# Results – Detailed Report

# -

Report Name:

Generated by

# Data Files

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  | | --- | --- | | **MS Sample** | | | Data File: |  | | Folder: |  | | Injection: |  | | |  |  | | --- | --- | | **MS Control #1** | | | Data File: |  | | Folder: |  | | Injection: |  | |
| |  |  | | --- | --- | | **MS Control #2** | | | Data File: |  | | Folder: |  | | Injection: |  | | |  |  | | --- | --- | | **MS Control #3** | | | Data File: |  | | Folder: |  | | Injection: |  | |
| |  |  | | --- | --- | | **MS Control #4** | | | Data File: |  | | Folder: |  | | Injection: |  | | |  |  | | --- | --- | | **MS Control #5** | | | Data File: |  | | Folder: |  | | Injection: |  | |

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  | | --- | --- | | **Analog Sample** | | | Data File: |  | | Folder: |  | | Injection: |  | | Channel: |  | | |  |  | | --- | --- | | **Analog Control #1** | | | Data File: |  | | Folder: |  | | Injection: |  | | Channel: |  | |
| |  |  | | --- | --- | | **Analog Control #2** | | | Data File: |  | | Folder: |  | | Injection: |  | | Channel: |  | | |  |  | | --- | --- | | **Analog Control #3** | | | Data File: |  | | Folder: |  | | Injection: |  | | Channel: |  | |
| |  |  | | --- | --- | | **Analog Control #4** | | | Data File: |  | | Folder: |  | | Injection: |  | | Channel: |  | | |  |  | | --- | --- | | **Analog Control #5** | | | Data File: |  | | Folder: |  | | Injection: |  | | Channel: |  | |

|  |  |
| --- | --- |
| **Additional MS/MS Data** | |
| Data File: |  |
| Folder: |  |
| Injection: |  |

Dedicated MS/MS Data

# Potential Metabolites

None

| **Report** | **Peak ID** | **Name** | **Formula** | **Assigned** | **Neutral Mass** | ***m/z*** | **Charge** | **Peak Index** | **ppm** | **R.T. (min)** | **Peak Area** | **% Area** | **% Score** | **Peak Area – Analog** | **% Area – Analog** | **R.T. (min) - Analog** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |

## Metabolite Chromatogram

## 

## Isotope Pattern Chromatogram



Analog Chromatogram



# Metabolite Details

None

|  |  |
| --- | --- |
| *-* | |
| Formula: |  |
| RT: | min |
| *m/z*: |  |
| ppm: |  |
| Score: | % |

## Metabolite XIC



## Mass Defect Chromatogram



## Product Ions Chromatogram



## Neutral Losses Chromatogram



Fragment Isotope Pattern Chromatogram



## MS Spectrum



## ***MS/MS Spectrum***

***Chart, line chart

Description automatically generated***

### Common Product Ions (m/z):

### Common Neutral Losses

| **Loss (Da)** | **Metabolite *m/z*** |
| --- | --- |
|  |  |

Additional MS/MS Spectrum

Chart, line chart

Description automatically generated

**Common Product Ions (m/z):**

### Common Neutral Losses

| **Loss (Da)** | **Metabolite *m/z*** |
| --- | --- |
|  |  |

# Processing Parameters

## Compound Information

|  |  |
| --- | --- |
| Compound name: |  |
| Chemical formula: |  |
| Isotopic enrichment: |  |
| Adduct: |  |
| Charge State: | From: To: |
| *m/z*: |  |

## Structure



## Peak Finding Strategy

The following algorithms were used:

|  |  |
| --- | --- |
| TOF MS   * Predicted metabolites * Generic peak finding   + Mass Defect Filter   + Charge State Filter * Mass defect * Isotope pattern | TOF MSMS   * Characteristic product ions   + Find all specified ions   + Find at least ions * Characteristic neutral losses   + Find all specified losses   + Find at least losses * Internal Neutral Losses * Isotope Pattern (SWATH only) |

## Generic Parameters

### Biotransformations (Set used: )

| **Name** | **Mass Shift** | **Description** |
| --- | --- | --- |
|  |  |  |

### Chromatographic Data

*Chromatographic Peak*

Retention time window: to min

|  |  |  |
| --- | --- | --- |
|  | **MS Data** | **Analog Data** |
| XIC Width: Use mDaAutomatic | Wavelength (UV only): to nm  Time offset from MS: min |
| LC Peak Separation |  |  |
| Minimum peak width | sec. | sec. |
| Minimum peak intensity | |  |  | | --- | --- | | TOF MS: | cps | | TOF MSMS: | cps | |  |
| Use smoothing |  |  |
| Sample-control offset | min | min |
| Sample/control ratio | times greater than control signal |  |

### MS Parameters

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  | | --- | --- | | *m/z Tolerance* |  | | MS m/z Tolerance: |  | | Minimum MS peak intensity: |  | |  |  | | *Isotope Pattern Tolerances* |  | | Intensity tolerance: | % | | MS m/z tolerance: | mDa | |  |  | | *Limits* |  | | Maximum number of unexpected metabolites: |  | | Mass range window (*m/z*): to | | | *Generic LC/MS Peak Finding*  Perform background subtraction:  *Chosen Adducts*   | **Ion Type** | **Charge** | **Radical** | | --- | --- | --- | |  |  |  | |

