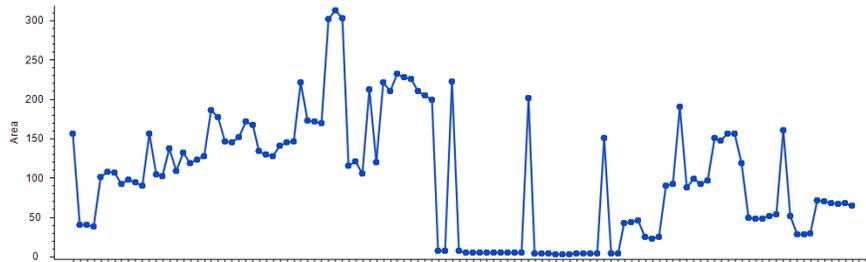
7 time points

Plot as box-whisker chart grouped by 7 time points ...

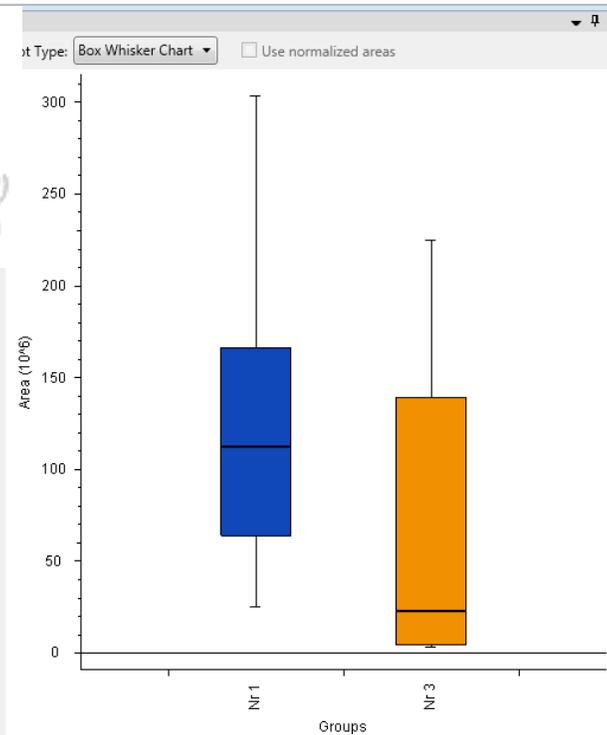
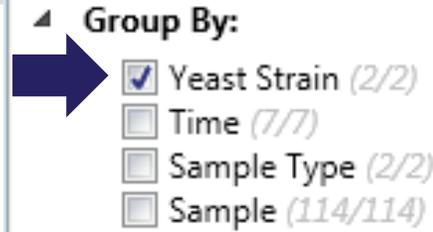
Utilize Study Factors for Statistics and Interactive Visualizations



Tryptophan



Relative abundance in 114 samples
(7 time points, 2 yeast strains x biol. replicates)

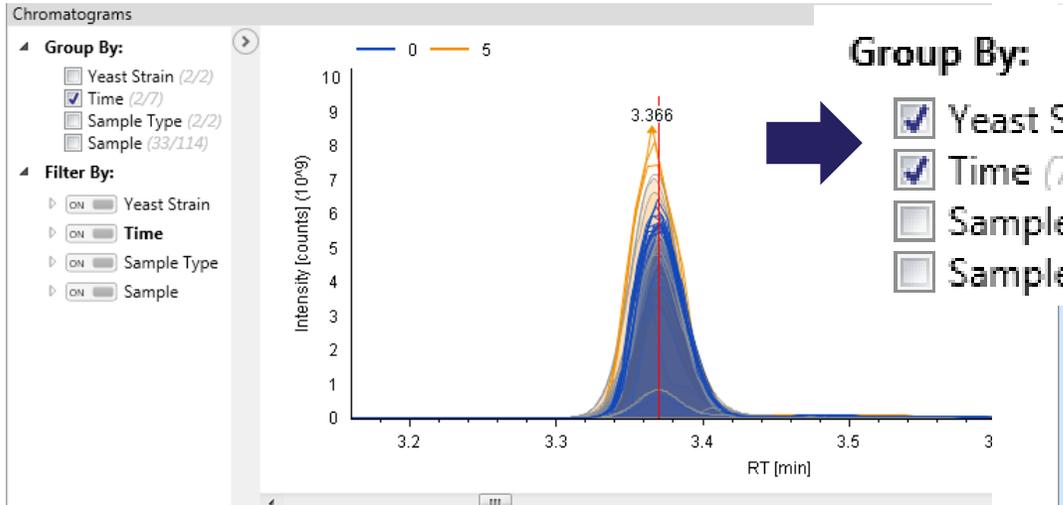


2 yeast strains



... or grouped by the two yeast strains

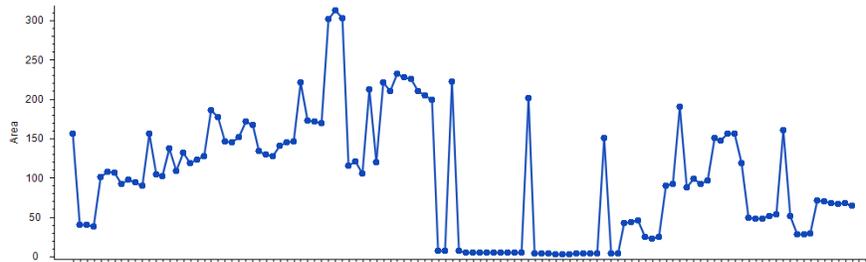
Utilize Study Factors for Statistics and Interactive Visualizations



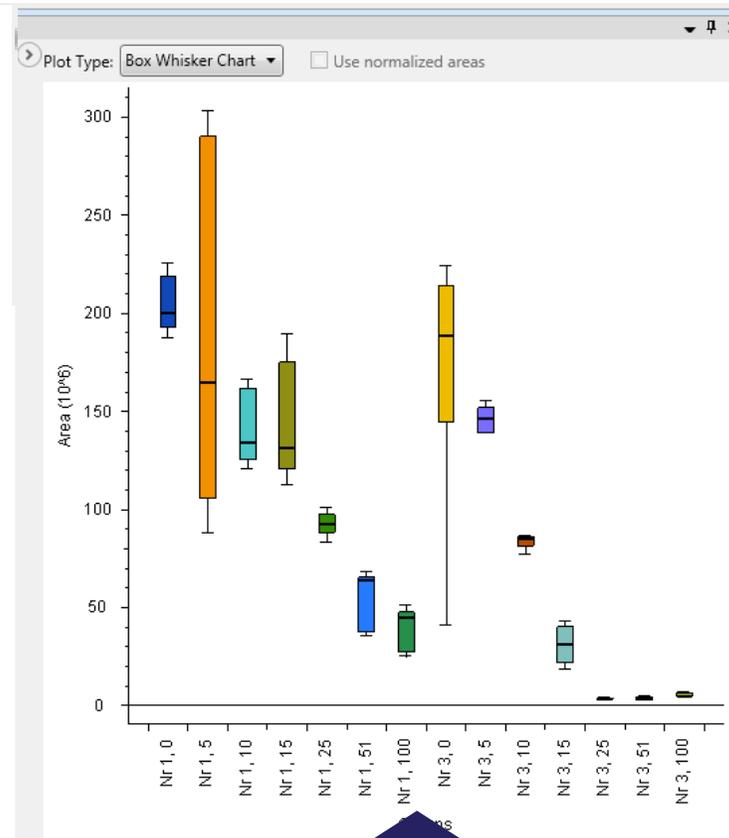
Group By:

- Yeast Strain (2/2)
- Time (7/7)
- Sample Type (2/2)
- Sample (114/114)

Tryptophan



Relative abundance in 114 samples
(7 time points, 2 yeast strains x biol. replicates)



2 yeast strains

7 time points



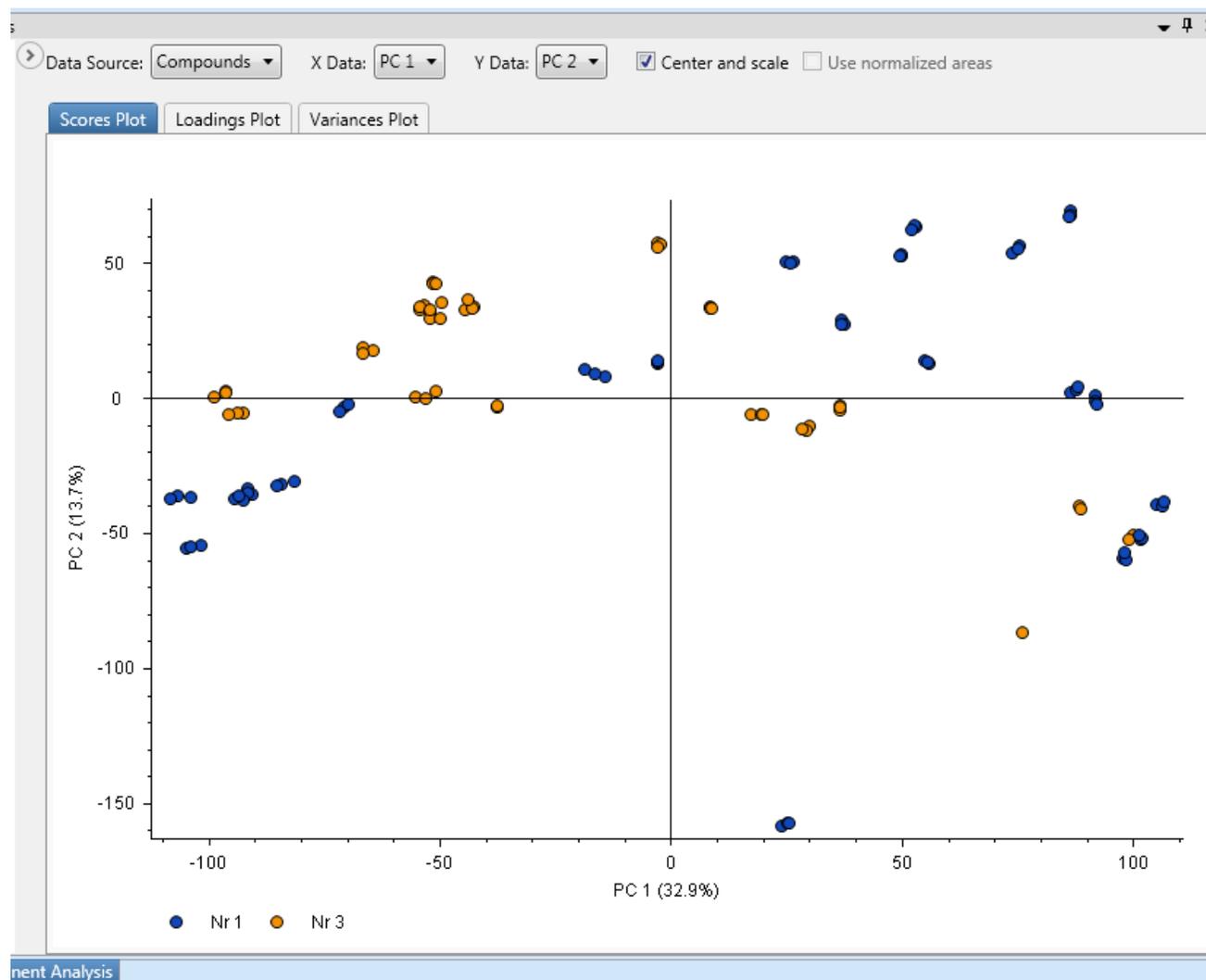
... or both at the same time

Utilize Study Factors for Statistics and Interactive Visualizations - PCA

Color By:

- Yeast Strain (2/2)
- Time (7/7)
- Sample Type (2/2)
- Sample (114/114)

PCA scores plot –
samples colored using
the two yeast strains ...



