# Interpretation – Detailed Report

# -

Report Name:

Generated by

# Compound Information

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

# Structure



# 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



# Interpretation Results

No interpretation data

## –

|  |  |
| --- | --- |
| Formula: |  |
| ppm: |  |
| RDB: |  |

### Applied Metabolite Structure

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | |  |  | | --- | --- | | Composition: |  | | Mass: |  | |

|  |  |
| --- | --- |
| MS/MS No spectrum  Shape  Description automatically generated with low confidence | Reference MS/MS No spectrum  Shape  Description automatically generated with low confidence |

**Common product ions (m/z)**:

**Peaks selected for assignment (m/z)**:

### Metabolite Options

|  |  |
| --- | --- |
| Number of fragment peaks selected for assignment: |  |
| Minimum signal-to-noise ratio: |  |
| MS/MS m/z tolerance: |  |
| *Fragmentation Settings* |  |
| Break aromatic rings: |  |
| Maximum number of bonds to break: |  |
| Maximum number of C-C bonds to break: |  |
| *Label Settings* |  |
| Label peaks with: |  |

|  |  |
| --- | --- |
| Additional MS/MS No spectrum  Shape  Description automatically generated with low confidence | Additional Reference MS/MS No spectrum  Shape  Description automatically generated with low confidence |

**Common product ions (m/z)**:

**Peaks selected for assignment (m/z)**:

### Metabolite Options

|  |  |
| --- | --- |
| Number of fragment peaks selected for assignment: |  |
| Minimum signal-to-noise ratio: |  |
| MS/MS m/z tolerance: |  |
| *Fragmentation Settings* |  |
| Break aromatic rings: |  |
| Maximum number of bonds to break: |  |
| Maximum number of C-C bonds to break: |  |
| *Label Settings* |  |
| Label peaks with: |  |

### Fragment Filters

None

|  |  |
| --- | --- |
| RDB | Integer value (even-electron)Non-integer value (odd-electron) |
| Mass Range (m/z) | To |
| Mass Accuracy within |  |
| Intensity above | cps |
| Score above |  |
| Fragments with assigned structures |  |

**Fragment Details**

No Structures Assigned

| **Fragment Details** | **Structure Details** |
| --- | --- |
| |  |  | | --- | --- | | Mass (m/z): |  | | Ion Formula: |  | | Error (): |  | | Intensity (cps): |  | | RDB: |  | | Score: |  | | Fragmentation Type: |  | | |  |  |  |  |  |  |  |  |  |  |  |  | | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | |  | |  |  | | --- | --- | | Selected: |  | | Mass: |  | | Broken Bonds: |  | | Delta H: |  | | Score: |  | |   **Contained Neutral Losses**  No contained neutral losses   |  |  | | --- | --- | | **Mass** | **Formula** | |  |  | |