# Direct mass spectrometry analysis of protein complexes and intact proteins up to >70 kDa from tissue

Rian L. Griffiths[1#], Albert Konijnenberg[2], Rosa Viner[3] and Helen J. Cooper[1]*

[1]School of Biosciences, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK.

[2]Thermo Fisher Scientific, Achtseweg Noord 5, 5651 GG Eindhoven, The Netherlands

[3]Thermo Fisher Scientific, River Oaks Parkway 355, San Jose, 95134, California, U.S.A

#Current address: School of Pharmacy, University of Nottingham, University Park, Nottingham NG7 2RD, UK.

*To whom correspondence should be addressed: h.j.cooper@bham.ac.uk

**Supplementary Information:**

**Supplemental Figure 1.** Comparison of deconvoluted native LESA mass spectra from **A)** two separate cerebellum locations sampled with 10 mM ammonium acetate, 5% MeOH; **B)** two separate cerebellum locations sampled with 10 mM ammonium acetate, 0.125% C8E4; **C)** two separate cerebellum locations one sampled with 10 mM ammonium acetate, 5% MeOH and one with 10 mM ammonium acetate, 0.125% C8E4; **D)** one cerebellum location and one cerebral cortex location sampled with 10 mM ammonium acetate, 0.125% C8E4; **E)** two separate medulla (kidney) locations one sampled with 10 mM ammonium acetate, 0.125% C8E4; **F)** one medulla (kidney) location and one cortex (kidney) location sampled with 10 mM ammonium acetate, 0.125% C8E4.

**Supplemental Figure 2.** Native LESA MS of rat brain tissue. A) Sampling location: cerebral cortex. LESA extraction/ionisation solvent: 10 mM ammonium acetate, 5% MeOH. B) Detail from main figure 1C. Sampling location cerebral cortex. LESA extraction/ionisation solvent: 10 mM ammonium acetate, 0.125% C8E4.

**Supplemental Figure 3.** Native LESA MS of rat kidney tissue. Sampling location: outer cortex. LESA extraction/ionisation solvent: 10 mM ammonium acetate, 5% MeOH.

**Supplemental Figure 4.** Native LESA HCD MS/MS of rat kidney tissue. Sampling location: outer cortex. LESA extraction/ionisation solvent: 10 mM ammonium acetate, 5% MeOH. HCD energy = 80%.

**Supplemental File 1:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 1A. (Cerebellum, 10 mM ammonium acetate, 5% MeOH).

**Supplemental File 2:** Biopharma Finder search parameters and outputs for LESA mass spectrum obtained from separate cerebellum location (Cerebellum, 10 mM ammonium acetate, 5% MeOH).

**Supplemental File 3:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 1B. (Cerebellum, 10 mM ammonium acetate, 0.125% C8E4).

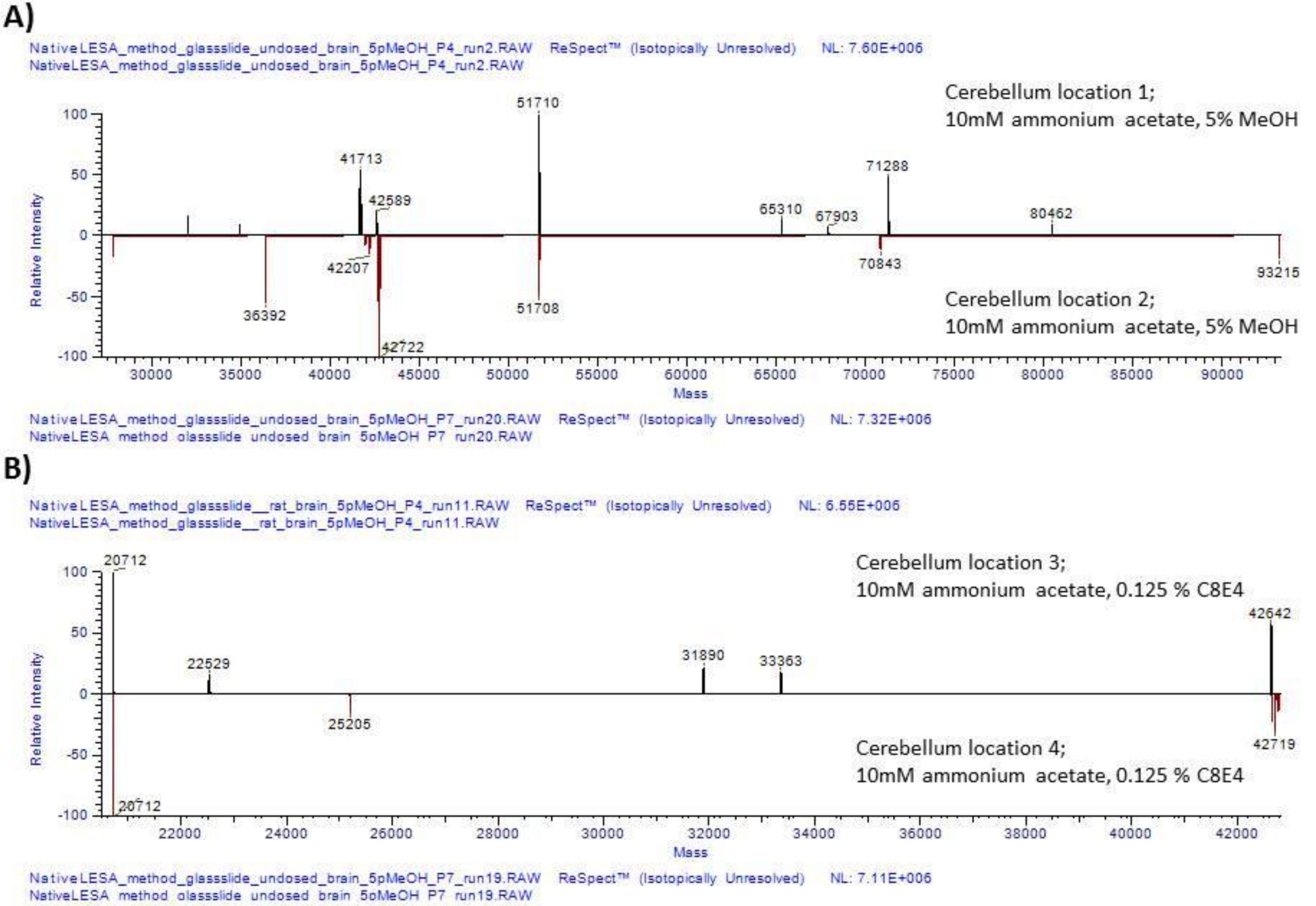
**Supplemental File 4:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 1C. (Cerebral cortex, 10 mM ammonium acetate, 0.125% C8E4).

**Supplemental File 5:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 2A. (Kidney outer cortex, 10 mM ammonium acetate, 0.125% C8E4).

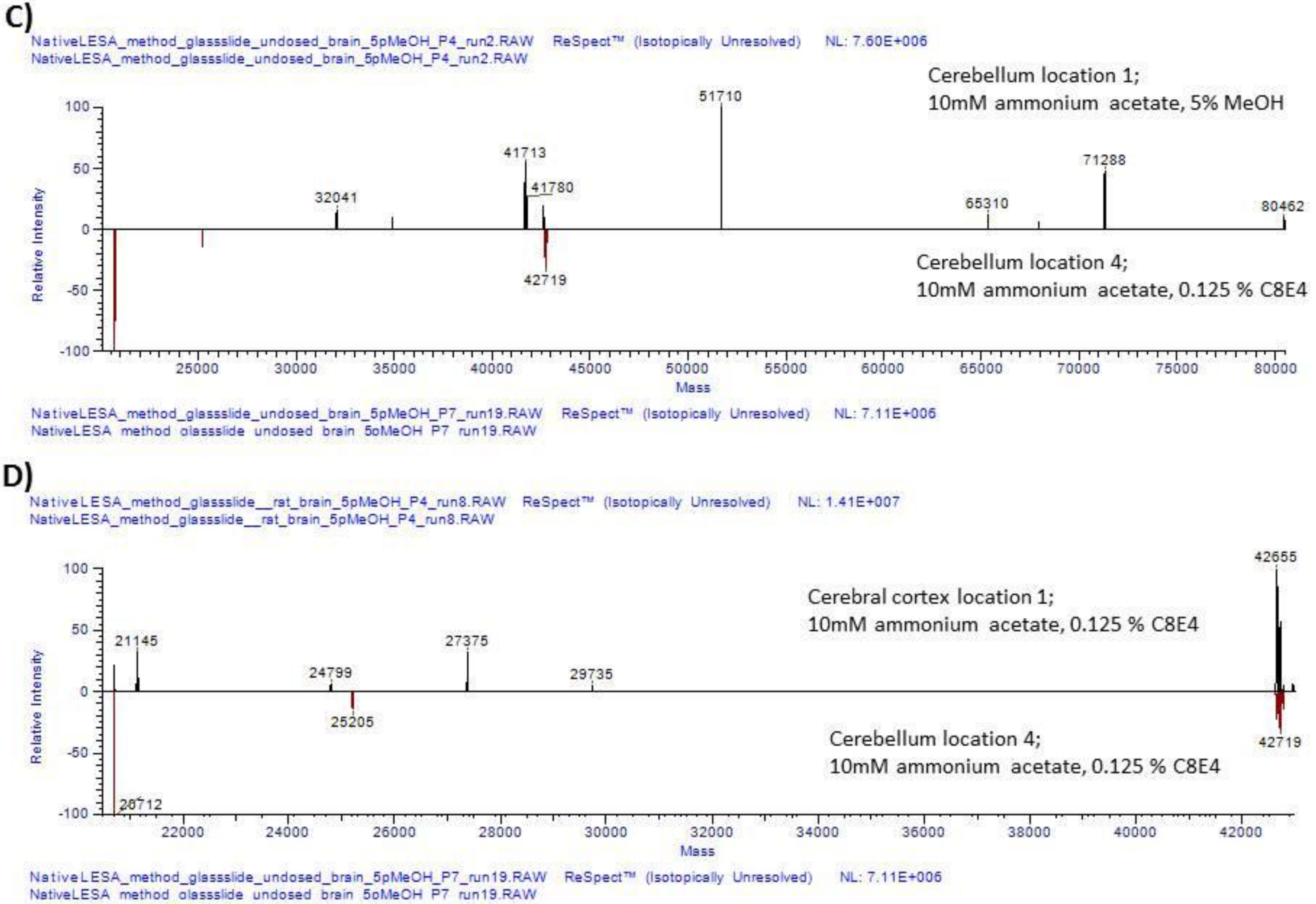
**Supplemental File 6:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Suppl Fig 3. (Kidney outer cortex, 10 mM ammonium acetate, 5% MeOH).

**Supplemental File 7:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 2C. (Kidney medulla, 10 mM ammonium acetate, 0.125% C8E4).