2 yeast strains

7 time points

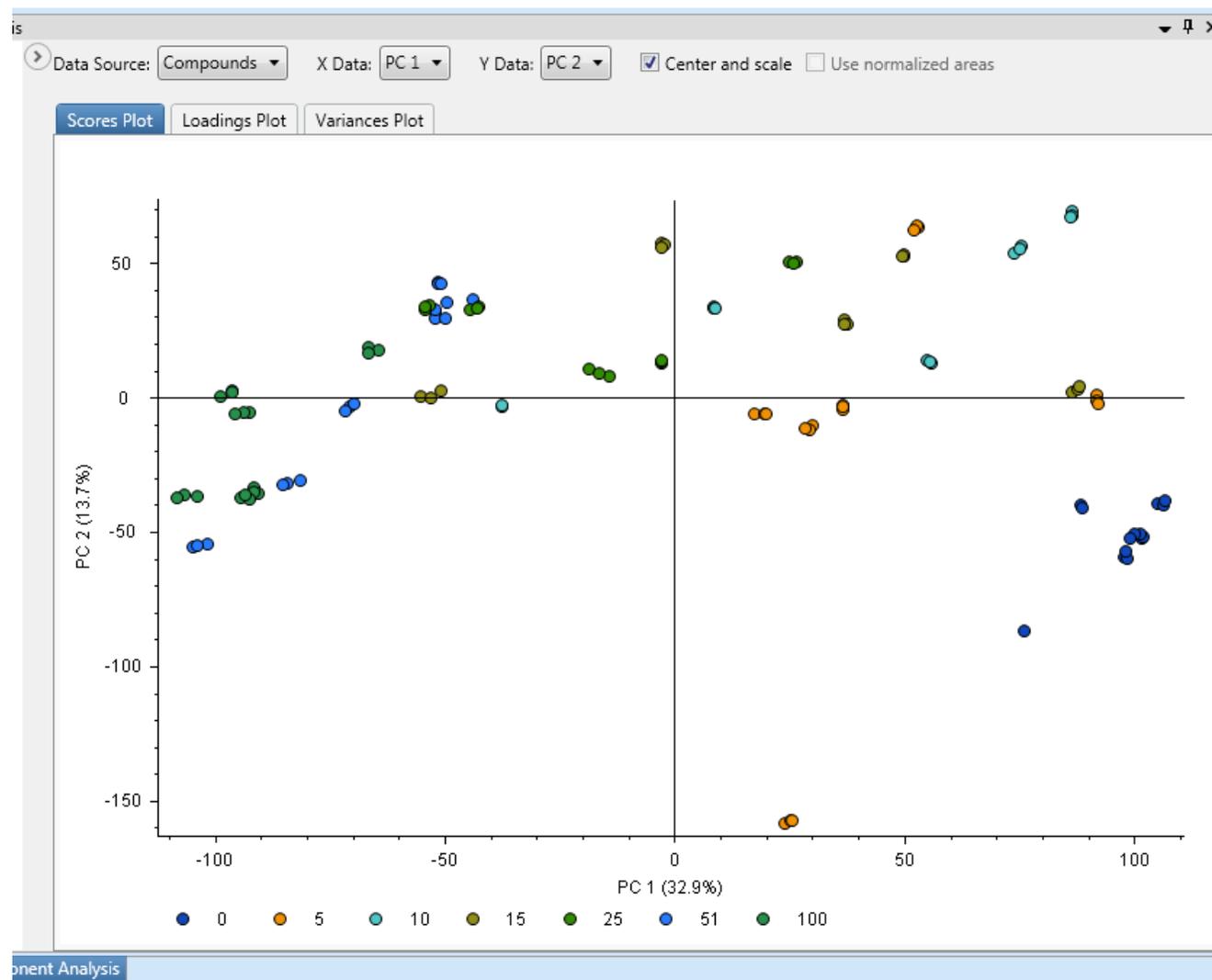


Utilize Study Factors for Statistics and Interactive Visualizations - PCA

Color By:

- Yeast Strain (2/2)
- Time (7/7)
- Sample Type (2/2)
- Sample (114/114)

PCA scores plot –
samples colored using
the 7 time points ...



2 yeast strains



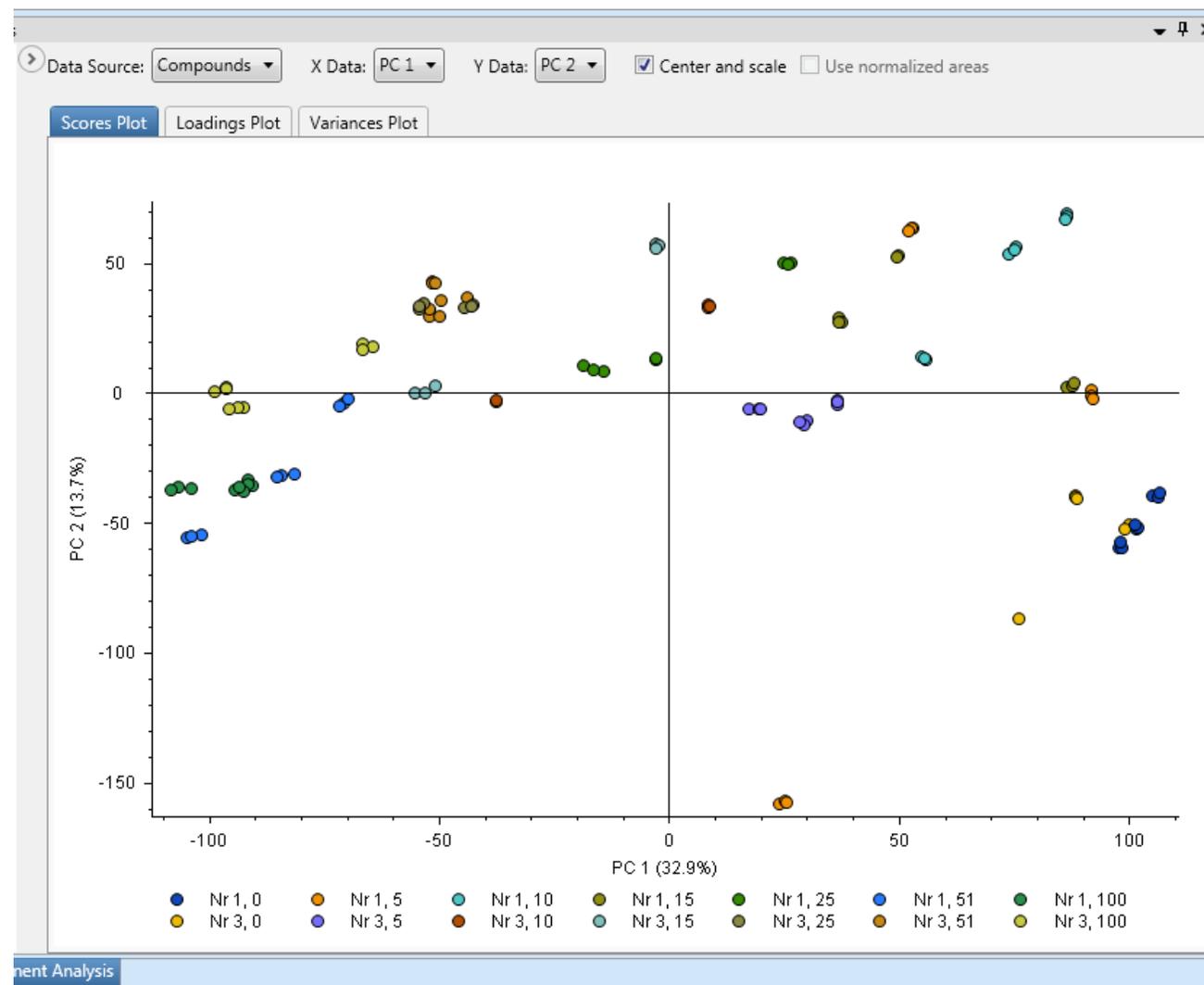
Utilize Study Factors for Statistics and Interactive Visualizations - PCA

Color By:



- Yeast Strain (2/2)
- Time (7/7)
- Sample Type (2/2)
- Sample (114/114)

PCA scores plot –
samples colored using
both yeast strain and
time point information



2 yeast strains

7 time points



PROTOCOL

Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry

Warwick B Dunn¹⁻³, David Broadhurst^{2,4}, Paul Begley², Eva Zelena², Sue Francis-McIntyre², Nadine Anderson², Marie Brown², Joshau D Knowles⁵, Antony Halsall², John N Haselden⁶, Andrew W Nicholls⁶, Ian D Wilson⁷, Douglas B Kell², Royston Goodacre^{1,2} & The Human Serum Metabolome (HUSERMET) Consortium

- Large experiments with hundreds of samples often require data acquisition in multiple batches
- QC metrics and filtering using pooled samples as QCs
- Correct “batch-effects” – independently for each compound

- QC-based normalization
 - State of the art method for normalization (correction of batch-effects)
 - Based on pooled samples used as QCs
 - Correction applied independently for each (unknown) compound
 - Also filters compounds based on QC criteria

PROTOCOL

Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry

Warwick B Dunn¹⁻³, David Broadhurst^{2,4}, Paul Begley², Eva Zelena², Sue Francis-McIntyre², Nadine Anderson², Marie Brown², Joshau D Knowles⁵, Antony Halsall², John N Haselden⁶, Andrew W Nicholls⁶, Ian D Wilson⁷, Douglas B Kell², Royston Goodacre^{1,2} & The Human Serum Metabolome (HUSERMET) Consortium

¹Manchester Centre for Integrative Systems Biology, Manchester Interdisciplinary Biocentre, University of Manchester, Manchester, UK. ²School of Chemistry, Manchester Interdisciplinary Biocentre, University of Manchester, Manchester, UK. ³Centre for Advanced Discoveries and Experimental Therapeutics, Manchester Biomedical Research Centre and School of Biomedicine, Manchester, UK. ⁴Department of Medicine, Katz Group Centre for Pharmacy & Health, University of Alberta, Edmonton, Alberta, Canada. ⁵School of Computer Science, The University of Manchester, Manchester, UK. ⁶Department of Investigative Preclinical Toxicology, GlaxoSmithKline, Hertfordshire, UK. ⁷Department of Clinical Pharmacology, Drug Metabolism and Pharmacokinetics, AstraZeneca, Cheshire, UK. Correspondence should be addressed to W.B.D. (warwick.dunn@manchester.ac.uk).

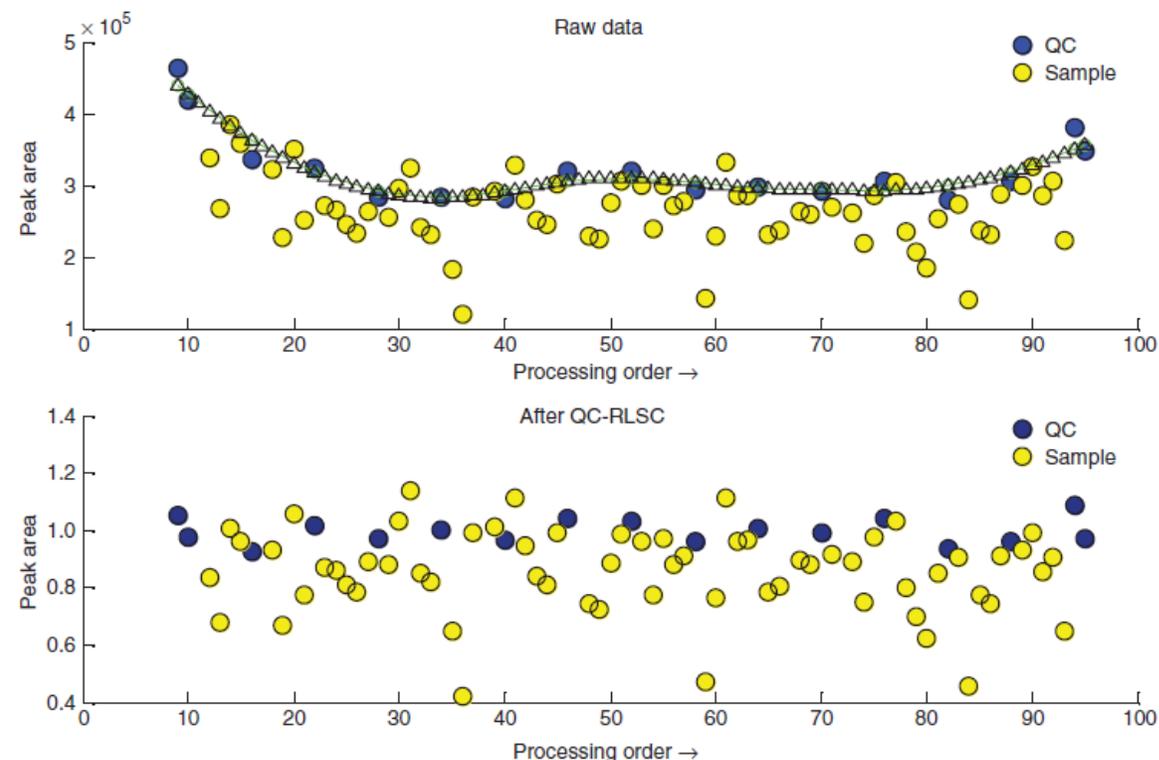
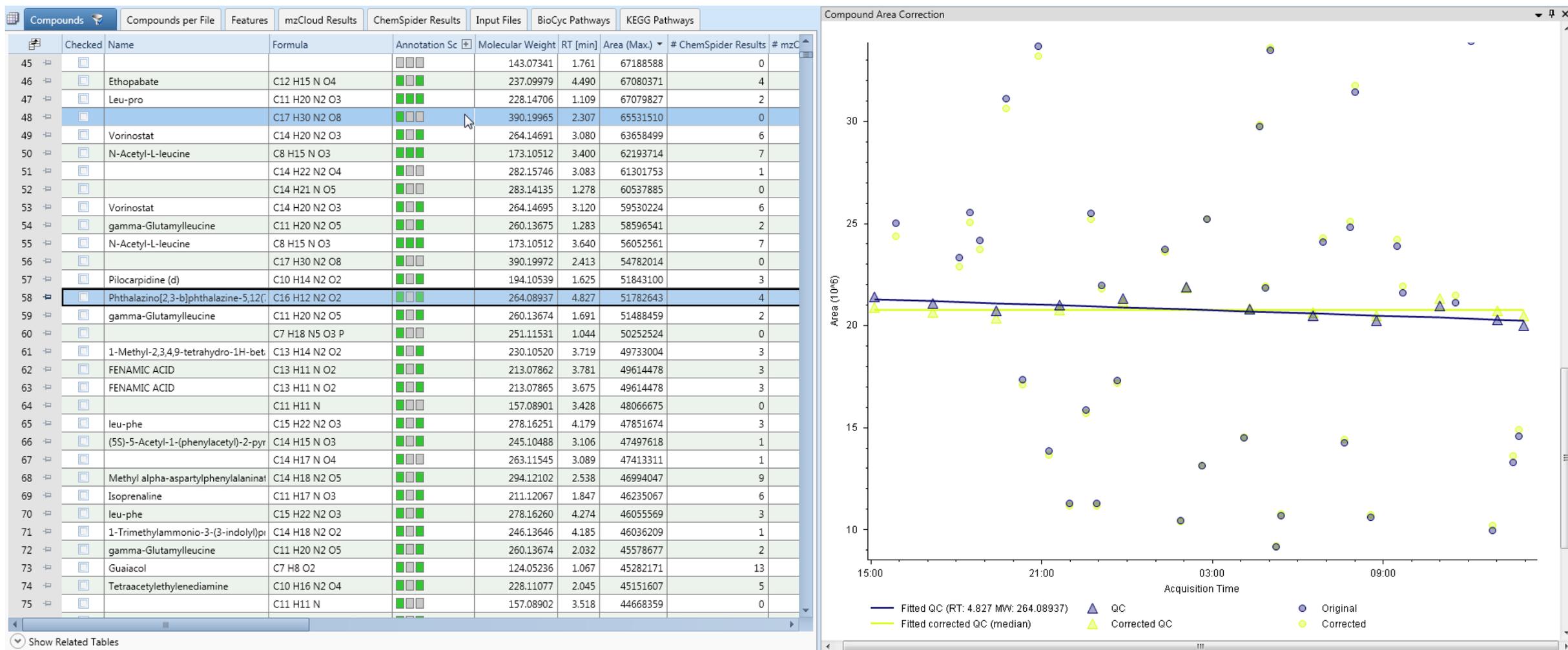


