

ProteinDeconvolution Report

Created: 24/02/2021 11:48:54

Sample Information

| | |
|-----------------------|---|
| Original File Name | C:\Xcalibur\Data\20210224_AA_QF_QBN.raw |
| Instrument Method | C:\Xcalibur\methods\Current Orbitrap Methods\Orbi_IntactFlowInjLR_01fast.meth |
| Vial | GE7 |
| Injection Volume (µL) | 1 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 1 |

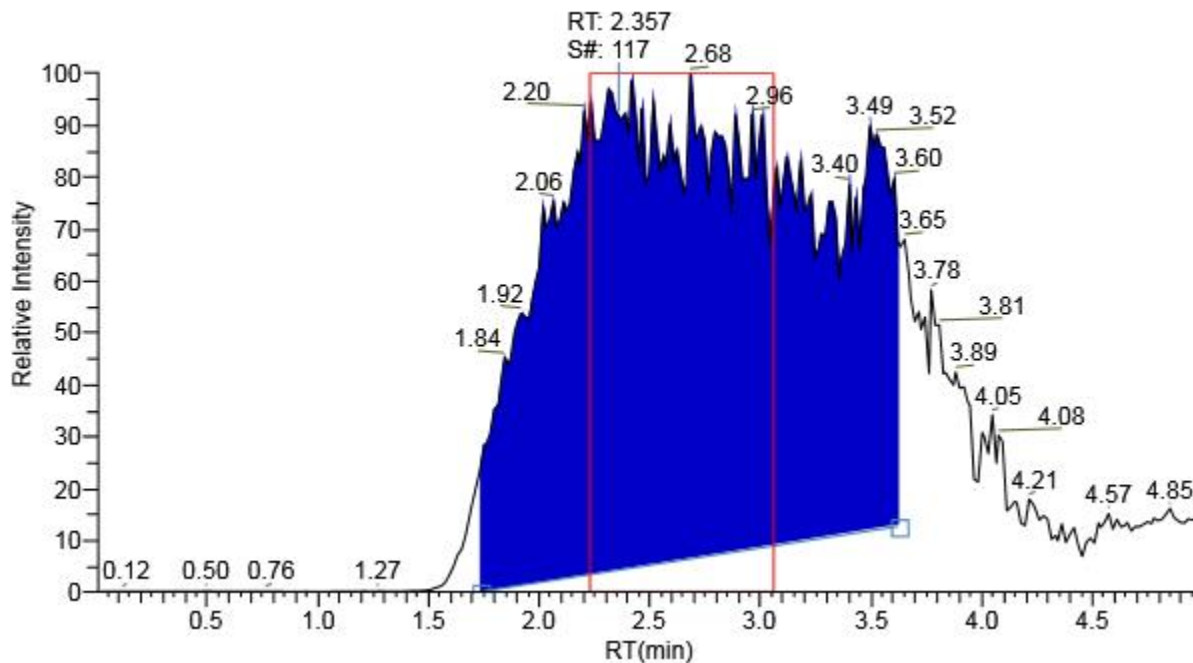
Chromatogram Parameters

| | |
|------------------------------|-----------------------|
| Use restricted time. | False |
| Time Range | 0.003 - 4.992 Minutes |
| Rel. Intensity Threshold (%) | 1 |
| Type | Unknown |
| Sensitivity | High |
| Chromatogram m/z Range | 1000 - 2000 |
| Use Auto Spectral Averaging | False |

Source Chromatogram

20210224_AA_QF_QBN ProteinDeconvolution NL: 1.71E7

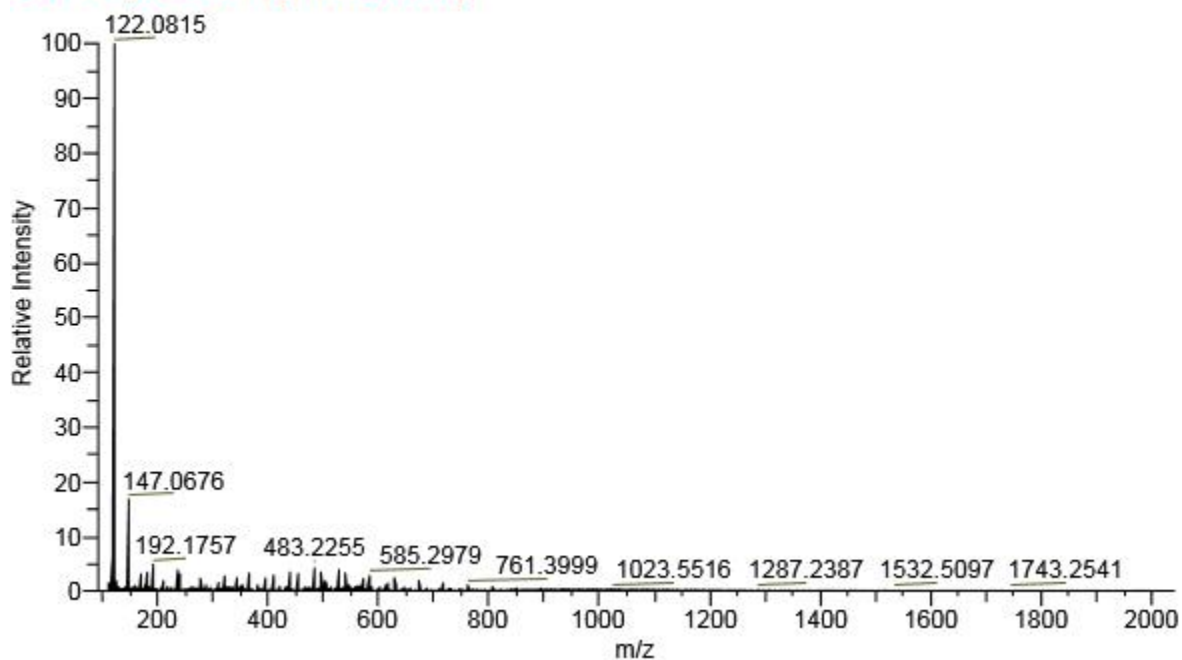
F:

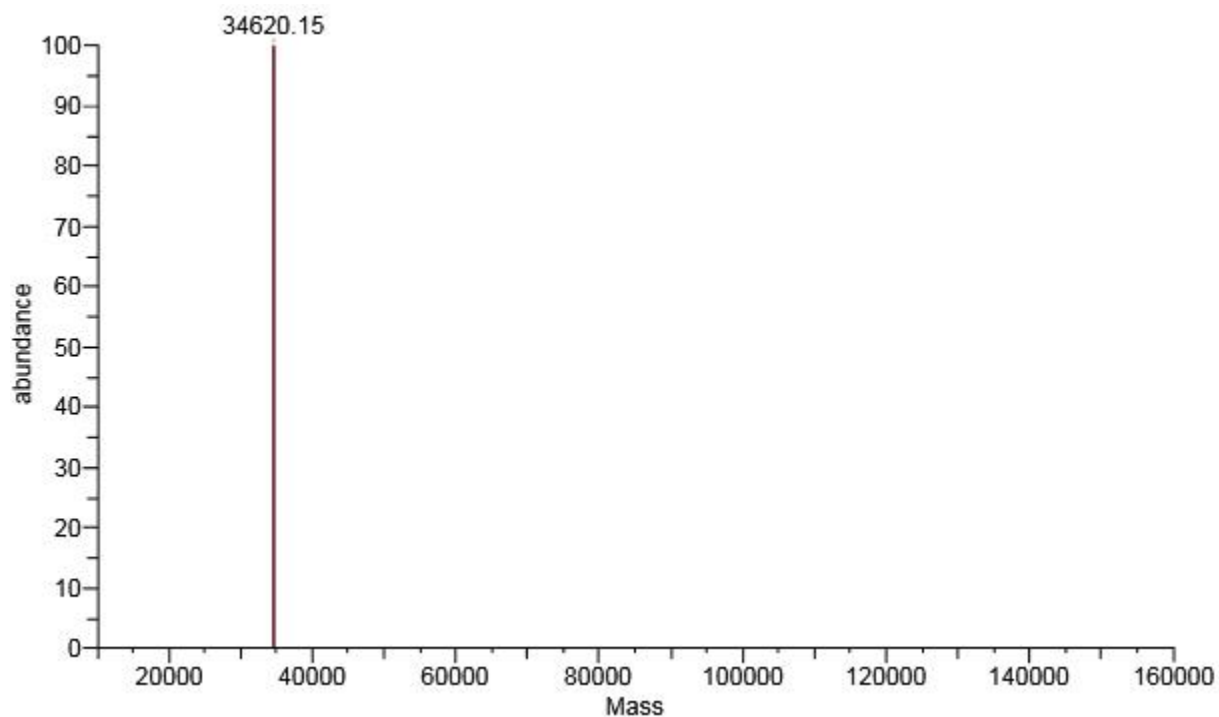


| Main Parameters (ReSpect™) | |
|----------------------------------|-----------------------|
| Negative Charge | False |
| Minimum Adjacent Charges | 6 - 10 |
| Noise Rejection | 95% Confidence |
| Rel. Abundance Threshold (%) | 0 |
| Calculate XIC | True |
| Quality Score Threshold | 0 |
| m/z Range | 750 - 2000 |
| Output Mass Range | 10000 - 160000 |
| Mass Tolerance | 20 ppm |
| Target Mass | 15000 Da |
| Charge State Range | 5 - 100 |
| Choice of Peak Model | Intact Protein |
| Advanced Parameters (ReSpect™) | |
| Minimum Peak Significance | 1 |
| Use Relative Intensities | True |
| Peak Width | 0 |
| Feature Width | 0 |
| Degree of Fit | 0 |
| Number of Iterations | 3 |
| Noise Compensation | True |
| Charge Carrier | H+ (1.00727663) |
| Number of Peak Models | 1 |
| Resolution at 400 m/z | 15000 |
| Left/Right Peak Shape | 2:2 |
| Sliding Window Parameters | |
| Use Sliding Window | False |
| RT Range | 0.003 - 4.992 Minutes |
| Target Avg Spectrum Width | 0.1 Minutes |
| Target Avg Spectrum Offset (%) | 50 |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 Minutes |
| Min Num of Detected Intervals | 3 |

20210224_AA_QF_QBN #109-162 RT:2.233-3.057 AV:54

F:FTMS + p NSI Full ms [110.00-2000.00]





| ReSpect Masses Table | | | | | | | | | | |
|----------------------|-----------|-------------------------|--------------|-------------|------------|--------------------|----------------------|-------------|---------|---------|
| Average Mass | Intensity | Number of Charge States | Mass Std Dev | PPM Std Dev | Delta Mass | Relative Abundance | Fractional Abundance | RT Range | Apex RT | Score |
| 34620.15 | 934900.56 | 13 | 1.62 | 46.84 | 0.00 | 100.0000 | 100.0000 | 2.233-3.057 | 2.295 | 76.4000 |