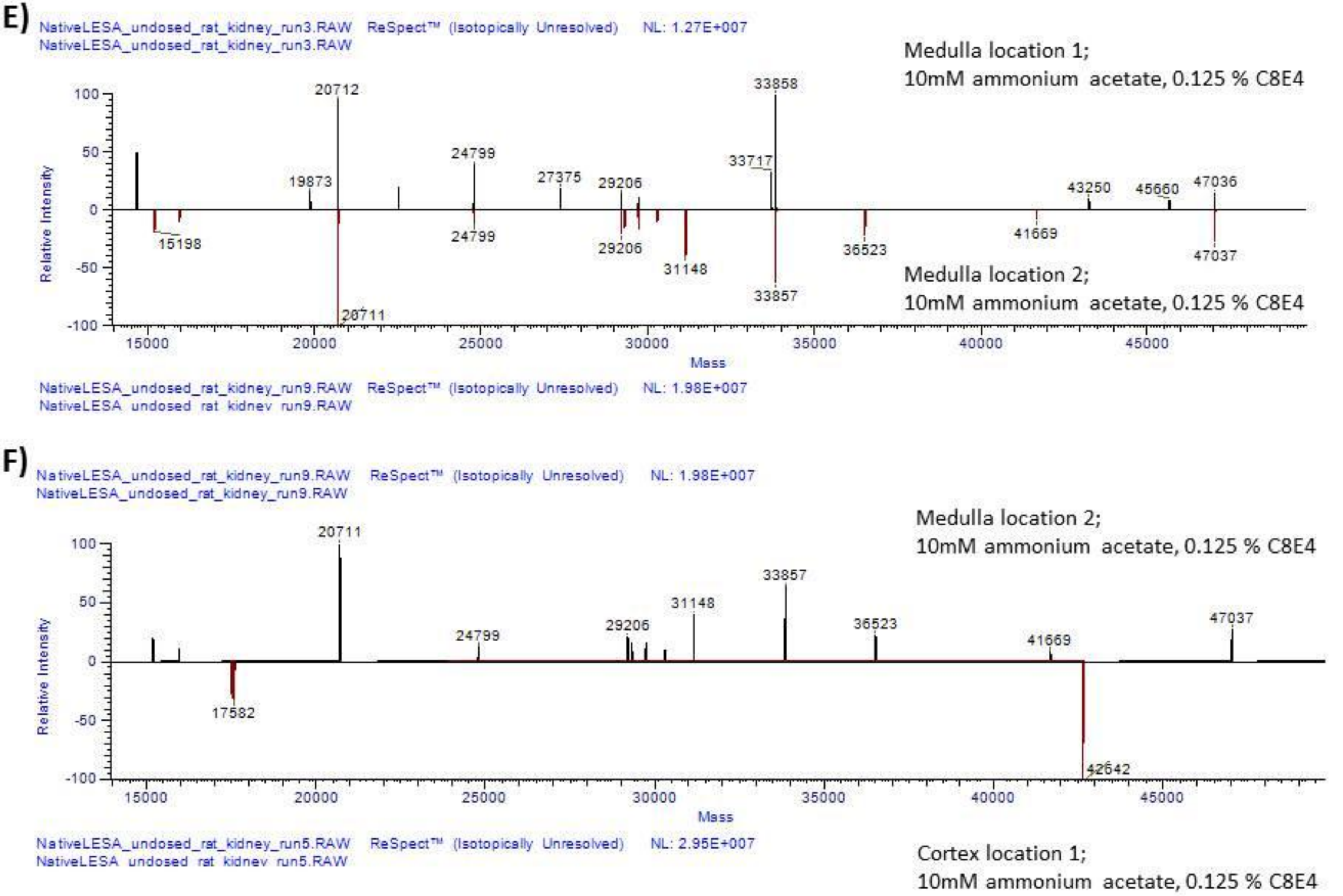
**Supplemental File 8:** Biopharma Finder search parameters and outputs for LESA mass spectrum obtained from a separate medulla location. (Kidney medulla, 10 mM ammonium acetate, 0.125% C8E4).



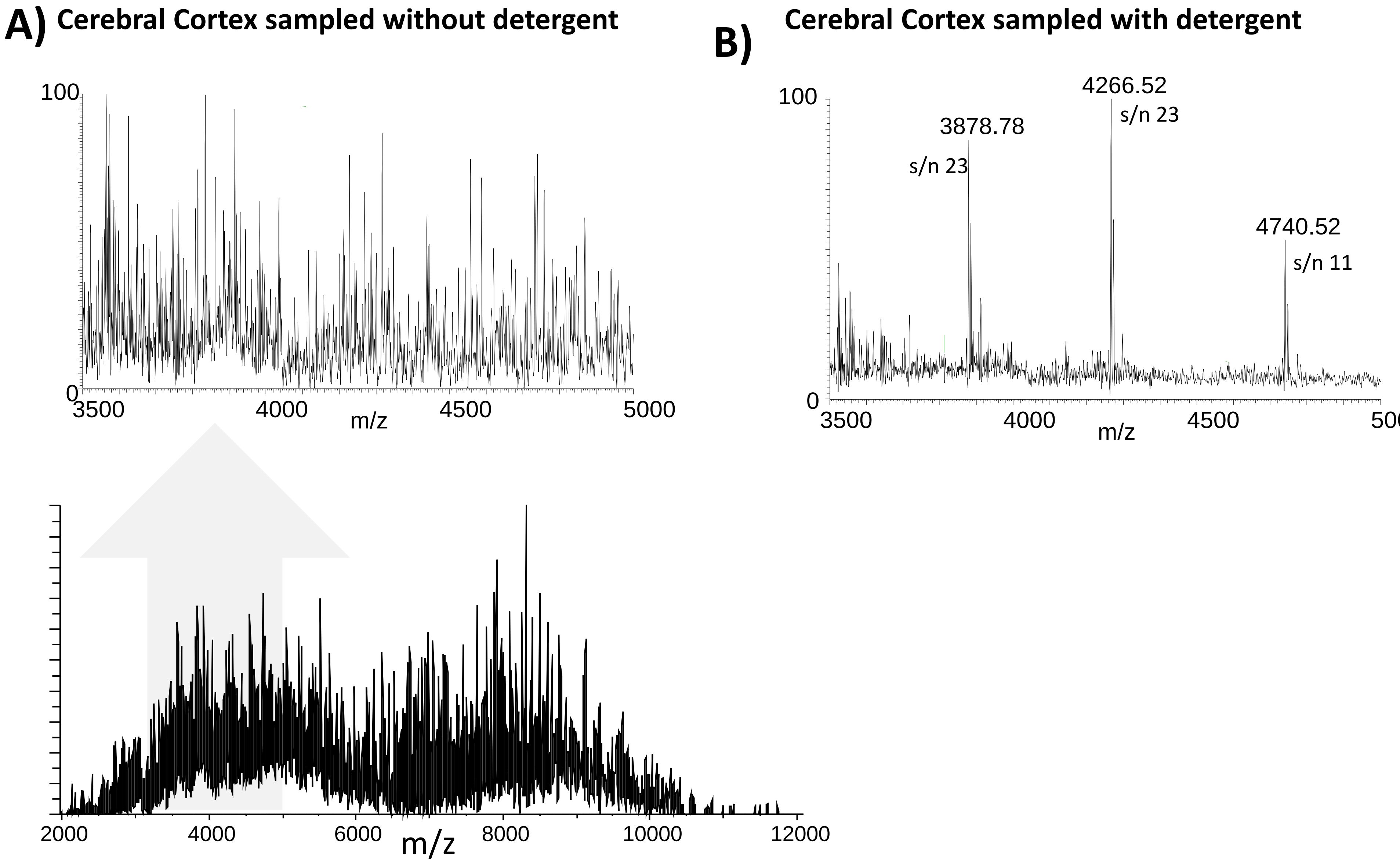
**Supplemental Figure 1.** Comparison of deconvoluted native LESA mass spectra from **A)** two separate cerebellum locations sampled with 10 mM ammonium acetate, 5% MeOH and **B)** two separate cerebellum locations sampled with 10 mM ammonium acetate, 0.125% C8E4



**Supplemental Figure 1 ctd.** Comparison of deconvoluted native LESA mass spectra from **C)** two separate cerebellum locations one sampled with 10 mM ammonium acetate, 5% MeOH and one with 10 mM ammonium acetate, 0.125% C8E4 **D)** one cerebellum location and one cerebral cortex location sampled with 10 mM ammonium acetate, 0.125% C8E4 .



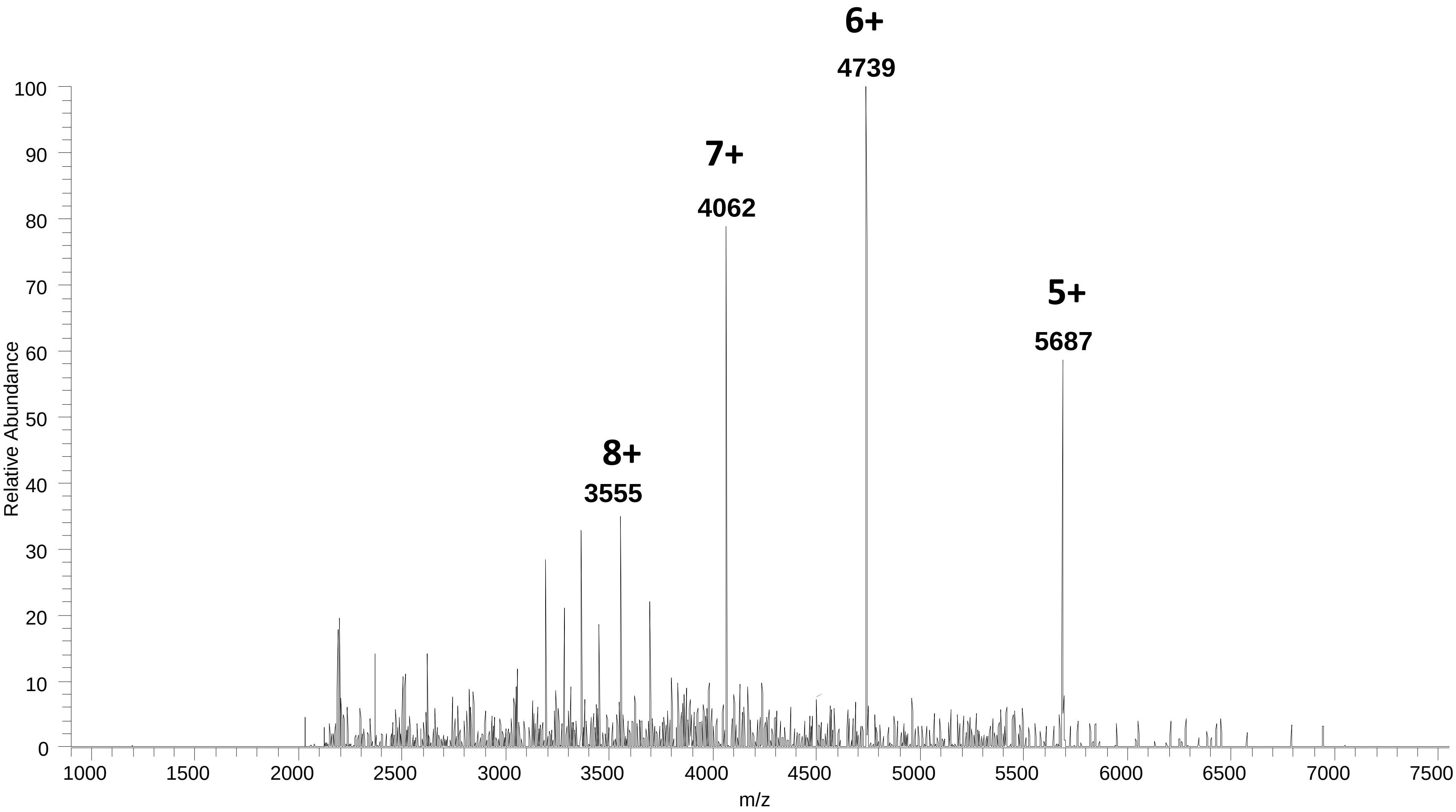
**Supplemental Figure 1 ctd.** Comparison of deconvoluted native LESA mass spectra from **E)** two separate medulla (kidney) locations one sampled with 10 mM ammonium acetate, 0.125% C8E4 and **F)** one medulla (kidney) location and one cortex (kidney) location sampled with 10 mM ammonium acetate, 0.125% C8E4 .