### MS/MS Parameters

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  | | --- | --- | | *MS/MS Finding* |  | | MS/MS m/z tolerance: | mDa | | Minimum MS/MS peak intensity: | cps | |  |  | | *MS/MS Isotope Finding* |  | | Intensity tolerance: | % | | MS/MS m/z tolerance: | mDa | |  |  | | *Source of Reference MS/MS Spectrum* |  | |  |  | | *MS/MS Spectrum* |  | | Use advanced MS/MS filter: |  | | Advanced MS/MS filter value: |  | | |  |  |  | | --- | --- | --- | | *Similarity and Fragment Interpretation* | |  | | MS/MS m/z tolerance: |  | | |  |  |  | | *Fragment Interpretation Options* | CID Values: | EAD Values: | | Minimum signal-to-noise ratio: |  |  | | Number of fragment peaks  selected for assignment |  |  | | Break aromatic rings |  |  | | Maximum number of bonds to break: |  |  | | Maximum number of C-C bonds to break: |  |  | |

### Formula Prediction

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  | | --- | --- | | *Search Constraints* |  | | Elements from: |  | | Elements to: |  | |  |  | | *Isotope Pattern Tolerance* |  | | Intensity tolerance: | % | | MS m/z tolerance: | ppm | |  |  | | *Ranking* |  | | Contribution  (from MS to MS/MS data): |  | | Automatically weight MS/MS |  | | |  |  | | --- | --- | | *Rings and Double Bonds* |  | | RDB from: |  | | RDB to: |  | |  |  | | *Element Ratios* |  | | Oxygen/phosphorus count: | >= | | Oxygen/sulphur count: | >= | |

## Confirmation Scoring

| **Property** | **Maximum Score** |
| --- | --- |
| Mass defect |  |
| Isotope pattern |  |
| MS/MS |  |
| Mass accuracy |  |
| *Total confirmation score* |  |

## Compound-Specific Parameters

### Cleavage Metabolites

Maximum bonds to break:

Break ring bonds:

Only break C-N bonds:

The table of selected cleavage metabolites exceeds 200 rows. To view the table, please refer to the processing method via the software.

Selected Cleavage Metabolites:

| **Loss From Parent** | **Formula** | **#CleavageMetaboliteHeader#** | **#CleavageMetaboliteHeader#** | **#CleavageMetaboliteHeader#** | **#CleavageMetaboliteHeader#** | **#CleavageMetaboliteHeader#** |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | #CleavageMetaboliteField# | #CleavageMetaboliteField# | #CleavageMetaboliteField# | #CleavageMetaboliteField# | #CleavageMetaboliteField# |

| **Loss From Parent** | **Formula** | **#CleavageMetaboliteHeader#** | **#CleavageMetaboliteHeader#** | **#CleavageMetaboliteHeader#** | **#CleavageMetaboliteHeader#** | **#CleavageMetaboliteHeader#** |
| --- | --- | --- | --- | --- | --- | --- |
|  |  | #CleavageMetaboliteField# | #CleavageMetaboliteField# | #CleavageMetaboliteField# | #CleavageMetaboliteField# | #CleavageMetaboliteField# |

### Mass Defect

| **Name** | **Formula** | ***m/z*** | **Defect** | **Mass Defect Window (mDa)** | | **Mass Range** | |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Below** | **Above** | **From *m/z*** | **To *m/z*** |
|  |  |  |  |  |  |  |  |

### Isotope Pattern

****

Isotopes

| ***m/z*** | **Intensity (%)** | **Mass Offset** |
| --- | --- | --- |
|  |  |  |

|  |
| --- |
| Intensity tolerance: % |
| MS *m/z* tolerance: mDa |

Isotope Enrichment

| **Element** | **Enrichment (%)** |
| --- | --- |
|  |  |

### CID Product Ions and Neutral Losses

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Reference MS/MS spectrum: | *Filters*   |  |  |  | | --- | --- | --- | |  | **From** | **To** | | **m/z** |  |  | | **Charge State** |  |  |   Show only product ions above: %  Mass accuracy within: mDa |
|  |
| Add product ions, neutral losses from Phase II metabolites: |

| **m/z** | **Z** | **Formula** | **Error** | **Neutral Loss** | **PI** | **NL** | **IP** |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |

### EAD Product Ions and Neutral Losses

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Reference MS/MS spectrum: | *Filters*   |  |  |  | | --- | --- | --- | |  | **From** | **To** | | **m/z** |  |  | | **Charge State** |  |  |   Show only product ions above: %  Mass accuracy within: mDa |
|  |
| Add product ions, neutral losses from Phase II metabolites: |

| **m/z** | **Z** | **Formula** | **Error** | **Neutral Loss** | **PI** | **NL** | **IP** |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |  |  |