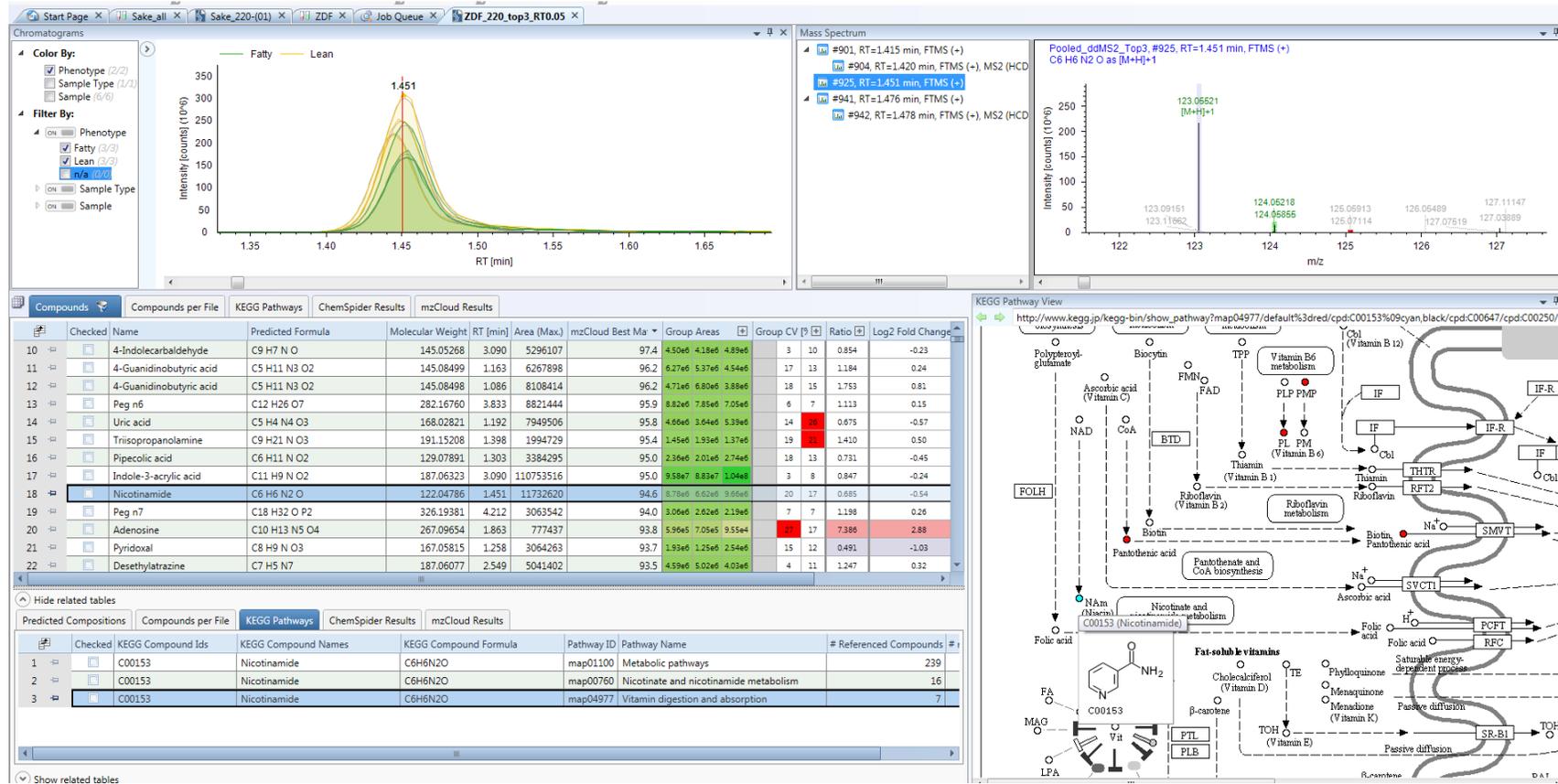
Figure 2 | The QC-RLSC protocol for a metabolic feature detected in UPLC-MS (ES+) with signal attenuation across a given analytical batch. A cross-validated LOESS curve (upper plot) is fitted to the QC samples, the correction curve interpolated (triangles), to which the total data set for that peak is corrected (lower plot).

Compound Discoverer 2.1 Software – QC-based Normalization



Compound area correction plot for each compound

Compound Discoverer 2.1 Software: Pathway Mapping using KEGG and BioCyc



KEGG and BioCyc pathways: global and context-specific

Pathway Mapping to BioCyc with Omics Data Overlay

Compound Discoverer 2.1.0.388

File Reporting Libraries View Window Help

Start Page X ZDF_2 X Job Queue X Configuration X ZDF_b388_1e6_BC (3) X Soy_CD2.1_378_regular_only_2-(2) X Soy X

Compounds Compounds per File Features mzCloud Results

ChemSpider Results BioCyc Results Input Files KEGG Pathways BioCyc Pathways

| Checked | Pathway ID | Pathway Name | # Referenced Compou |
|-------------------------------------|------------------------|--|---------------------|
| <input type="checkbox"/> | META:PWY-6954 | superpathway of aromatic compound degradation via 2-oxopent-4-enoate | 23 |
| <input type="checkbox"/> | META:TRNA-CHARGING-PWY | tRNA charging | 21 |
| <input type="checkbox"/> | META:PWY-4201 | volatile cinnamoic ester biosynthesis | 19 |
| <input type="checkbox"/> | META:PWY-5882 | epoxypseudoisoeugenol-2-methylbutanoate biosynthesis | 19 |
| <input checked="" type="checkbox"/> | META:PWY-5183 | superpathway of aerobic toluene degradation | 17 |
| <input type="checkbox"/> | META:PWY-5991 | superpathway of linamarin and lotaustralin biosynthesis | 17 |
| <input type="checkbox"/> | META:PWY-361 | phenylpropanoid biosynthesis | 15 |
| <input type="checkbox"/> | META:PWY-2504 | superpathway of aromatic compound degradation via 3-oxoadipate | 15 |
| <input type="checkbox"/> | META:PWY-5327 | superpathway of L-lysine degradation | 15 |
| <input type="checkbox"/> | META:PWY-7698 | 2,5-xyleneol and 3,5-xyleneol degradation | 15 |
| <input type="checkbox"/> | META:PWY-7667 | apicidin biosynthesis | 15 |
| <input type="checkbox"/> | META:PWY-7114 | tea aroma glycosidic precursor bioactivation | 13 |
| <input type="checkbox"/> | META:PWY-5532 | nucleoside and nucleotide degradation (archaea) | 13 |
| <input type="checkbox"/> | META:PWY-4203 | volatile benzenoid biosynthesis I (ester formation) | 13 |
| <input type="checkbox"/> | META:PWY-3621 | γ-butyrobetaine degradation | 13 |
| <input type="checkbox"/> | META:PWY-7648 | 4-methyl-proline biosynthesis | 13 |
| <input type="checkbox"/> | META:PWY-6806 | carotenoid cleavage | 12 |
| <input type="checkbox"/> | META:PWY-5990 | lotaustralin biosynthesis | 12 |
| <input type="checkbox"/> | META:PWY-6080 | 4-ethylphenol degradation (anaerobic) | 12 |
| <input type="checkbox"/> | META:PWY-7703 | 2,4-xyleneol degradation to protocatechuate | 12 |
| <input type="checkbox"/> | META:PWY-5975 | furaneol biosynthesis | 12 |
| <input type="checkbox"/> | META:PWY-7076 | 3,5-dimethoxytoluene biosynthesis | 12 |
| <input type="checkbox"/> | META:PWY-4021 | β-alanine betaine biosynthesis | 12 |
| <input type="checkbox"/> | META:PWY-5005 | biotin biosynthesis II | 11 |
| <input type="checkbox"/> | META:PWY-1782 | superpathway of indole-3-acetate conjugate biosynthesis | 11 |
| <input type="checkbox"/> | META:PWY-6342 | noradrenaline and adrenaline degradation | 11 |
| <input type="checkbox"/> | META:PWY-3661-1 | glycine betaine degradation II (mammalian) | 11 |
| <input type="checkbox"/> | META:PWY-3661 | glycine betaine degradation I | 11 |
| <input type="checkbox"/> | META:PWY-5079 | L-phenylalanine degradation III | 11 |
| <input type="checkbox"/> | META:PWY-5178 | toluene degradation IV (aerobic) (via catechol) | 11 |
| <input type="checkbox"/> | META:PWY30-4108 | L-tyrosine degradation III | 11 |
| <input type="checkbox"/> | META:PWY-6234 | superpathway of jasmonoyl-amino acid conjugates biosynthesis | 11 |
| <input type="checkbox"/> | META:PWY-7694 | zwittericin A biosynthesis | 11 |
| <input type="checkbox"/> | META:PWY-5328 | superpathway of L-methionine salvage and degradation | 10 |
| <input type="checkbox"/> | META:PWY-5428 | m-xylene degradation to m-toluate | 10 |
| <input type="checkbox"/> | META:PWY-5429 | p-xylene degradation to p-toluate | 10 |
| <input type="checkbox"/> | META:PWY-5181 | toluene degradation III (aerobic) (via p-cresol) | 10 |

Show Related Tables

BioCyc Pathway (beta) <https://biocyc.org/META/new-image?type=PATHWAY&object=PWY-5183> Omics-Overlay: Log2 Fold Change

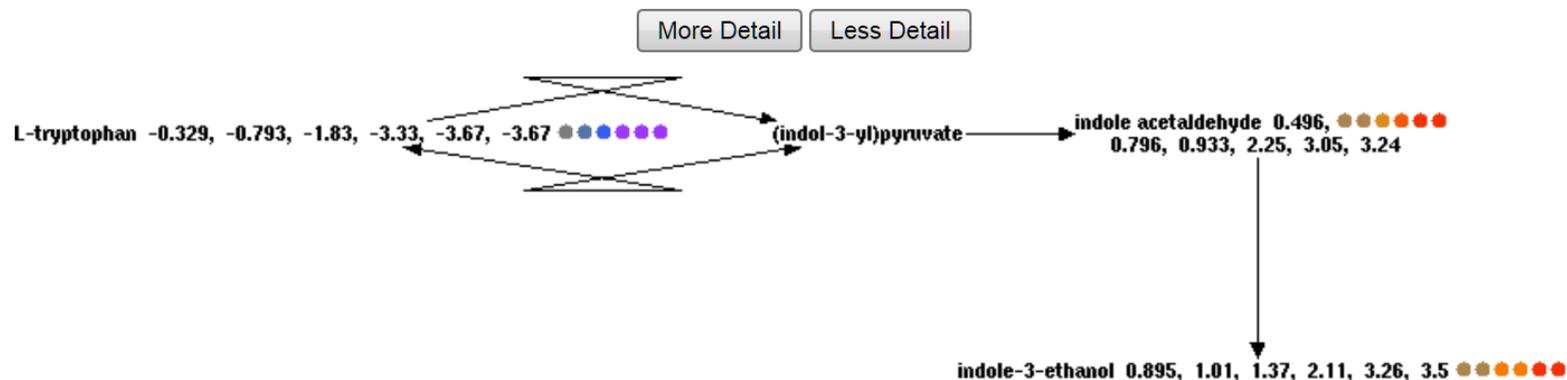
MetaCyc Chimeric Pathway: superpathway of aerobic toluene degradation

Compound: 4-hydroxybenzyl alcohol
 Synonyms: p-hydroxybenzyl alcohol, 4-(hydroxymethyl) phenol

If an enzyme name is shown in bold, there is experimental evidence for this enzymatic activity.