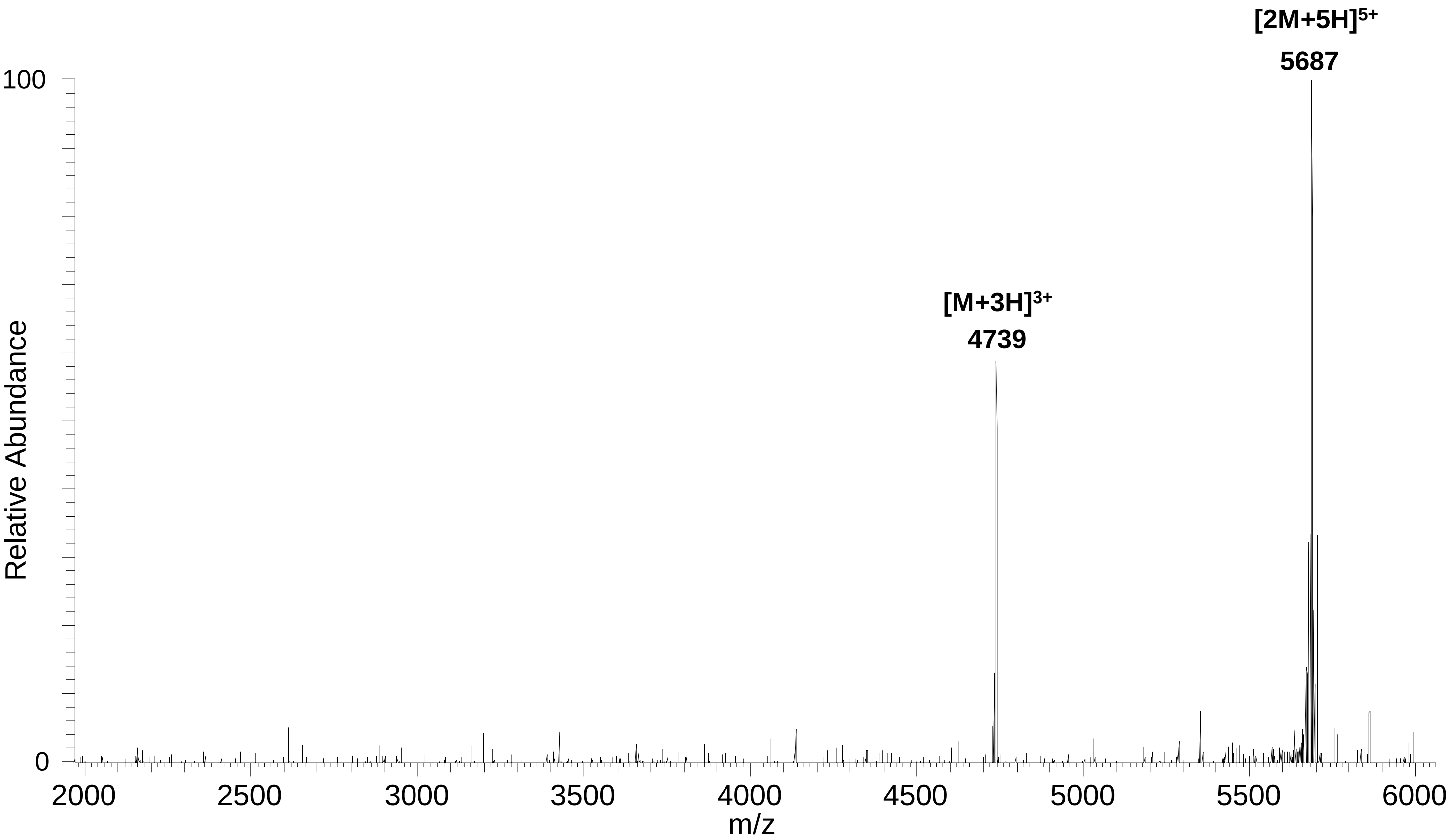
Cerebral Cortex sampled without detergent

Cerebral Cortex sampled with detergent

**Supplemental Figure 2.** Native LESA MS of rat brain tissue. A) Sampling location: cerebral cortex. LESA extraction/ionisation solvent: 10 mM ammonium acetate, 5% MeOH. B) Detail from main figure 1C. Sampling location cerebral cortex. LESA extraction/ionisation solvent: 10 mM ammonium acetate, 0.125% C8E4.



**Supplemental Figure 3.** Native LESA MS of rat kidney tissue. Sampling location: outer cortex. LESA extraction/ionisation solvent: 10 mM ammonium acetate, 5% MeOH.



**Supplemental Figure 4.** Native LESA HCD MS/MS of rat kidney tissue. Sampling location: outer cortex. LESA extraction/ionisation solvent: 10 mM ammonium acetate, 5% MeOH. HCD energy = 80%.

**Supplemental File 1:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 1A. (Cerebellum, 10 mM ammonium acetate, 5% MeOH).

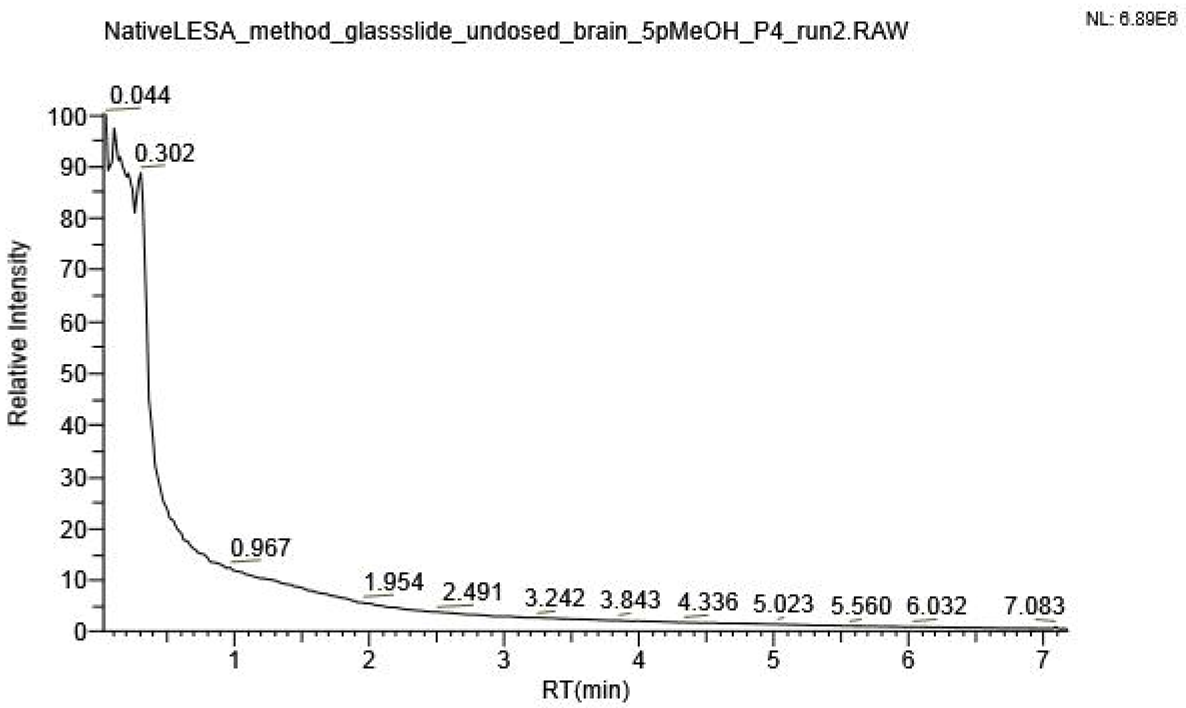
# BioPharma Finder Report

Created: 08/04/2019 09:56:45

| Sample Information | |
|---|---|
| Raw File Name | C:\Xcalibur\Data\ms2LESA\NativeLESA_method_glassslide_undosed_brain_5pMeOH_P4_run2.RAW |
| Instrument Method | |
| Vial | |
| Injection Volume (µL) | 0 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 0 |

| Chromatogram Parameters | |
|---|---|
| Use Restricted Time | False |
| Time Limits | 0.023 - 7.169 minutes |
| Scan Range | 1 - 334 |
| m/z Range | 400 - 20000 |
| Chromatogram Trace Type | TIC |
| Sensitivity | High |
| Rel. Intensity Threshold (%) | 1 |

