# Interpretation – Detailed Report

# -

Report Name:

Generated by

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

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Antibody Information  |  |  |  | | --- | --- | --- | | Enzyme: |  |  | | Break disulfide bonds: |  |  | | Site of conjugation: |  |  | | Type of conjugation: |  |  | | Maximum AA count: |  |  |  |  |  | | --- | --- | | Custom Amino Acids: |  | | Custom Modifications: |  | | Protein Sequence |

# 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: |  | |

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  | | --- | --- | | **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: |  | |

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: |  |

### Applied Metabolite Structure

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

### Applied Metabolite Sequence

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

|  |  |
| --- | --- |
| Metabolite MS/MS No spectrum | Parent MS/MS No spectrum |

**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: |  |
| *Structure Fragment Settings* |  |
| Break aromatic rings: |  |
| Maximum number of bonds to break: |  |
| Maximum number of C-C bonds to break: |  |
| *Sequence Fragment Settings* |  |
| Fragment Types: | None |
| Maximum number of bonds to break: |  |
| Break Linkages: |  |
| *Label Settings* |  |
| Label peaks with: |  |

### Fragment Filters

None

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

**Structure Fragment Details**

None

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

**Sequence Fragment Details**

None

| **Mass (m/z)** | **Sequence** | **Ion** | **Charge** | **Error ()** | **Intensity (cps)** |
| --- | --- | --- | --- | --- | --- |
|  |  |  |  |  |  |