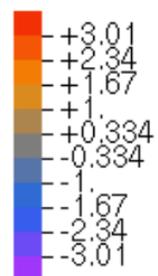
Pathway Mapping to BioCyc with Omics Data Overlay

[Add to SmartTable](#) ***Saccharomyces cerevisiae* S288c Pathway: tryptophan degradation VIII (to tryptophol)** 



If an enzyme name is shown in bold, there is experimental evidence for this enzymatic activity.

Key to Omics Data Colors:

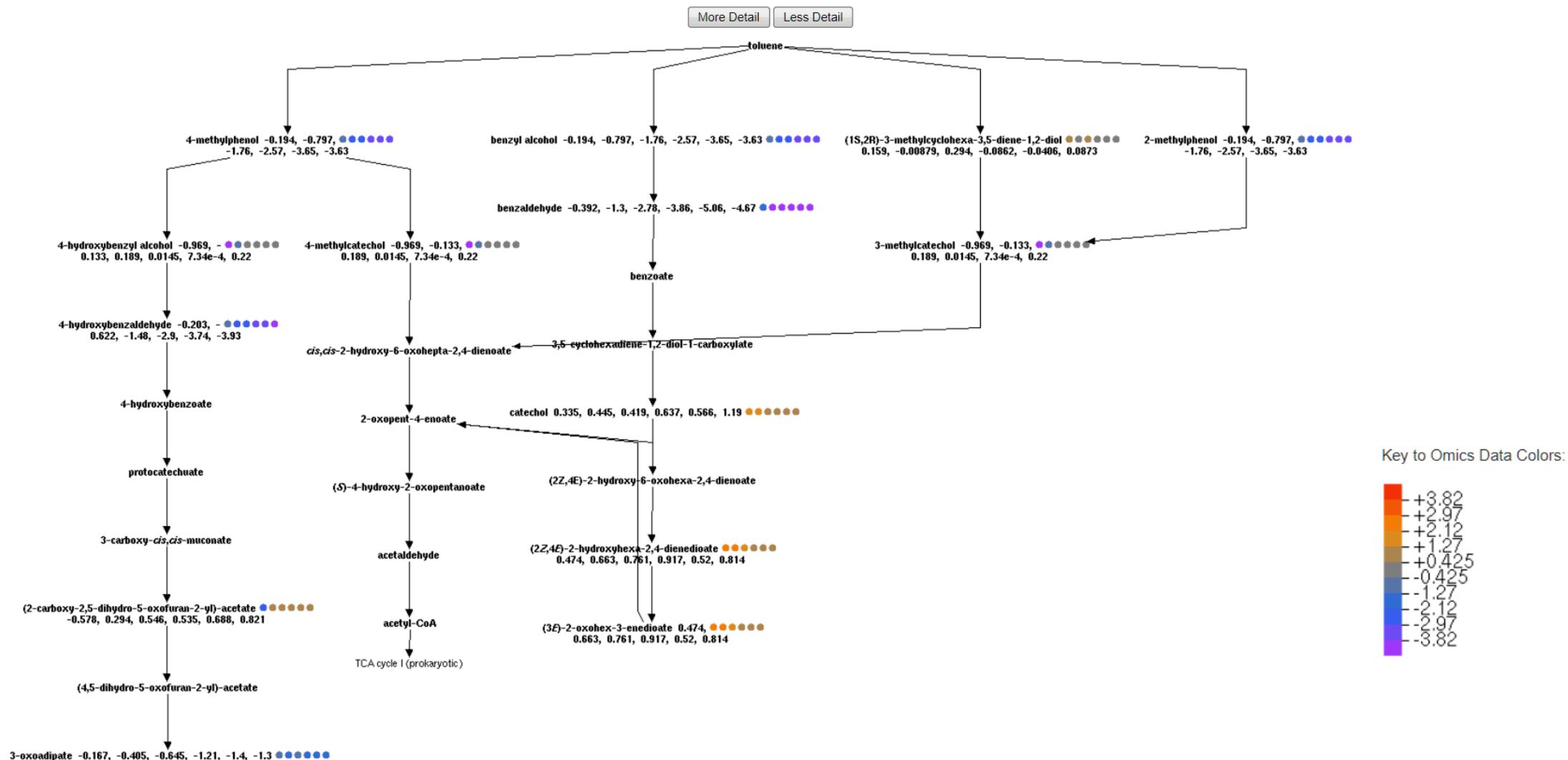


Synonyms: Ehrlich pathway

Pathway Mapping to BioCyc with Omics Data Overlay

[Add to SmartTable](#)

MetaCyc Chimeric Pathway: superpathway of aerobic toluene degradation



Compound Discoverer
Integrated solutions for small molecule structure identification

thermo scientific

HOME WHAT IS COMPOUND DISCOVERER? HELP BUTTON REQUEST FEATURE... RESOURCES TUTORIALS

Compound Discoverer 2.1 Released! Get your Demo here.

JUL 31 Posted by [Tim Stratton](#)

For current Compound Discoverer 2.0 users:
The electronic upgrade to Compound Discoverer 2.1 is free! Follow the download instructions below and use the instructions for the CD 2.0 to CD 2.1 upgrade.

For new users:
To download the Compound Discoverer 2.1 Demo (CD 2.1 demo), go to the Thermo Scientific Software Portal (Flexera) and download it from the "Compound Discoverer 2.1 Demo" folder.

[CLICK HERE FOR FULL INSTRUCTIONS.](#)

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Compound Discoverer at ASMS 2017

APR 14 Posted by [Tim Stratton](#)

mycompounddiscoverer.com

- News on Compound Discoverer
- Quick Videos
- Request a feature
- “Help button” - contact the team



Questions?

Appendix

Compound Discoverer 2.1 Software – QC-based Normalization

| Study File ID | File Name | Creation Date | Instrument Name | Ref. File ID | Sample Type |
|---------------|-------------------------|-------------------|------------------------|--------------|-----------------|
| F1 | Blank_1_Replicate_1.raw | 10/4/2016 2:34 PM | Q Exactive HF Orbitrap | F5 | Blank |
| F2 | Blank_1_Replicate_2.raw | 10/4/2016 2:45 PM | Q Exactive HF Orbitrap | F5 | Blank |
| F3 | Blank_1_Replicate_3.raw | 10/4/2016 2:57 PM | Q Exactive HF Orbitrap | F5 | Blank |
| F5 | QC_1.raw | 10/4/2016 3:08 PM | Q Exactive HF Orbitrap | F35 | Quality Control |
| F98 | Soy_28_Replicate_1.raw | 10/4/2016 3:19 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F41 | Soy_9_Replicate_1.raw | 10/4/2016 3:30 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F91 | Soy_25_Replicate_3.raw | 10/4/2016 3:41 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F28 | Soy_4_Replicate_3.raw | 10/4/2016 3:52 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F32 | Soy_6_Replicate_1.raw | 10/4/2016 4:03 PM | Q Exactive HF Orbitrap | F35 | Sample |
| F38 | Soy_8_Replicate_1.raw | 10/4/2016 4:15 PM | Q Exactive HF Orbitrap | F35 | Sample |
| F69 | Soy_18_Replicate_2.raw | 10/4/2016 4:26 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F30 | Soy_5_Replicate_2.raw | 10/4/2016 4:37 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F42 | Soy_9_Replicate_2.raw | 10/4/2016 4:48 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F60 | Soy_15_Replicate_2.raw | 10/4/2016 4:59 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F6 | QC_2.raw | 10/4/2016 5:10 PM | Q Exactive HF Orbitrap | F5 | Quality Control |
| F51 | Soy_12_Replicate_2.raw | 10/4/2016 5:33 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F52 | Soy_12_Replicate_3.raw | 10/4/2016 5:44 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F92 | Soy_26_Replicate_1.raw | 10/4/2016 5:55 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F109 | Soy_31_Replicate_3.raw | 10/4/2016 6:06 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F21 | Soy_2_Replicate_2.raw | 10/4/2016 6:17 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F117 | Soy_34_Replicate_2.raw | 10/4/2016 6:28 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F112 | Soy_32_Replicate_3.raw | 10/4/2016 6:39 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F48 | Soy_11_Replicate_2.raw | 10/4/2016 6:50 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F26 | Soy_4_Replicate_1.raw | 10/4/2016 7:02 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F97 | Soy_27_Replicate_3.raw | 10/4/2016 7:13 PM | Q Exactive HF Orbitrap | F84 | Sample |
| F7 | QC_3.raw | 10/4/2016 7:24 PM | Q Exactive HF Orbitrap | F5 | Quality Control |

- Use sample type “Quality Control” for QC samples
- Correct order is detected automatically
- Needs one QC sample at the beginning of the sequence and one at the end and at constant intervals (every 5-10 injections)

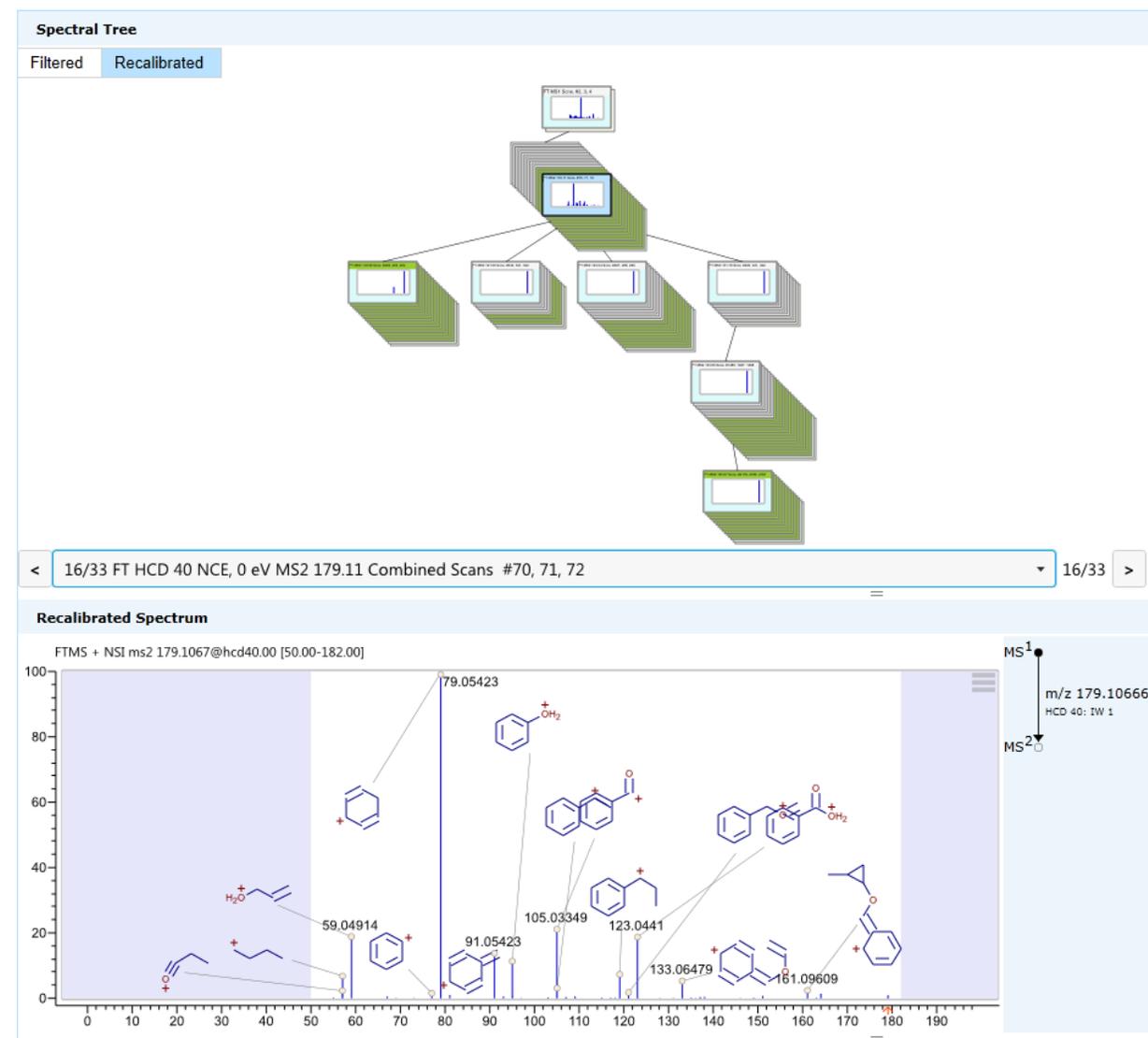
Compound Discoverer 2.1 Software – mzCloud Search Using Stepped Collision Energy