Chromatogram

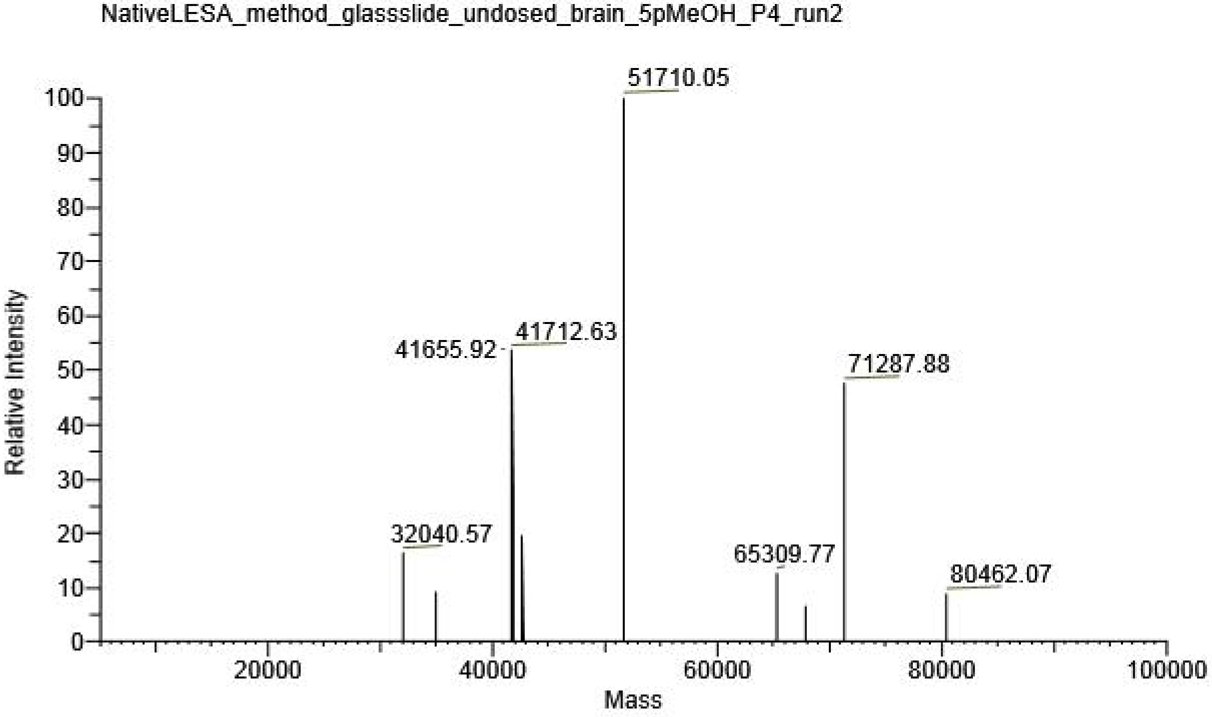


| Main Parameters ( ReSpect™ ) | |
|---|---|
| Deconvolution Results Filter | |
| Output Mass Range | 5000 - 100000 |
| Deconvoluted Spectra Display Mode | Isotopic Profile (new) |
| Charge State Distribution | |
| Deconvolution Mass Tolerance | 30 ppm |
| Choice of Peak Model | |
| Choice of Peak Model | Intact Protein |
| Resolution at 400 m/z | |
| Raw File Specific | 6187 |
| Generate XIC for Each Component | |
| Calculate XIC | False |

| Advanced Parameters ( ReSpect™) | |
|---|---|
| Charge State Distribution | |
| Model Mass Range | 10000 - 120000 |
| Charge State Range | 5 - 40 |
| Minimum Adjacent Charges (low & high model mass) | 3 - 3 |
| Noise Parameters | |
| Rel. Abundance Threshold (%) | 15 |
| Deconvolution Quality | |
| Quality Score Threshold | 0 |
| Choice of Peak Model | |
| Target Mass | 120000 Da |
| Peak Model Parameters | |
| Number of Peak Models | 1 |
| Left/Right Peak Shape | 2:2 |
| Peak Filter Parameters | |
| Peak Detection Minimum Significance Measure | 1 Standard Deviations |
| Peak Detection Quality Measure | 95% |
| Specialized Parameters | |
| Peak Model Width Factor | 1 |
| Intensity Threshold Scale | 0.01 |
| Deconvolution Parameters | |
| Noise Compensation | True |
| Charge Carrier | H |
| Negative Charge | False |

| Source Spectra Parameters | |
|---|---|
| Source Spectra Method | Sliding Windows |
| Sliding Windows Definition | |
| RT Range | 0.500 - 3.000 minutes |
| Target Avg Spectrum Width | 0.2 minutes |
| Target Avg Spectrum Offset Scan | 1 |
| Sliding Windows Merging Parameters | |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 minutes |
| Min. Number of Detected Intervals | 40 |

Deconvoluted Spectrum



Sliding Windows ReSpect Masses Table

| Row Number | Average Mass | Sum Intensity | Relative Abundance | Fractional Abundance | Score | Number of Charge States | Charge State Distribution | Number of Detected Intervals | Mass Std Dev | PPM Std Dev | Delta Mass | Scan Range | Start Time (min) | Stop Time (min) | Apex RT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 51710.05 | 7604135.09 | 100.00 | 28.79 | 23.63 | 5 | 13 - 17 | 67 | 4.50 | 87.11 | 0.00 | 23 - 138 | 0.495 | 2.984 | 0.849 |
| 2 | 41712.63 | 4073971.52 | 53.58 | 15.43 | 21.32 | 4 | 12 - 15 | 102 | 2.57 | 61.59 | -9997.42 | 24 - 135 | 0.516 | 2.920 | 1.171 |
| 3 | 71287.88 | 3610938.80 | 47.49 | 13.67 | 19.10 | 3 | 16 - 18 | 108 | 4.65 | 65.20 | 19577.84 | 23 - 138 | 0.495 | 2.984 | 0.999 |
| 4 | 41655.92 | 2885603.68 | 37.95 | 10.93 | 22.57 | 5 | 11 - 15 | 106 | 2.15 | 51.62 | -10054.13 | 25 - 138 | 0.538 | 2.984 | 0.892 |
| 5 | 41779.80 | 1954143.29 | 25.70 | 7.40 | 24.03 | 5 | 11 - 15 | 88 | 2.96 | 70.86 | -9930.25 | 37 - 136 | 0.795 | 2.941 | 1.343 |
| 6 | 42589.13 | 1479714.78 | 19.46 | 5.60 | 20.84 | 5 | 10 - 14 | 78 | 3.38 | 79.36 | -9120.91 | 26 - 138 | 0.559 | 2.984 | 1.450 |
| 7 | 32040.57 | 1239853.23 | 16.30 | 4.69 | 16.68 | 3 | 8 - 10 | 51 | 2.15 | 67.16 | -19669.48 | 37 - 100 | 0.795 | 2.169 | 1.600 |
| 8 | 65309.77 | 950060.43 | 12.49 | 3.60 | 21.82 | 4 | 17 - 20 | 58 | 5.48 | 83.87 | 13599.72 | 72 - 138 | 1.546 | 2.984 | 1.943 |
| 9 | 42656.79 | 761224.11 | 10.01 | 2.88 | 17.86 | 3 | 11 - 13 | 49 | 3.45 | 80.79 | -9053.26 | 23 - 138 | 0.495 | 2.984 | 0.591 |
| 10 | 34900.39 | 690711.47 | 9.08 | 2.62 | 18.11 | 3 | 8 - 10 | 50 | 2.43 | 69.71 | -16809.65 | 74 - 134 | 1.589 | 2.899 | 1.836 |
| 11 | 80462.07 | 669635.99 | 8.81 | 2.54 | 18.69 | 3 | 23 - 25 | 58 | 2.64 | 32.84 | 28752.02 | 58 - 131 | 1.246 | 2.834 | 2.094 |
| 12 | 67902.81 | 491095.13 | 6.46 | 1.86 | 15.81 | 3 | 21 - 23 | 41 | 3.69 | 54.36 | 16192.76 | 56 - 125 | 1.203 | 2.705 | 2.029 |

**Supplemental File 2:** Biopharma Finder search parameters and outputs for LESA mass spectrum obtained from separate cerebellum location (Cerebellum, 10 mM ammonium acetate, 5% MeOH).

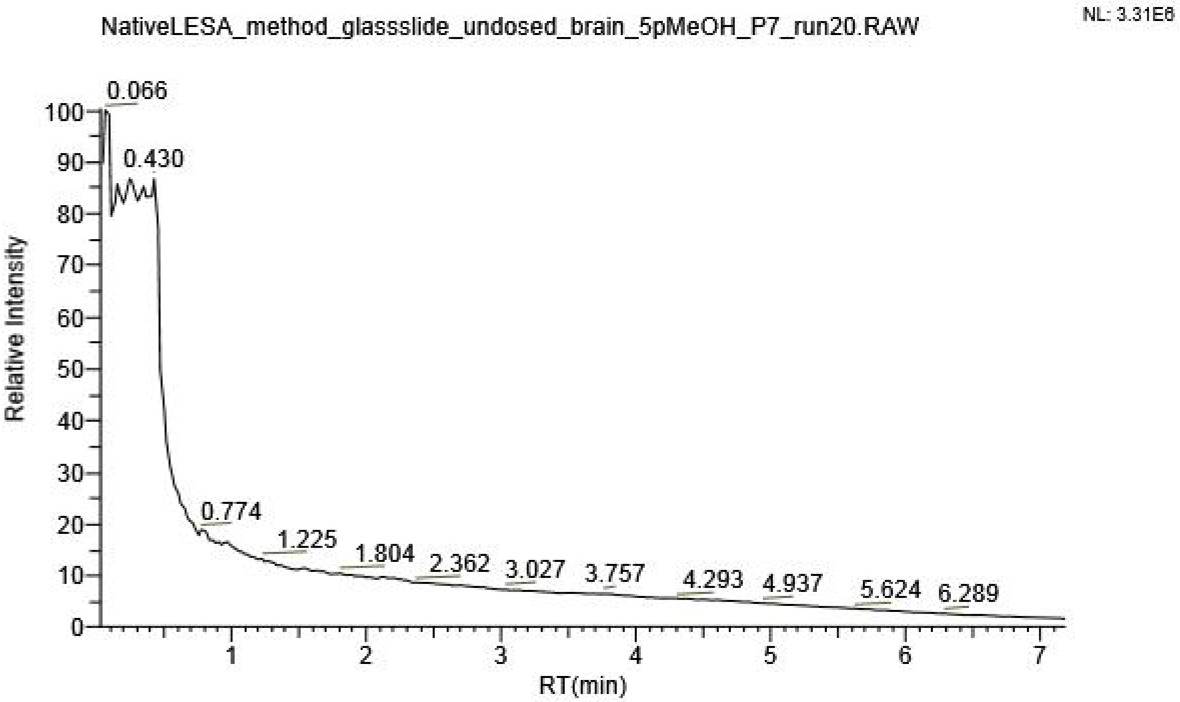
# BioPharma Finder Report

Created: 08/04/2019 10:20:13

| Sample Information | |
|---|---|
| Raw File Name | C:\Xcalibur\Data\ms2LESA\NativeLESA_method_glassslide_undosed_brain_5pMeOH_P7_run20.RAW |
| Instrument Method | |
| Vial | |
| Injection Volume (µL) | 0 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 0 |

| Chromatogram Parameters | |
|---|---|
| Use Restricted Time | False |
| Time Limits | 0.023 - 7.169 minutes |
| Scan Range | 1 - 334 |
| m/z Range | 400 - 20000 |
| Chromatogram Trace Type | TIC |
| Sensitivity | High |
| Rel. Intensity Threshold (%) | 1 |

Chromatogram



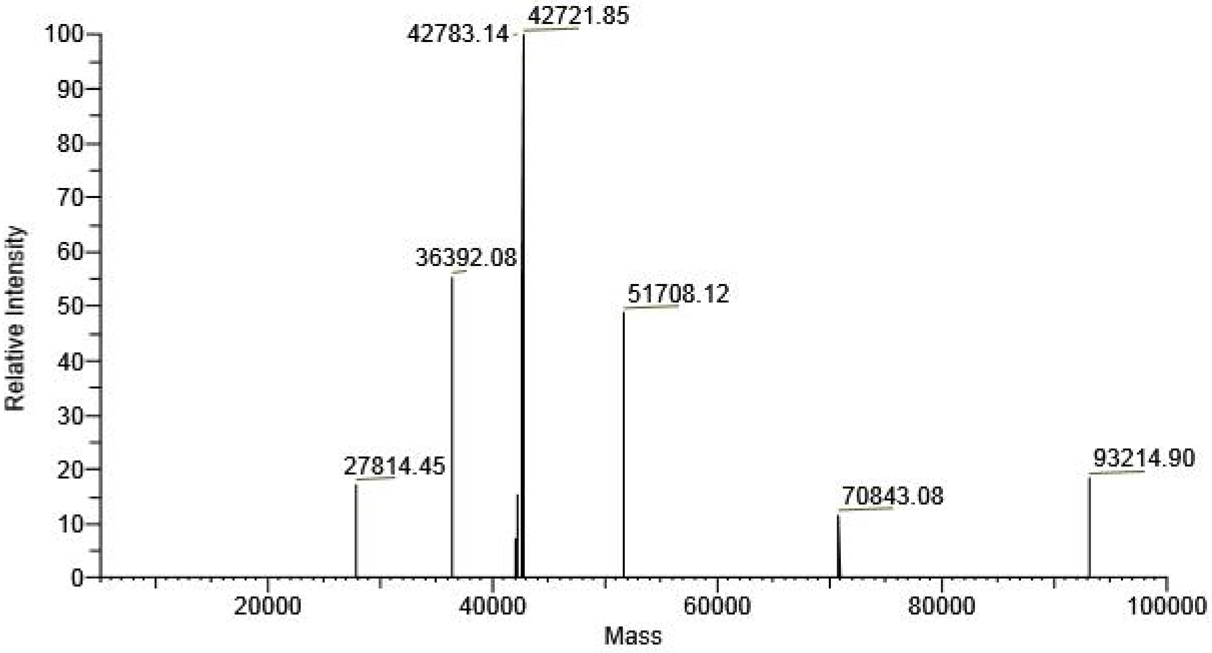
| Main Parameters ( ReSpect™ ) | |
|---|---|
| Deconvolution Results Filter | |
| Output Mass Range | 5000 - 100000 |
| Deconvoluted Spectra Display Mode | Isotopic Profile (new) |
| Charge State Distribution | |
| Deconvolution Mass Tolerance | 30 ppm |
| Choice of Peak Model | |
| Choice of Peak Model | Intact Protein |
| Resolution at 400 m/z | |
| Raw File Specific | 6187 |
| Generate XIC for Each Component | |
| Calculate XIC | False |

| Advanced Parameters ( ReSpect™) | |
|---|---|
| Charge State Distribution | |
| Model Mass Range | 10000 - 120000 |
| Charge State Range | 5 - 40 |
| Minimum Adjacent Charges (low & high model mass) | 3 - 3 |
| Noise Parameters | |
| Rel. Abundance Threshold (%) | 15 |
| Deconvolution Quality | |
| Quality Score Threshold | 0 |
| Choice of Peak Model | |
| Target Mass | 120000 Da |
| Peak Model Parameters | |
| Number of Peak Models | 1 |
| Left/Right Peak Shape | 2:2 |
| Peak Filter Parameters | |
| Peak Detection Minimum Significance Measure | 1 Standard Deviations |
| Peak Detection Quality Measure | 95% |
| Specialized Parameters | |
| Peak Model Width Factor | 1 |
| Intensity Threshold Scale | 0.01 |
| Deconvolution Parameters | |
| Noise Compensation | True |
| Charge Carrier | H |
| Negative Charge | False |

| Source Spectra Parameters | |
|---|---|
| Source Spectra Method | Sliding Windows |
| Sliding Windows Definition | |
| RT Range | 2.000 - 9.000 minutes |
| Target Avg Spectrum Width | 0.2 minutes |
| Target Avg Spectrum Offset Scan | 1 |
| Sliding Windows Merging Parameters | |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 minutes |
| Min. Number of Detected Intervals | 100 |

Deconvoluted Spectrum

NativeLESA_method_glassslide_undosed_brain_5pMeOH_P7_run20



Sliding Windows ReSpect Masses Table

| Row Number | Average Mass | Sum Intensity | Relative Abundance | Fractional Abundance | Score | Number of Charge States | Charge State Distribution | Number of Detected Intervals | Mass Std Dev | PPM Std Dev | Delta Mass | Scan Range | Start Time (min) | Stop Time (min) | Apex RT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 42721.85 | 7320974.19 | 100.00 | 27.11 | 19.39 | 4 | 11 - 14 | 275 | 2.90 | 67.78 | 0.00 | 93 - 417 | 1.997 | 8.972 | 2.308 |
| 2 | 36392.08 | 4033161.76 | 55.09 | 14.93 | 26.19 | 6 | 7 - 12 | 287 | 2.70 | 74.18 | -6329.77 | 93 - 416 | 1.997 | 8.951 | 2.995 |
| 3 | 42653.26 | 3874901.33 | 52.93 | 14.35 | 22.10 | 4 | 11 - 14 | 195 | 3.18 | 74.51 | -68.59 | 93 - 345 | 1.997 | 7.427 | 2.802 |
| 4 | 51708.12 | 3572900.98 | 48.80 | 13.23 | 18.93 | 4 | 13 - 16 | 281 | 2.82 | 54.58 | 8986.27 | 129 - 417 | 2.770 | 8.972 | 3.038 |
| 5 | 42783.14 | 3141993.21 | 42.92 | 11.63 | 17.54 | 4 | 10 - 13 | 253 | 3.41 | 79.81 | 61.29 | 93 - 356 | 1.997 | 7.663 | 2.459 |
| 6 | 93214.90 | 1344648.89 | 18.37 | 4.98 | 27.12 | 6 | 24 - 29 | 128 | 7.84 | 84.10 | 50493.05 | 116 - 282 | 2.491 | 6.075 | 3.596 |
| 7 | 27814.45 | 1249522.35 | 17.07 | 4.63 | 18.36 | 3 | 8 - 10 | 195 | 0.97 | 34.93 | -14907.40 | 124 - 328 | 2.662 | 7.062 | 3.360 |
| 8 | 42206.97 | 1115973.10 | 15.24 | 4.13 | 18.89 | 4 | 10 - 13 | 114 | 3.16 | 74.94 | -514.88 | 131 - 255 | 2.813 | 5.495 | 3.746 |
| 9 | 70843.08 | 832450.64 | 11.37 | 3.08 | 19.79 | 4 | 17 - 20 | 110 | 6.70 | 94.63 | 28121.23 | 194 - 377 | 4.165 | 8.114 | 4.862 |
| 10 | 41966.52 | 519591.40 | 7.10 | 1.92 | 17.76 | 3 | 11 - 13 | 116 | 2.18 | 52.04 | -755.33 | 164 - 297 | 3.521 | 6.397 | 3.789 |

**Supplemental File 3:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 1B. (Cerebellum, 10 mM ammonium acetate, 0.125% C8E4).

# BioPharma Finder Report

Created: 08/04/2019 11:20:38

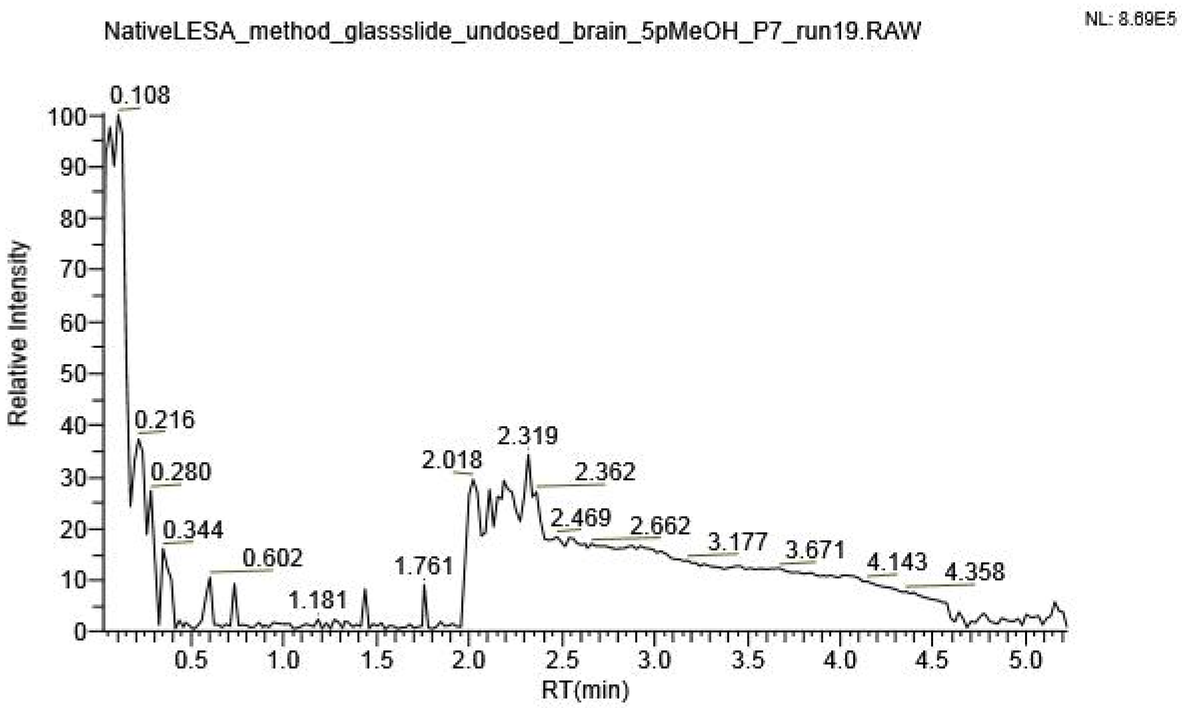
## Sample Information

| | |
|---|---|
| Raw File Name | C:\Xcalibur\Data\ms2LESA\NativeLESA_method_glassslide_undosed_brain_5pMeOH_P7_run19.RAW |
| Instrument Method | |
| Vial | |
| Injection Volume (µL) | 0 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 0 |

## Chromatogram Parameters

| | |
|---|---|
| Use Restricted Time | False |
| Time Limits | 0.023 - 7.169 minutes |
| Scan Range | 1 - 334 |
| m/z Range | 400 - 20000 |
| Chromatogram Trace Type | TIC |
| Sensitivity | High |
| Rel. Intensity Threshold (%) | 1 |