Advanced Mass Spectral Database

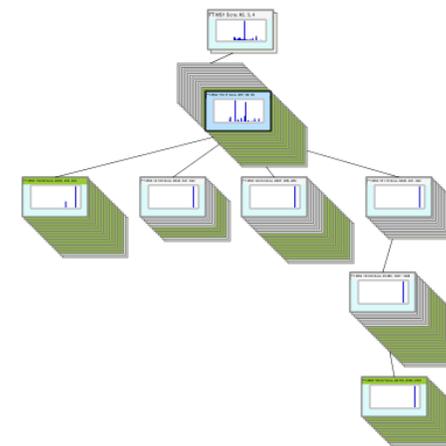
| | | | |
|--|-----------------------|--------------------------------|-------------------------------|
| 6,819 (+44) compounds <small>(+ added in the last 14 days)</small> | 10,672 (+64) trees | 2,382,231 (+32,439) spectra | 706,837 (+1,210) QM models |
|--|-----------------------|--------------------------------|-------------------------------|

> 10,000 spectral trees
> 2.4 million spectra



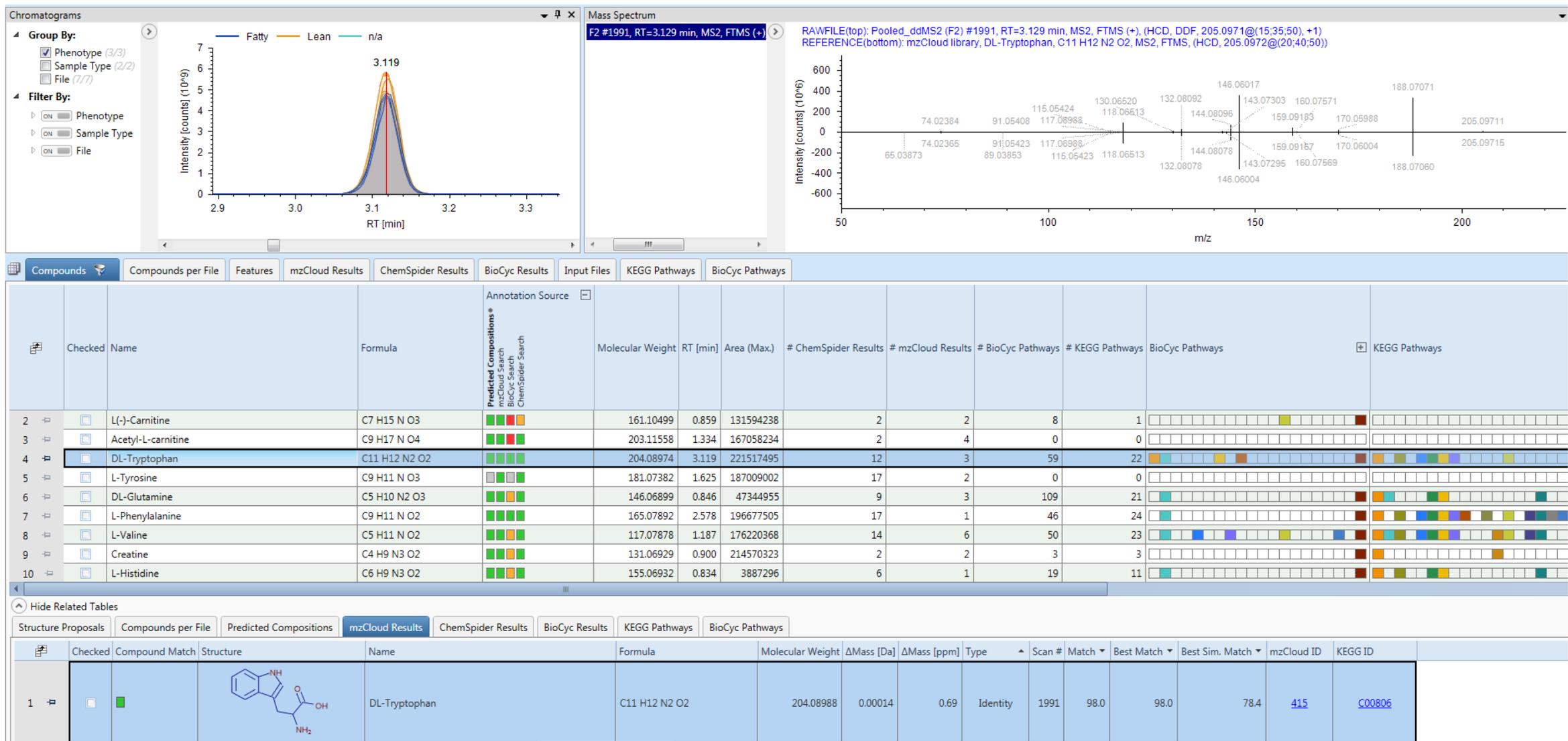
Compound Discoverer 2.1 Software – mzCloud Search Using Stepped Collision Energy

- CID 10, 15, 20, ... , 100 NCE
- HCD 10, 20, 30, ... , 200 NCE
- mzCloud search automatically matches your experimental conditions
- mzCloud automatically combines multiple scans during the search to match your experimental conditions for stepped collision energy

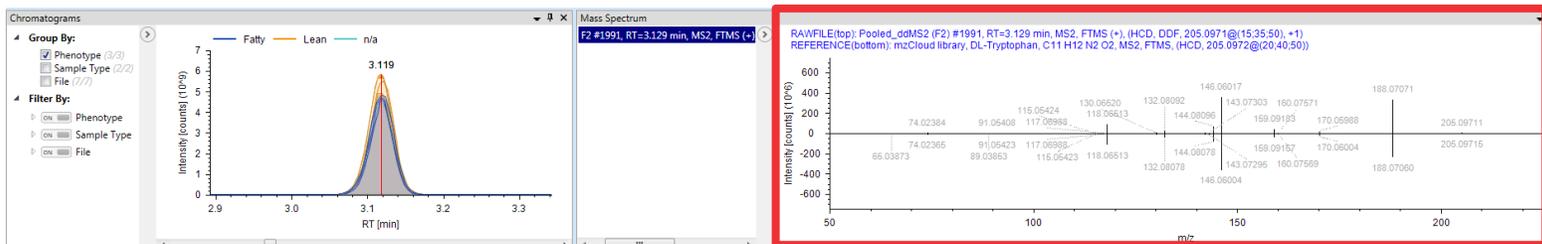


| 15/33 FT HCD 30 NCE, 0 eV MS2 179.11 Combined Scans #67, 68, 69 | |
|--|--|
| 1/33 FT CID 10 NCE, 0 eV MS2 179.11 Combined Scans #8, 9, 10 | |
| 2/33 FT CID 15 NCE, 0 eV MS2 179.11 Combined Scans #48, 49, 50 | |
| 3/33 FT CID 20 NCE, 0 eV MS2 179.11 Combined Scans #11, 12, 13 | |
| 4/33 FT CID 25 NCE, 0 eV MS2 179.11 Combined Scans #53, 54, 55 | |
| 5/33 FT CID 30 NCE, 0 eV MS2 179.11 Combined Scans #16, 17, 18 | |
| 6/33 FT CID 40 NCE, 0 eV MS2 179.11 Combined Scans #19, 20, 21 | |
| 7/33 FT CID 50 NCE, 0 eV MS2 179.11 Combined Scans #24, 25, 26 | |
| 8/33 FT CID 60 NCE, 0 eV MS2 179.11 Combined Scans #27, 28, 29 | |
| 9/33 FT CID 70 NCE, 0 eV MS2 179.11 Combined Scans #32, 33, 34 | |
| 10/33 FT CID 80 NCE, 0 eV MS2 179.11 Combined Scans #35, 36, 37 | |
| 11/33 FT CID 90 NCE, 0 eV MS2 179.11 Combined Scans #40, 41, 42 | |
| 12/33 FT CID 100 NCE, 0 eV MS2 179.11 Combined Scans #43, 44, 45 | |
| 13/33 FT HCD 10 NCE, 0 eV MS2 179.11 Combined Scans #59, 60, 61 | |
| 14/33 FT HCD 20 NCE, 0 eV MS2 179.11 Combined Scans #62, 63, 64 | |
| 15/33 FT HCD 30 NCE, 0 eV MS2 179.11 Combined Scans #67, 68, 69 | |
| 16/33 FT HCD 40 NCE, 0 eV MS2 179.11 Combined Scans #70, 71, 72 | |
| 17/33 FT HCD 50 NCE, 0 eV MS2 179.11 Combined Scans #75, 76, 77 | |
| 18/33 FT HCD 60 NCE, 0 eV MS2 179.11 Combined Scans #78, 79, 80 | |
| 19/33 FT HCD 70 NCE, 0 eV MS2 179.11 Combined Scans #83, 84, 85 | |
| 20/33 FT HCD 80 NCE, 0 eV MS2 179.11 Combined Scans #86, 87, 88 | |

Compound Discoverer 2.1 Software – mzCloud Search Using Stepped Collision Energy



Compound Discoverer 2.1 Software – mzCloud Search Using Stepped Collision Energy

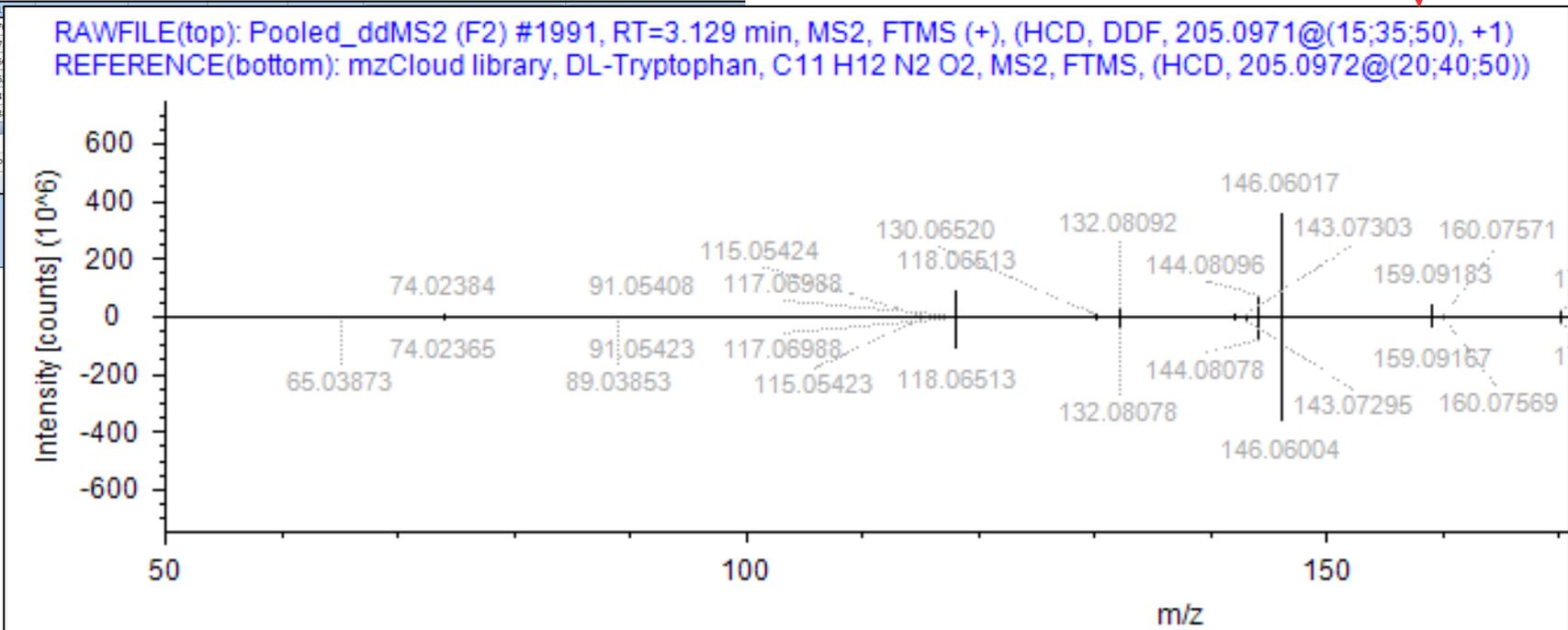


| Checked | Name | Formula | Molecular Weight | RT [min] | Area (Max.) | # ChemSpider Results | # mzCloud Results | # BioCyc Pathways | # KEGG Pathways | BioCyc Pathways | KEGG Pathways |
|-------------------------------------|--------------------|---------------|------------------|----------|-------------|----------------------|-------------------|-------------------|-----------------|-----------------|---------------|
| <input type="checkbox"/> | L(-)-Carnitine | C7 H15 N O3 | 161.10499 | 0.859 | 131594238 | 2 | 2 | 8 | 1 | | |
| <input type="checkbox"/> | Acetyl-L-carnitine | C9 H17 N O4 | 203.11558 | 1.334 | 167058234 | 2 | 4 | 0 | 0 | | |
| <input checked="" type="checkbox"/> | DL-Tryptophan | C11 H12 N2 O2 | 204.08974 | 3.119 | 221 | | | | | | |
| <input type="checkbox"/> | L-Tyrosine | C9 H11 N O3 | 181.07382 | 1.625 | 187 | | | | | | |
| <input type="checkbox"/> | DL-Glutamine | C5 H10 N2 O3 | 146.06899 | 0.846 | 47 | | | | | | |
| <input type="checkbox"/> | L-Phenylalanine | C9 H11 N O2 | 165.07892 | 2.578 | 196 | | | | | | |
| <input type="checkbox"/> | L-Valine | C5 H11 N O2 | 117.07878 | 1.187 | 176 | | | | | | |
| <input type="checkbox"/> | Creatine | C4 H9 N3 O2 | 131.06929 | 0.900 | 214 | | | | | | |
| <input type="checkbox"/> | L-Histidine | C6 H9 N3 O2 | 155.06932 | 0.834 | 3 | | | | | | |

Hide Related Tables

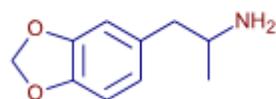
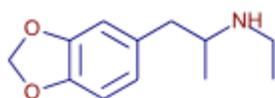
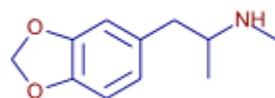
Structure Proposals | Compounds per File | Predicted Compositions | **mzCloud Results** | ChemSpider Results | BioCyc Results | KEGG Pathways | BioCyc P

| Checked | Compound Match | Structure | Name | Formula |
|-------------------------------------|-------------------------------------|-----------|---------------|---------------|
| <input checked="" type="checkbox"/> | <input checked="" type="checkbox"/> | | DL-Tryptophan | C11 H12 N2 O2 |

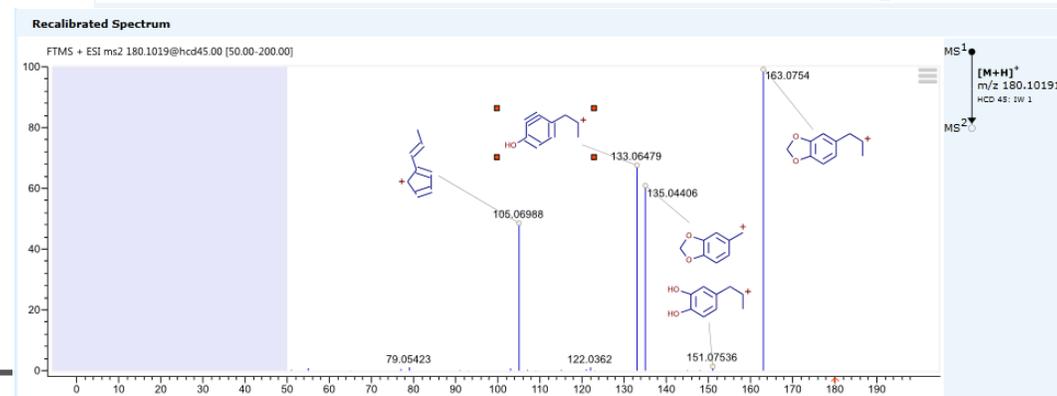
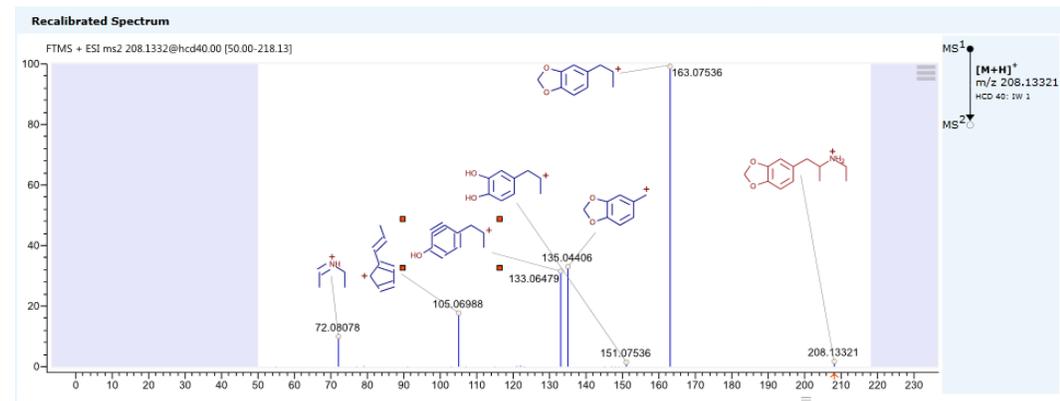
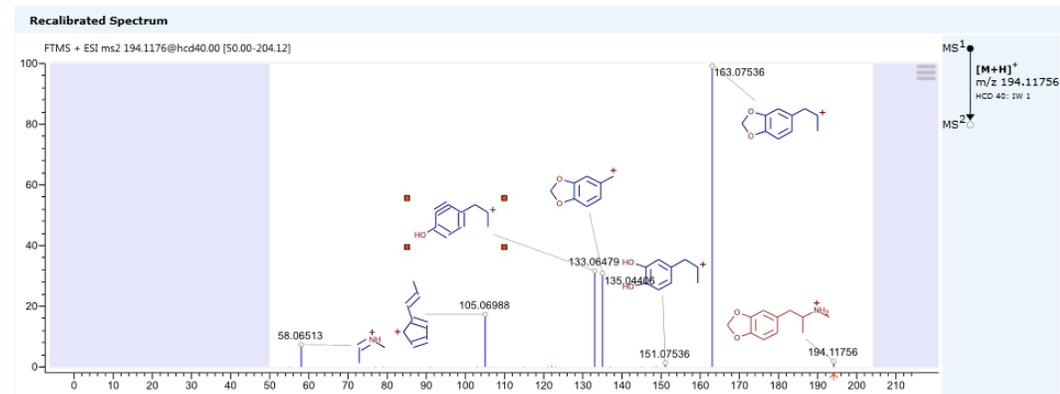


Compound Class Scoring

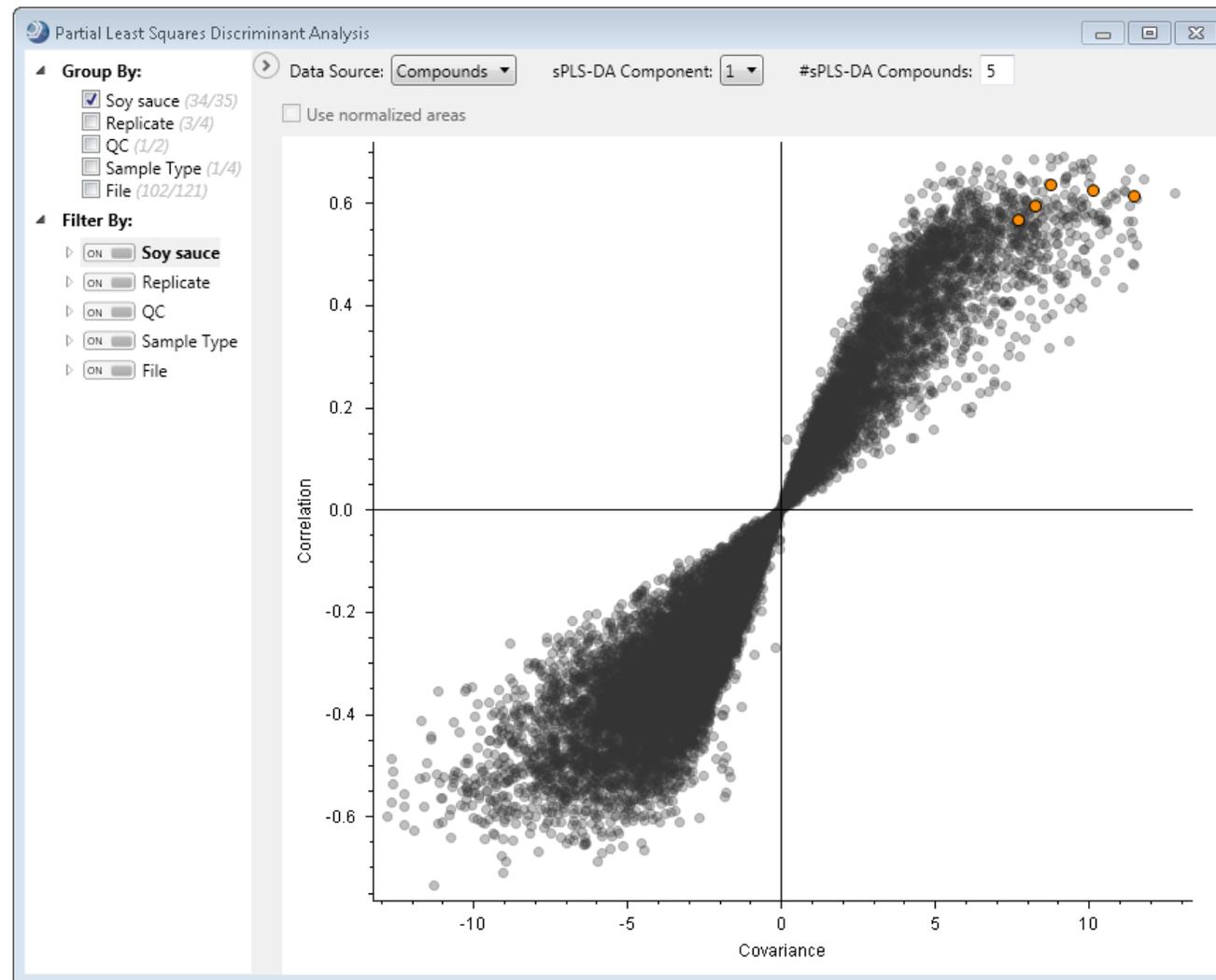
- Detects and scores similarities based on common fragments
- forensic applications
- e.g., detecting new designer drugs



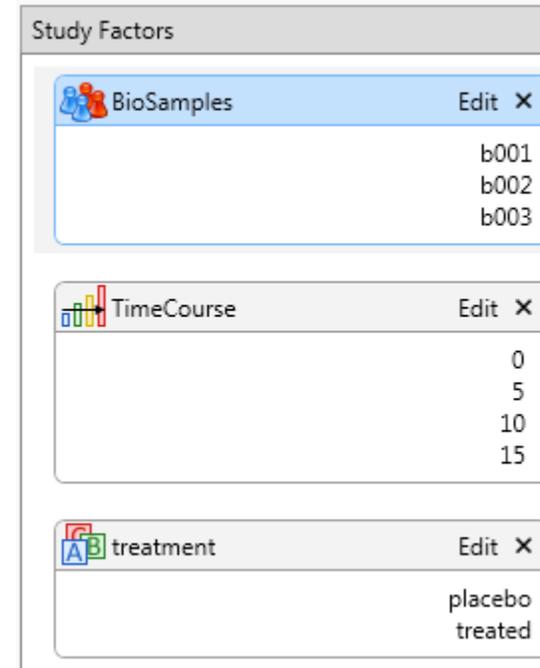
Substituted methylenedioxy-phenethylamines (MDxx)