## Chromatogram

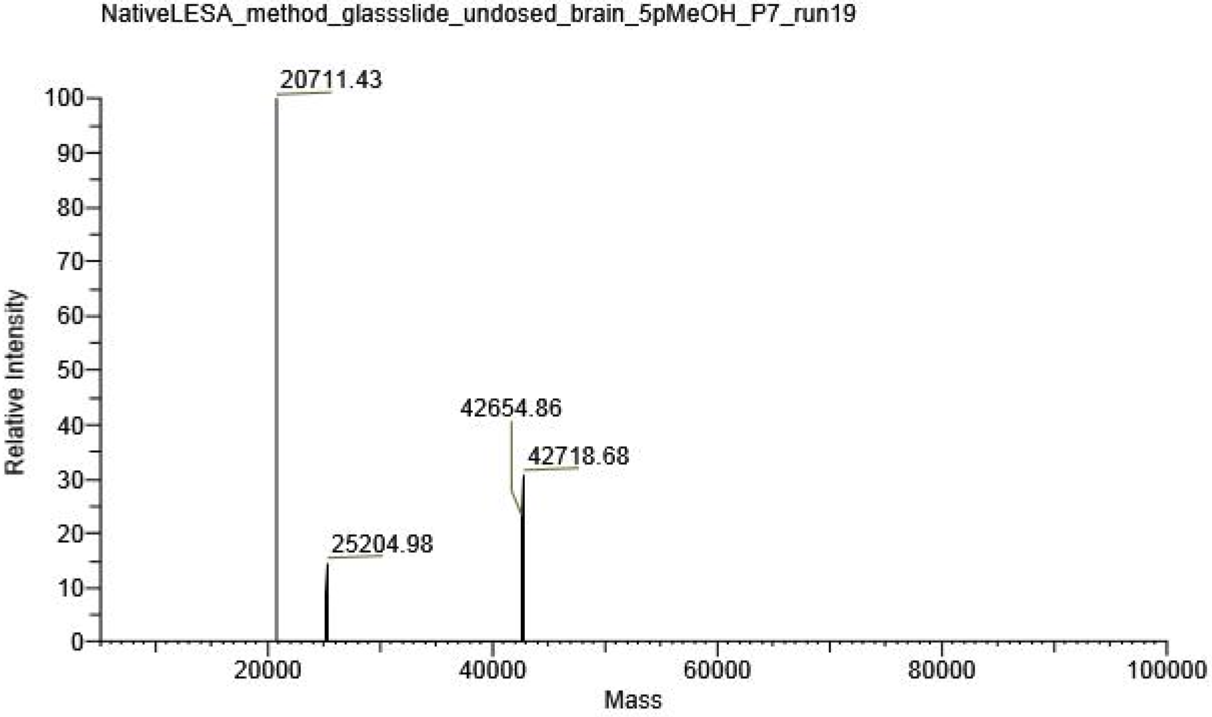


| Main Parameters ( ReSpect™ ) | |
|---|---|
| Deconvolution Results Filter | |
| Output Mass Range | 5000 - 100000 |
| Deconvoluted Spectra Display Mode | Isotopic Profile (new) |
| Charge State Distribution | |
| Deconvolution Mass Tolerance | 30 ppm |
| Choice of Peak Model | |
| Choice of Peak Model | Intact Protein |
| Resolution at 400 m/z | |
| Raw File Specific | 6187 |
| Generate XIC for Each Component | |
| Calculate XIC | False |

| Advanced Parameters ( ReSpect™) | |
|---|---|
| Charge State Distribution | |
| Model Mass Range | 10000 - 120000 |
| Charge State Range | 5 - 40 |
| Minimum Adjacent Charges (low & high model mass) | 3 - 3 |
| Noise Parameters | |
| Rel. Abundance Threshold (%) | 15 |
| Deconvolution Quality | |
| Quality Score Threshold | 0 |
| Choice of Peak Model | |
| Target Mass | 120000 Da |
| Peak Model Parameters | |
| Number of Peak Models | 1 |
| Left/Right Peak Shape | 2:2 |
| Peak Filter Parameters | |
| Peak Detection Minimum Significance Measure | 1 Standard Deviations |
| Peak Detection Quality Measure | 95% |
| Specialized Parameters | |
| Peak Model Width Factor | 1 |
| Intensity Threshold Scale | 0.01 |
| Deconvolution Parameters | |
| Noise Compensation | True |
| Charge Carrier | H |
| Negative Charge | False |

| Source Spectra Parameters | |
|---|---|
| Source Spectra Method | Sliding Windows |
| Sliding Windows Definition | |
| RT Range | 2.000 - 4.500 minutes |
| Target Avg Spectrum Width | 0.2 minutes |
| Target Avg Spectrum Offset Scan | 1 |
| Sliding Windows Merging Parameters | |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 minutes |
| Min. Number of Detected Intervals | 40 |

Deconvoluted Spectrum



Sliding Windows ReSpect Masses Table

| Row Number | Average Mass | Sum Intensity | Relative Abundance | Fractional Abundance | Score | Number of Charge States | Charge State Distribution | Number of Detected Intervals | Mass Std Dev | PPM Std Dev | Delta Mass | Scan Range | Start Time (min) | Stop Time (min) | Apex RT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 20711.43 | 7111245.16 | 100.00 | 55.09 | 23.47 | 4 | 5 - 8 | 108 | 0.48 | 23.24 | 0.00 | 93 - 208 | 1.997 | 4.486 | 2.780 |
| 2 | 42718.68 | 2174219.29 | 30.57 | 16.84 | 17.62 | 4 | 9 - 12 | 90 | 2.27 | 53.17 | 22007.25 | 96 - 194 | 2.061 | 4.186 | 2.630 |
| 3 | 42654.86 | 1593266.17 | 22.40 | 12.34 | 16.77 | 3 | 9 - 11 | 91 | 2.43 | 57.01 | 21943.43 | 110 - 208 | 2.362 | 4.486 | 2.716 |
| 4 | 25204.98 | 1016270.92 | 14.29 | 7.87 | 17.29 | 3 | 6 - 8 | 62 | 1.73 | 68.49 | 4493.56 | 108 - 189 | 2.319 | 4.079 | 2.587 |
| 5 | 42782.08 | 1013706.97 | 14.25 | 7.85 | 18.77 | 4 | 9 - 12 | 40 | 2.91 | 68.07 | 22070.66 | 93 - 173 | 1.997 | 3.735 | 2.609 |

**Supplemental File 4:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 1C. (Cerebral cortex, 10 mM ammonium acetate, 0.125% C8E4).

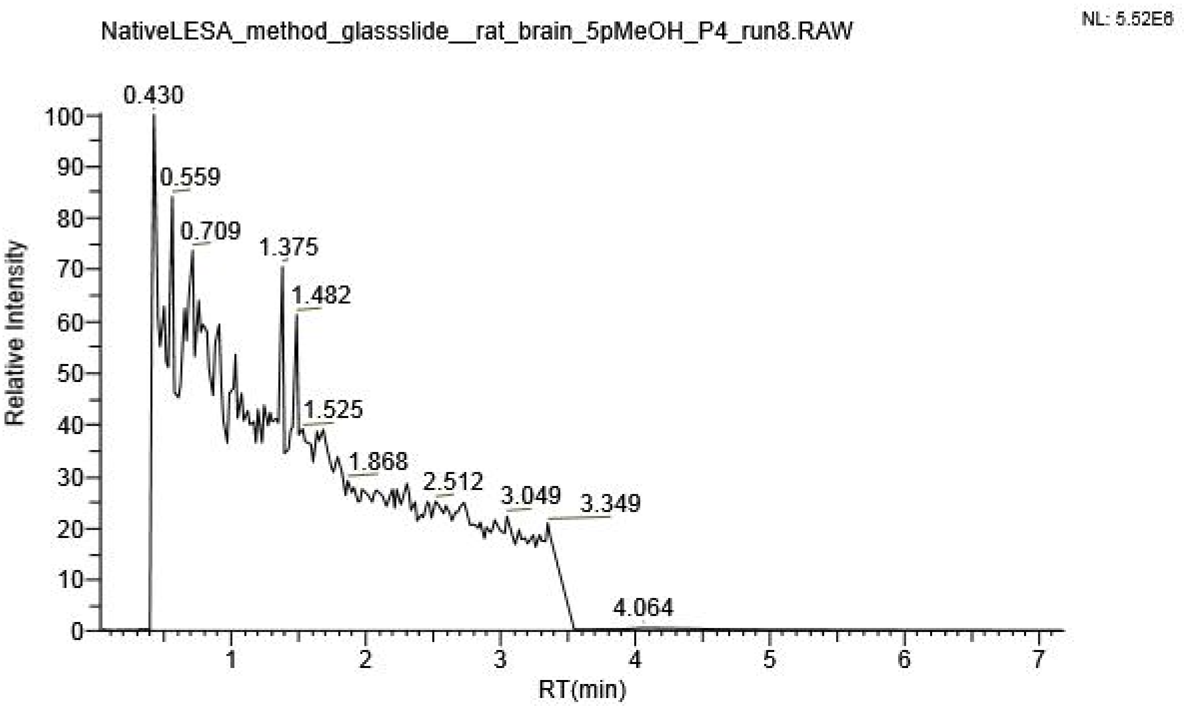
# BioPharma Finder Report

Created: 08/04/2019 12:25:49

| Sample Information | |
|---|---|
| Raw File Name | C:\Xcalibur\Data\ms2LESA\NativeLESA_method_glassslide__rat_brain_5pMeOH_P4_run8.RAW |
| Instrument Method | |
| Vial | |
| Injection Volume (µL) | 0 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 0 |

| Chromatogram Parameters | |
|---|---|
| Use Restricted Time | False |
| Time Limits | 0.023 - 7.169 minutes |
| Scan Range | 1 - 334 |
| m/z Range | 400 - 20000 |
| Chromatogram Trace Type | TIC |
| Sensitivity | High |
| Rel. Intensity Threshold (%) | 1 |

## Chromatogram

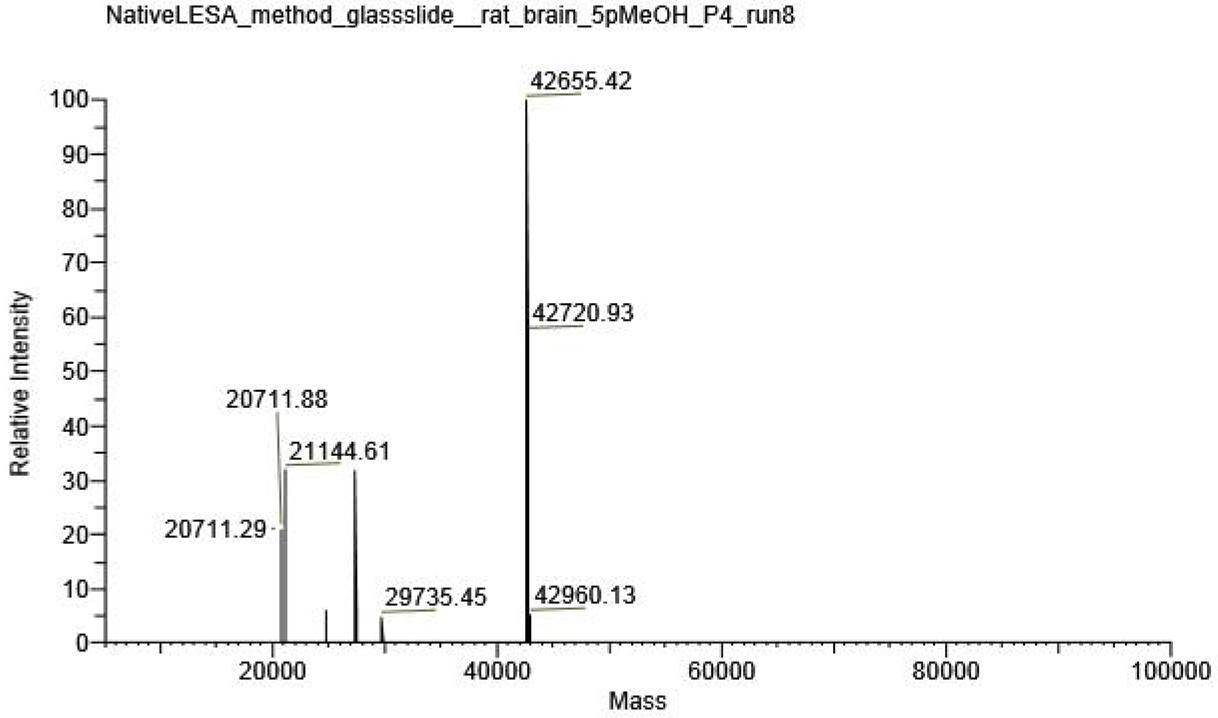


| Main Parameters ( ReSpect™ ) | |
|---|---|
| Deconvolution Results Filter | |
| Output Mass Range | 5000 - 100000 |
| Deconvoluted Spectra Display Mode | Isotopic Profile (new) |
| Charge State Distribution | |
| Deconvolution Mass Tolerance | 30 ppm |
| Choice of Peak Model | |
| Choice of Peak Model | Intact Protein |
| Resolution at 400 m/z | |
| Raw File Specific | 6187 |
| Generate XIC for Each Component | |
| Calculate XIC | False |