- PLS – DA
 - Partial Least Squares Discriminant Analysis
 - What are the *compounds* that best describe the differences between the groups?
 - Biomarker discovery



- Support for biological vs. technical replicates
 - New type of study factor
- Support for nested study design
 - Paired tests



Compound Discoverer 2.1 Software - Statistics

- Support for biological vs. technical replicates
 - New type of study factor
- Support for nested study design
 - Paired tests

Generated Sample Groups

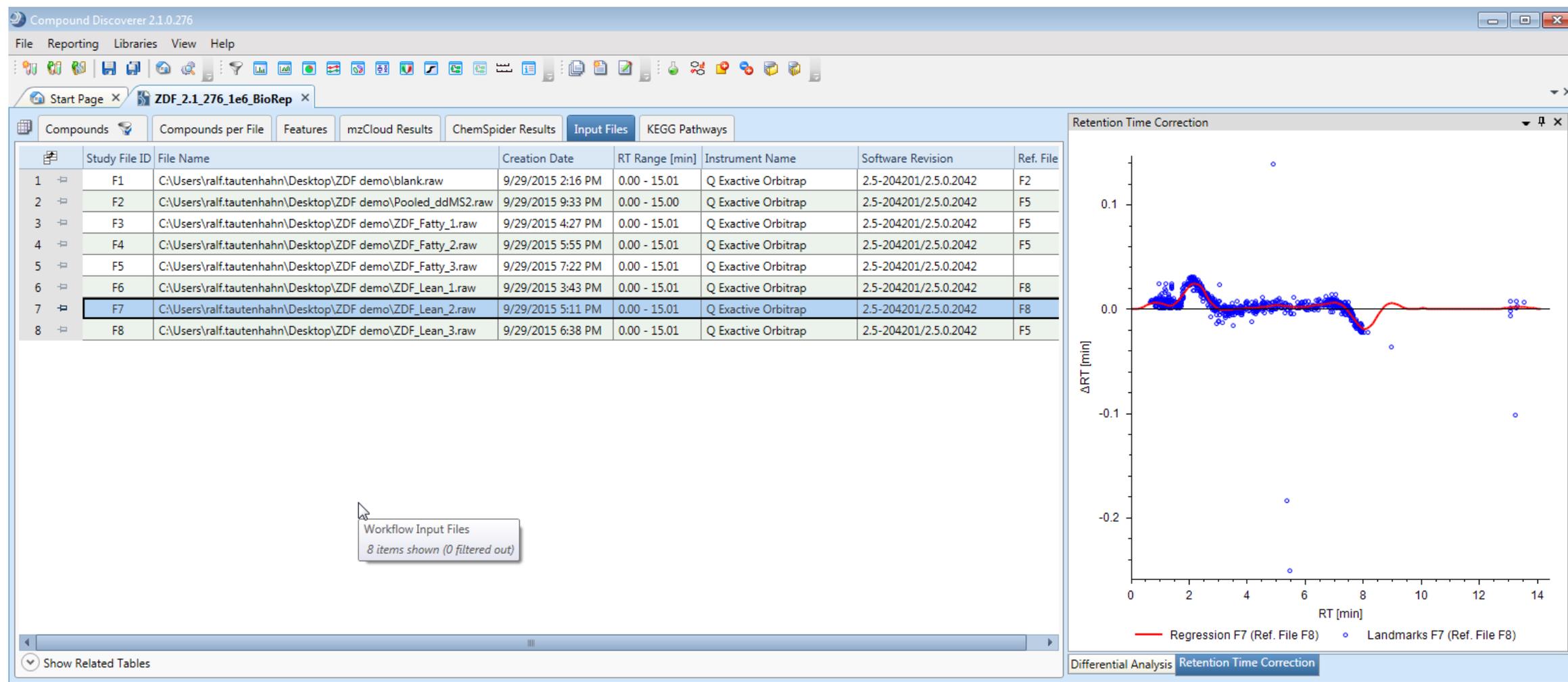
| Group | Sample | Treatment | Replicate | Sample ID | Sample Name |
|-----------|-----------|-----------|-----------|-----------|-------------------------------|
| placebo 0 | Sample | placebo | 0 | b001 | F1: BeerMetabolome1_0minA_01 |
| | Sample | placebo | 0 | b001 | F2: BeerMetabolome1_0minA_02 |
| | Sample | placebo | 0 | b001 | F3: BeerMetabolome1_0minA_03 |
| | Sample | placebo | 0 | b002 | F4: BeerMetabolome1_0minB_02 |
| | Sample | placebo | 0 | b002 | F5: BeerMetabolome1_0minB_03 |
| | Sample | placebo | 0 | b003 | F6: BeerMetabolome1_0minC_01 |
| | Sample | placebo | 0 | b003 | F7: BeerMetabolome1_0minC_02 |
| | Sample | placebo | 0 | b003 | F8: BeerMetabolome1_0minC_03 |
| | treated 0 | Sample | treated | 0 | b001 |
| Sample | | treated | 0 | b001 | F37: BeerMetabolome3_0minA_02 |
| Sample | | treated | 0 | b002 | F38: BeerMetabolome3_0minA_03 |
| Sample | | treated | 0 | b002 | F39: BeerMetabolome3_0minB_01 |
| Sample | | treated | 0 | b003 | F40: BeerMetabolome3_0minB_02 |
| Sample | | treated | 0 | b003 | F41: BeerMetabolome3_0minB_03 |

Generated Ratios (Nested Design)

| Ratio | Treatment | Replicate | Sample ID | Sample Name |
|---------------------------|-----------|-----------|-----------|-------------------------------|
| X treated 0 / placebo 0 | treated | 0 | b001 | F1: BeerMetabolome1_0minA_01 |
| | treated | 0 | b002 | F4: BeerMetabolome1_0minB_02 |
| | treated | 0 | b003 | F6: BeerMetabolome1_0minC_01 |
| X treated 5 / placebo 5 | treated | 5 | b001 | F36: BeerMetabolome3_0minA_01 |
| | treated | 5 | b002 | F38: BeerMetabolome3_0minA_03 |
| | treated | 5 | b003 | F40: BeerMetabolome3_0minB_02 |
| X treated 10 / placebo 10 | treated | 10 | b001 | F36: BeerMetabolome3_0minA_01 |
| | treated | 10 | b002 | F38: BeerMetabolome3_0minA_03 |
| | treated | 10 | b003 | F40: BeerMetabolome3_0minB_02 |
| X treated 15 / placebo 15 | treated | 15 | b001 | F36: BeerMetabolome3_0minA_01 |
| | treated | 15 | b002 | F38: BeerMetabolome3_0minA_03 |
| | treated | 15 | b003 | F40: BeerMetabolome3_0minB_02 |

| Group CV [%] | | | | | | Ratio | | | | Bio. Rep. Ratio | | | | | | | | | | | | | |
|--------------|---|----|---|----|----|-------------------------------|----|-------|-------|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0, placebo* | | | | | | 0, treated / (0, placebo)* | | | | 0, treated, b001 / (0, placebo, b001)* | | | | | | | | | | | | | |
| 0, treated | | | | | | (5, treated) / (5, placebo) | | | | (0, treated, b002) / (0, placebo, b002) | | | | | | | | | | | | | |
| 5, placebo | | | | | | (10, treated) / (10, placebo) | | | | (0, treated, b003) / (0, placebo, b003) | | | | | | | | | | | | | |
| 5, treated | | | | | | (15, treated) / (15, placebo) | | | | (5, treated, b001) / (5, placebo, b001) | | | | | | | | | | | | | |
| 10, placebo | | | | | | | | | | (5, treated, b002) / (5, placebo, b002) | | | | | | | | | | | | | |
| 10, treated | | | | | | | | | | (5, treated, b003) / (5, placebo, b003) | | | | | | | | | | | | | |
| 15, placebo | | | | | | | | | | (10, treated, b001) / (10, placebo, b001) | | | | | | | | | | | | | |
| 15, treated | | | | | | | | | | (10, treated, b002) / (10, placebo, b002) | | | | | | | | | | | | | |
| | | | | | | | | | | (10, treated, b003) / (10, placebo, b003) | | | | | | | | | | | | | |
| | | | | | | | | | | (15, treated, b001) / (15, placebo, b001) | | | | | | | | | | | | | |
| | | | | | | | | | | (15, treated, b002) / (15, placebo, b002) | | | | | | | | | | | | | |
| | | | | | | | | | | (15, treated, b003) / (15, placebo, b003) | | | | | | | | | | | | | |
| 3 | 6 | 41 | 4 | 12 | 6 | 21 | 27 | 0.982 | 0.823 | 0.406 | 0.074 | 0.982 | 1.026 | 0.925 | 1.364 | 0.520 | 0.823 | 0.406 | 0.437 | 0.318 | 0.034 | 0.074 | 0.074 |
| 3 | 6 | 41 | 4 | 12 | 7 | 21 | 27 | 0.982 | 0.822 | 0.442 | 0.075 | 0.982 | 1.027 | 0.924 | 1.365 | 0.521 | 0.822 | 0.442 | 0.470 | 0.337 | 0.034 | 0.075 | 0.075 |
| 3 | 4 | 96 | 4 | 12 | 5 | 21 | 13 | 1.023 | 0.909 | 0.296 | 0.075 | 1.023 | 1.008 | 1.032 | 1.385 | 0.162 | 0.909 | 0.308 | 0.296 | 0.237 | 0.044 | 0.077 | 0.075 |
| 6 | 4 | 55 | 2 | 12 | 10 | 40 | 11 | 1.005 | 0.739 | 0.286 | 0.095 | 1.041 | 0.957 | 1.005 | 1.712 | 0.425 | 0.739 | 0.286 | 0.319 | 0.222 | 0.039 | 0.095 | 0.099 |

Improved Alignment and New RT Correction Plot



Export to Thermo Scientific Xcalibur and TraceFinder Software

| Checked | Name | Formula | Annotation Sc | Mol | Rest | # mzCloud Results | # Kegg Pathways | # BioCyc Pathway |
|--------------------------|--------------------------|----------------|---------------|-----------|-------|-------------------|-----------------|------------------|
| <input type="checkbox"/> | | C8 H20 N6 O2 S | ■ ■ ■ | | 49 | 0 | 8 | |
| <input type="checkbox"/> | TBHQ | C10 H14 O2 | ■ ■ ■ | | 41 | 0 | 4 | |
| <input type="checkbox"/> | TBHQ | C10 H14 O2 | ■ ■ ■ | | 41 | 0 | 4 | |
| <input type="checkbox"/> | Eugenol | C10 H12 O2 | ■ ■ ■ | | 35 | 0 | 4 | |
| <input type="checkbox"/> | Eugenol | C10 H12 O2 | ■ ■ ■ | | 35 | 0 | 4 | |
| <input type="checkbox"/> | (2E)-4-Hydroxy-2-nonenal | C9 H16 O2 | ■ ■ ■ | | 31 | 0 | 0 | |
| <input type="checkbox"/> | Diethylpyrocarbonate | C6 H10 O5 | ■ ■ ■ | | | | | |
| <input type="checkbox"/> | Diethylpyrocarbonate | C6 H10 O5 | ■ ■ ■ | 162.05267 | 0.878 | 5728389 | | |
| <input type="checkbox"/> | veratraldehyde | C9 H10 O3 | ■ ■ ■ | 166.06306 | 2.910 | 761623 | | |
| <input type="checkbox"/> | veratraldehyde | C9 H10 O3 | ■ ■ ■ | 166.06301 | 2.837 | 724028 | | |
| <input type="checkbox"/> | veratraldehyde | C9 H10 O3 | ■ ■ ■ | 166.06303 | 2.669 | 551897 | | |
| | | | | | 28 | 0 | 10 | |

Check All ▶

Uncheck Selected ▶

Uncheck All ▶

Edit Compound Annotation

Clear Compound Annotation

Apply FISh Annotations

Export ▶

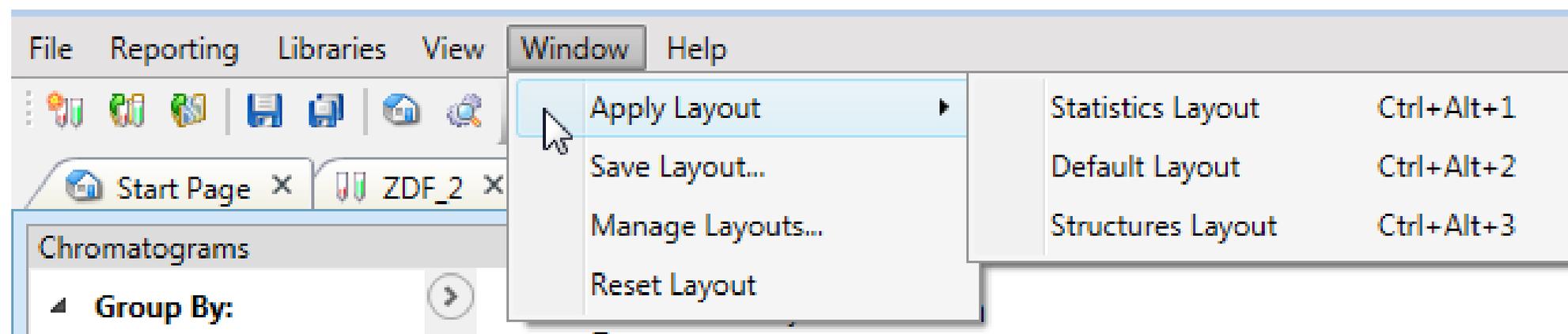
Export to Text File...

Export to Excel...

Export to Xcalibur Inclusion/Exclusion List...

Export to TraceFinder...

Compound Discoverer 2.1 Software – Layouts



The screenshot displays the Compound Discoverer 2.1.0.388 software interface. The top menu bar includes File, Reporting, Libraries, View, Window, and Help. The main workspace is divided into several panels:

- Chromatograms:** Shows a chromatogram with intensity (counts) on the y-axis (0 to 5) and retention time (RT [min]) on the x-axis (1.8 to 2.3). Two peaks are labeled with their retention times: 1.922 and 2.010. The legend indicates three categories: Fatty (blue), Lean (orange), and n/a (green).
- Mass Spectrum:** Shows a mass spectrum with intensity (counts) on the y-axis (0 to 6) and m/z on the x-axis (140 to 260). The title is "ZDF_Fatty_2 (F4) #381, RT=2.010 min, MS1, FTMS (+)". The base peak is at m/z 132.10181. Other significant peaks are labeled at m/z 133.10486, 154.08376, 176.06558, 177.00682, 199.16902, 204.12297, 218.13847, 219.14172, 216.05417, 257.11255, 259.24484, and 263.19623.
- Compounds Table:** A table listing identified compounds with columns for Checked, Name, Formula, Annotation, Molecular Weight, RT [min], Area (Max), # ChemSpider Results, # mzCloud Results, # BioCyc Pathways, # KEGG Pathways, BioCyc Pathways, and KEGG Pathways. The table is sorted by RT [min] in ascending order.

| Checked | Name | Formula | Annotation | Molecular Weight | RT [min] | Area (Max) | # ChemSpider Results | # mzCloud Results | # BioCyc Pathways | # KEGG Pathways | BioCyc Pathways | KEGG Pathways | mz |
|-------------------------------------|--|------------------|------------|------------------|----------|------------|----------------------|-------------------|-------------------|-----------------|-----------------|---------------|----|
| <input type="checkbox"/> | Ethylenediaminetetraacetic acid (EDTA) | C10 H16 N2 O8 | ■ ■ ■ ■ | 292.09007 | 0.940 | 1220352847 | 1 | 2 | 0 | 0 | | | |
| <input type="checkbox"/> | C15 H28 S | | ■ ■ ■ ■ | 240.19066 | 7.086 | 663551286 | 0 | 0 | 0 | 0 | | | |
| <input type="checkbox"/> | Phenyl sulfoxide | C12 H10 O S | ■ ■ ■ ■ | 202.04495 | 0.839 | 315836664 | 1 | 10 | 0 | 0 | | | |
| <input checked="" type="checkbox"/> | Isoleucine | C6 H13 N O2 | ■ ■ ■ ■ | 131.09453 | 2.014 | 273034057 | 18 | 16 | 39 | 21 | | | |
| <input type="checkbox"/> | Betaine | C5 H11 N O2 | ■ ■ ■ ■ | 117.07877 | 0.868 | 272533644 | 14 | 3 | 50 | 23 | | | |
| <input type="checkbox"/> | Ethylenediaminetetraacetic acid (EDTA) | C10 H16 N2 O8 | ■ ■ ■ ■ | 292.09005 | 0.848 | 245497612 | 1 | 1 | 0 | 0 | | | |
| <input type="checkbox"/> | DL-Tryptophan | C11 H12 N2 O2 | ■ ■ ■ ■ | 204.08974 | 3.119 | 221517495 | 12 | 3 | 59 | 22 | | | |
| <input type="checkbox"/> | Creatine | C4 H9 N3 O2 | ■ ■ ■ ■ | 131.06929 | 0.900 | 214570323 | 2 | 2 | 3 | 3 | | | |
| <input type="checkbox"/> | L-Phenylalanine | C9 H11 N O2 | ■ ■ ■ ■ | 165.07892 | 2.578 | 196677505 | 17 | 1 | 46 | 24 | | | |
| <input type="checkbox"/> | Creatinine | C4 H7 N3 O | ■ ■ ■ ■ | 113.05880 | 0.927 | 187929579 | 2 | 0 | 3 | 2 | | | |
| <input type="checkbox"/> | L-Tyrosine | C9 H11 N O3 | ■ ■ ■ ■ | 181.07382 | 1.625 | 187009002 | 17 | 2 | 0 | 0 | | | |
| <input type="checkbox"/> | L-Valine | C5 H11 N O2 | ■ ■ ■ ■ | 117.07878 | 1.187 | 176220368 | 14 | 6 | 50 | 23 | | | |
| <input type="checkbox"/> | Acetyl-L-carnitine | C9 H17 N O4 | ■ ■ ■ ■ | 203.11558 | 1.334 | 167058234 | 2 | 4 | 0 | 0 | | | |
| <input type="checkbox"/> | L-Isoleucine | C6 H13 N O2 | ■ ■ ■ ■ | 131.09453 | 1.926 | 135383791 | 18 | 4 | 39 | 21 | | | |
| <input type="checkbox"/> | Benzene | C6 H6 | ■ ■ ■ ■ | 78.04684 | 2.578 | 134647271 | 1 | 29 | 2 | 4 | | | |
| <input type="checkbox"/> | 3-Methylsulfolene | C5 H8 O2 S | ■ ■ ■ ■ | 132.02440 | 1.362 | 134209264 | 2 | 12 | 0 | 0 | | | |
| <input type="checkbox"/> | L(-)-Carnitine | C7 H15 N O3 | ■ ■ ■ ■ | 161.10499 | 0.859 | 131594238 | 2 | 2 | 8 | 1 | | | |
| <input type="checkbox"/> | Triadimefon | C14 H16 Cl N3 O2 | ■ ■ ■ ■ | 293.09259 | 0.934 | 129208301 | 2 | 0 | 0 | 0 | | | |
| <input type="checkbox"/> | L(-)-Methionine | C5 H11 N O2 S | ■ ■ ■ ■ | 149.05093 | 1.535 | 103824776 | 7 | 1 | 96 | 14 | | | |
| <input type="checkbox"/> | [Similar to: Fluoxymesterone; ΔMass: 56.0270 Da] | C12 H30 N2 O P2 | ■ ■ ■ ■ | 280.18306 | 7.266 | 102014803 | 0 | 38 | 0 | 0 | | | |
| <input type="checkbox"/> | Piperidine | C5 H11 N | ■ ■ ■ ■ | 85.08903 | 2.015 | 93672219 | 1 | 0 | 0 | 2 | | | |
| <input type="checkbox"/> | Dibutyl malate | C12 H22 O5 | ■ ■ ■ ■ | 246.14650 | 6.735 | 86177357 | 2 | 25 | 0 | 0 | | | |
| <input type="checkbox"/> | [Similar to: N-Acetyl-L-cysteine; ΔMass: 59.0344 Da] | | ■ ■ ■ ■ | 103.99588 | 0.713 | 69984429 | 0 | 2 | 0 | 0 | | | |

Compound Discoverer 2.1.0.388

File Reporting Libraries View Window Help

Start Page X ZDF_2 X Job Queue X Configuration X ZDF_b388_1e6_BC-(3) X

Compounds BioCyc Results Input Files KEGG Pathways BioCyc Pathways

| Checked | Name | Formula | Annotation Sc | Molecular Weight | RT [min] | Area (Max) | Group Areas | Group CV [%] | Ratio | Log2 Fold Change | P-value | Adj. P-value | mzCloud Best Match | mzCloud Best Sim. Match | # BioCyc Pathways | # KEGG Pathways |
|--------------------------|--------------------|---------------|---------------|------------------|----------|------------|---------------|--------------|-------|------------------|---------|--------------|--------------------|-------------------------|-------------------|-----------------|
| <input type="checkbox"/> | Isoleucine | C6 H13 N O2 | ■■■■■ | 131.09453 | 2.014 | 273034057 | 2.59e8 1.49e8 | 17 11 | 1.735 | 0.79 | 2.8e-2 | 1.4e-1 | 99.9 | 98.7 | 39 | 21 |
| <input type="checkbox"/> | L(-)-Carnitine | C7 H15 N O3 | ■■■■■ | 161.10499 | 0.859 | 131594238 | 7.90e7 7.37e7 | 60 24 | 1.072 | 0.10 | 9.8e-1 | 9.9e-1 | 98.7 | 98.1 | 8 | 1 |
| <input type="checkbox"/> | Acetyl-L-carnitine | C9 H17 N O4 | ■■■■■ | 203.11558 | 1.334 | 167058234 | 1.51e8 9.40e7 | 19 11 | 1.609 | 0.69 | 5.0e-2 | 2.0e-1 | 98.1 | 98.0 | 0 | 0 |
| <input type="checkbox"/> | DL-Tryptophan | C11 H12 N2 O2 | ■■■■■ | 204.08974 | 3.119 | 221517495 | 1.75e8 2.09e8 | 2 9 | 0.836 | -0.26 | 8.0e-2 | 2.6e-1 | 98.0 | 97.7 | 59 | 22 |
| <input type="checkbox"/> | L-Tyrosine | C9 H11 N O3 | ■■■■■ | 181.07382 | 1.625 | 187009002 | 1.29e8 1.69e8 | 18 8 | 0.761 | -0.39 | 6.3e-2 | 2.3e-1 | 97.7 | 97.6 | 0 | 0 |
| <input type="checkbox"/> | DL-Glutamine | C5 H10 N2 O3 | ■■■■■ | 105.04240 | 0.841 | 32328674 | 2.23e7 2.44e7 | 21 17 | 0.911 | -0.14 | 3.8e-1 | 6.3e-1 | 97.6 | 97.5 | 68 | 24 |
| <input type="checkbox"/> | DL-Glutamine | C5 H10 N2 O3 | ■■■■■ | 146.06899 | 0.846 | 47344955 | 3.28e7 3.66e7 | 18 17 | 0.896 | -0.16 | 4.4e-1 | 6.6e-1 | 97.6 | 97.4 | 109 | 21 |
| <input type="checkbox"/> | L-Phenylalanine | C9 H11 N O2 | ■■■■■ | 165.07892 | 2.578 | 196677505 | 1.89e8 1.45e8 | 9 9 | 1.303 | 0.38 | 4.8e-2 | 1.9e-1 | 97.5 | 97.4 | 46 | 24 |
| <input type="checkbox"/> | L-Valine | C5 H11 N O2 | ■■■■■ | 117.07878 | 1.187 | 176220368 | 1.76e8 1.01e8 | 15 8 | 1.740 | 0.80 | 1.8e-2 | 1.1e-1 | 97.4 | 96.8 | 50 | 23 |
| <input type="checkbox"/> | Creatine | C4 H9 N3 O2 | ■■■■■ | 131.06929 | 0.900 | 214570323 | 2.10e8 6.57e7 | 20 17 | 3.196 | 1.68 | 2.8e-3 | 5.4e-2 | 96.8 | 96.7 | 3 | 3 |
| <input type="checkbox"/> | L-Histidine | C6 H9 N3 O2 | ■■■■■ | 155.06932 | 0.834 | 3887296 | 2.08e6 3.25e6 | 14 21 | 0.640 | -0.64 | 5.9e-2 | 2.2e-1 | 96.7 | 96.4 | 19 | 11 |
| <input type="checkbox"/> | Propionylcarnitine | C10 H19 N O4 | ■■■■■ | 217.13119 | 2.010 | 34957470 | 2.99e7 1.86e7 | 38 13 | 1.612 | 0.69 | 2.9e-1 | 5.5e-1 | 96.4 | | 0 | 0 |

Show Related Tables

Differential Analysis

Data Source: Compounds

Comparison: Fatty vs. Lean

P-value: 0.001 Log2 Fold Change: 3

7 ↓ (21 ≤ PV, 35 ≤ -FC) 37 ↑ (86 ≤ PV, 177 ≥ FC)

Trend Chart Differential Analysis

Principal Component Analysis

Data Source: Compounds X Data: PC 1 Y Data: PC 2

Color By: Phenotype (2/3) Sample Type (1/2) File (6/7)

Filter By: Phenotype Sample Type File

Scores Plot Loadings Plot Variances Plot

Principal Component Analysis Partial Least Squares Discriminant Analysis