| Advanced Parameters ( ReSpect™) | |
|---|---|
| Charge State Distribution | |
| Model Mass Range | 10000 - 120000 |
| Charge State Range | 5 - 40 |
| Minimum Adjacent Charges (low & high model mass) | 3 - 3 |
| Noise Parameters | |
| Rel. Abundance Threshold (%) | 15 |
| Deconvolution Quality | |
| Quality Score Threshold | 0 |
| Choice of Peak Model | |
| Target Mass | 120000 Da |
| Peak Model Parameters | |
| Number of Peak Models | 1 |
| Left/Right Peak Shape | 2:2 |
| Peak Filter Parameters | |
| Peak Detection Minimum Significance Measure | 1 Standard Deviations |
| Peak Detection Quality Measure | 95% |
| Specialized Parameters | |
| Peak Model Width Factor | 1 |
| Intensity Threshold Scale | 0.01 |
| Deconvolution Parameters | |
| Noise Compensation | True |
| Charge Carrier | H |
| Negative Charge | False |

| Source Spectra Parameters | |
|---|---|
| Source Spectra Method | Sliding Windows |
| Sliding Windows Definition | |
| RT Range | 0.430 - 3.300 minutes |
| Target Avg Spectrum Width | 0.2 minutes |
| Target Avg Spectrum Offset Scan | 1 |
| Sliding Windows Merging Parameters | |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 minutes |
| Min. Number of Detected Intervals | 20 |

## Deconvoluted Spectrum



Sliding Windows ReSpect Masses Table

| Row Number | Average Mass | Sum Intensity | Relative Abundance | Fractional Abundance | Score | Number of Charge States | Charge State Distribution | Number of Detected Intervals | Mass Std Dev | PPM Std Dev | Delta Mass | Scan Range | Start Time (min) | Stop Time (min) | Apex RT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 42655.42 | 14067523.01 | 100.00 | 36.74 | 30.11 | 9 | 8 - 16 | 118 | 2.21 | 51.85 | 0.00 | 27 - 152 | 0.581 | 3.285 | 1.600 |
| 2 | 42720.93 | 7994026.90 | 56.83 | 20.88 | 30.32 | 9 | 7 - 15 | 106 | 1.94 | 45.42 | 65.51 | 25 - 152 | 0.538 | 3.285 | 2.158 |
| 3 | 21144.61 | 4472423.83 | 31.79 | 11.68 | 20.62 | 4 | 5 - 8 | 70 | 1.00 | 47.18 | -21510.81 | 20 - 114 | 0.430 | 2.469 | 0.527 |
| 4 | 27375.41 | 4450148.04 | 31.63 | 11.62 | 20.75 | 6 | 5 - 10 | 101 | 1.43 | 52.15 | -15280.01 | 23 - 151 | 0.495 | 3.263 | 2.008 |
| 5 | 20711.88 | 1667804.98 | 11.86 | 4.36 | 21.42 | 4 | 5 - 8 | 35 | 1.09 | 52.44 | -21943.53 | 24 - 112 | 0.516 | 2.426 | 0.785 |
| 6 | 20711.29 | 1260771.74 | 8.96 | 3.29 | 19.72 | 4 | 5 - 8 | 42 | 1.39 | 67.09 | -21944.13 | 20 - 149 | 0.430 | 3.220 | 1.986 |
| 7 | 21121.87 | 862100.36 | 6.13 | 2.25 | 22.92 | 4 | 5 - 8 | 21 | 1.34 | 63.53 | -21533.55 | 20 - 59 | 0.430 | 1.289 | 1.042 |
| 8 | 24798.65 | 828510.80 | 5.89 | 2.16 | 17.83 | 4 | 6 - 9 | 22 | 1.90 | 76.68 | -17856.77 | 21 - 82 | 0.452 | 1.783 | 0.591 |
| 9 | 21162.61 | 779314.56 | 5.54 | 2.04 | 21.99 | 4 | 5 - 8 | 24 | 1.33 | 62.80 | -21492.80 | 20 - 65 | 0.430 | 1.418 | 1.042 |
| 10 | 42960.13 | 727514.64 | 5.17 | 1.90 | 23.23 | 7 | 8 - 14 | 22 | 3.07 | 71.43 | 304.71 | 41 - 149 | 0.881 | 3.220 | 1.493 |
| 11 | 29735.45 | 648545.36 | 4.61 | 1.69 | 20.96 | 6 | 7 - 12 | 24 | 2.39 | 80.43 | -12919.97 | 22 - 99 | 0.473 | 2.147 | 0.978 |
| 12 | 42784.83 | 534673.34 | 3.80 | 1.40 | 26.27 | 7 | 9 - 15 | 21 | 3.19 | 74.64 | 129.42 | 102 - 152 | 2.190 | 3.285 | 2.866 |

**Supplemental File 5:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 2A. (Kidney outer cortex, 10 mM ammonium acetate, 0.125% C8E4).

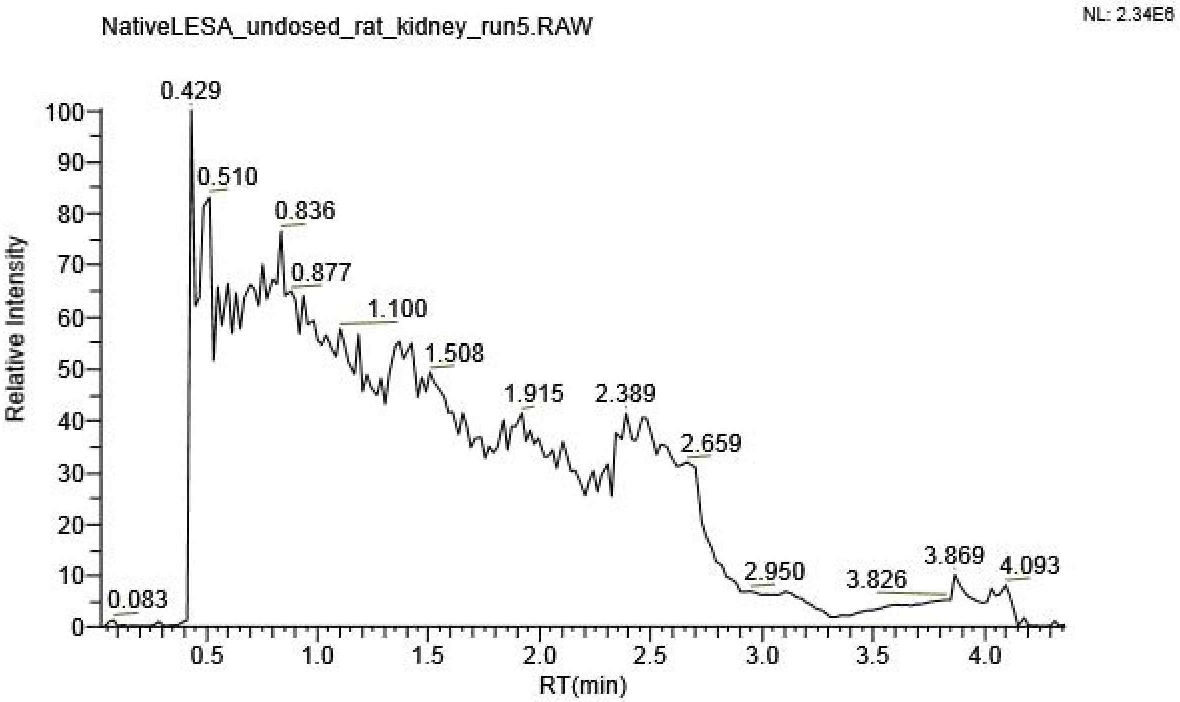
# BioPharma Finder Report

Created: 08/04/2019 13:52:58

| Sample Information | |
|---|---|
| Raw File Name | C:\Xcalibur\Data\ms2LESA\NativeLESA_undosed_rat_kidney_run5.RAW |
| Instrument Method | |
| Vial | |
| Injection Volume (µL) | 0 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 0 |

| Chromatogram Parameters | |
|---|---|
| Use Restricted Time | False |
| Time Limits | 0.023 - 7.169 minutes |
| Scan Range | 1 - 334 |
| m/z Range | 2000 - 20000 |
| Chromatogram Trace Type | TIC |
| Sensitivity | High |
| Rel. Intensity Threshold (%) | 1 |

## Chromatogram

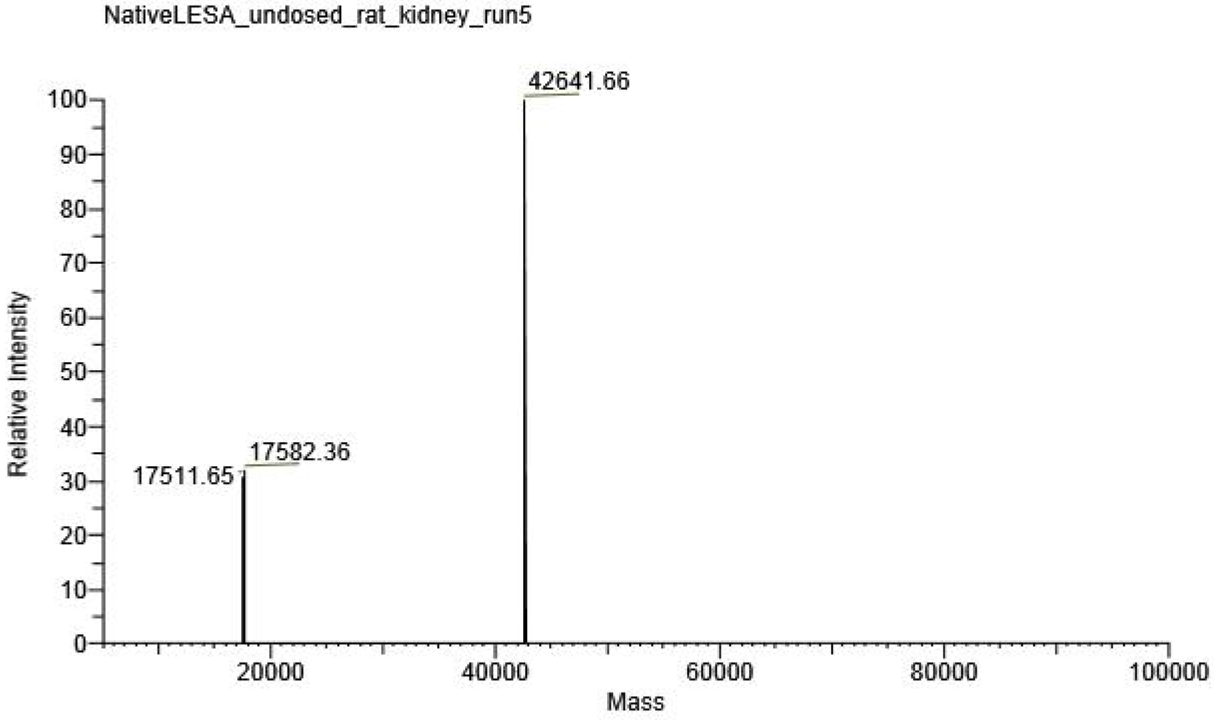


| Main Parameters ( ReSpect™ ) | |
|---|---|
| Deconvolution Results Filter | |
| Output Mass Range | 5000 - 100000 |
| Deconvoluted Spectra Display Mode | Isotopic Profile (new) |
| Charge State Distribution | |
| Deconvolution Mass Tolerance | 30 ppm |
| Choice of Peak Model | |
| Choice of Peak Model | Intact Protein |
| Resolution at 400 m/z | |
| Raw File Specific | 6187 |
| Generate XIC for Each Component | |
| Calculate XIC | False |

| Advanced Parameters ( ReSpect™) | |
|---|---|
| Charge State Distribution | |
| Model Mass Range | 10000 - 120000 |
| Charge State Range | 5 - 40 |
| Minimum Adjacent Charges (low & high model mass) | 3 - 3 |
| Noise Parameters | |
| Rel. Abundance Threshold (%) | 15 |
| Deconvolution Quality | |
| Quality Score Threshold | 0 |
| Choice of Peak Model | |
| Target Mass | 120000 Da |
| Peak Model Parameters | |
| Number of Peak Models | 1 |
| Left/Right Peak Shape | 2:2 |
| Peak Filter Parameters | |
| Peak Detection Minimum Significance Measure | 1 Standard Deviations |
| Peak Detection Quality Measure | 95% |
| Specialized Parameters | |
| Peak Model Width Factor | 1 |
| Intensity Threshold Scale | 0.01 |
| Deconvolution Parameters | |
| Noise Compensation | True |
| Charge Carrier | H |
| Negative Charge | False |

| Source Spectra Parameters | |
|---|---|
| Source Spectra Method | Sliding Windows |
| Sliding Windows Definition | |
| RT Range | 0.440 - 3.000 minutes |
| Target Avg Spectrum Width | 0.2 minutes |
| Target Avg Spectrum Offset Scan | 1 |
| Sliding Windows Merging Parameters | |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 minutes |
| Min. Number of Detected Intervals | 40 |

## Deconvoluted Spectrum



| Sliding Windows ReSpect Masses Table | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Row Number | Average Mass | Sum Intensity | Relative Abundance | Fractional Abundance | Score | Number of Charge States | Charge State Distribution | Number of Detected Intervals | Mass Std Dev | PPM Std Dev | Delta Mass | Scan Range | Start Time (min) | Stop Time (min) | Apex RT |
| 1 | 42641.66 | 29486568.19 | 100.00 | 61.60 | 25.46 | 10 | 6 - 15 | 114 | 1.58 | 37.01 | 0.00 | 22 - 143 | 0.449 | 2.995 | 0.815 |
| 2 | 17582.36 | 9383396.46 | 31.82 | 19.60 | 19.18 | 3 | 5 - 7 | 73 | 0.59 | 33.58 | -25059.30 | 22 - 104 | 0.449 | 2.139 | 1.426 |
| 3 | 17511.65 | 9001058.95 | 30.53 | 18.80 | 17.51 | 3 | 5 - 7 | 59 | 0.40 | 22.94 | -25130.01 | 22 - 89 | 0.449 | 1.833 | 1.447 |

**Supplemental File 6:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Suppl Fig 3. (Kidney outer cortex, 10 mM ammonium acetate, 5% MeOH).

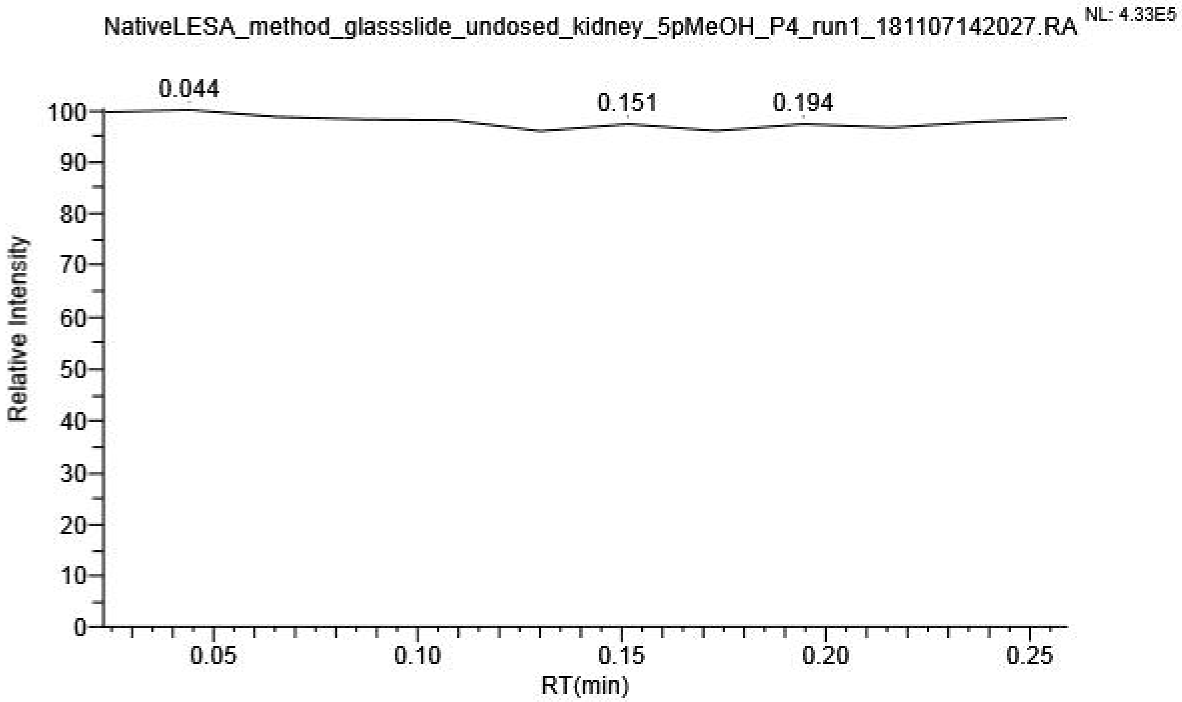
# BioPharma Finder Report

Created: 08/04/2019 14:03:48

| Sample Information | |
|---|---|
| Raw File Name | C:\Xcalibur\Data\ms2LESA\NativeLESA_method_glassslide_undosed_kidney_5pMeOH_P4_run1_181107142027.RAW |
| Instrument Method | |
| Vial | |
| Injection Volume (µL) | 0 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 0 |

| Chromatogram Parameters | |
|---|---|
| Use Restricted Time | False |
| Time Limits | 0.023 - 7.169 minutes |
| Scan Range | 1 - 334 |
| m/z Range | 400 - 20000 |
| Chromatogram Trace Type | TIC |
| Sensitivity | High |
| Rel. Intensity Threshold (%) | 1 |

## Chromatogram

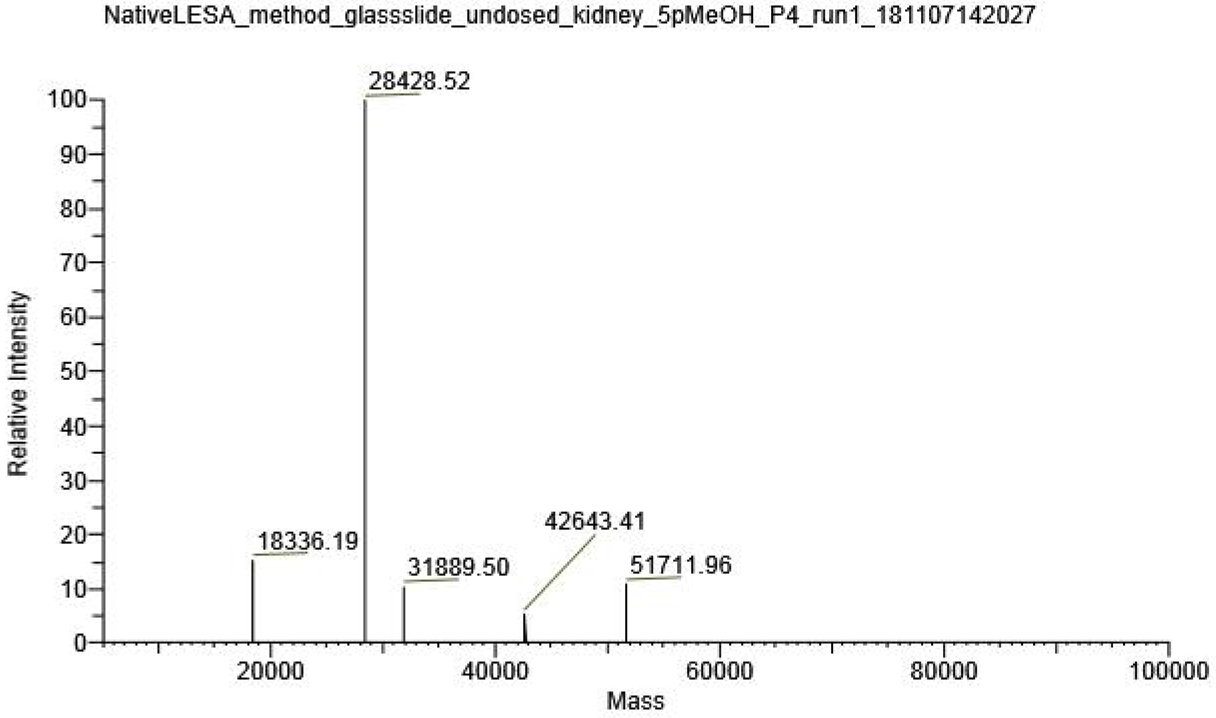


| Main Parameters ( ReSpect™ ) | |
|---|---|
| Deconvolution Results Filter | |
| Output Mass Range | 5000 - 100000 |
| Deconvoluted Spectra Display Mode | Isotopic Profile (new) |
| Charge State Distribution | |
| Deconvolution Mass Tolerance | 30 ppm |
| Choice of Peak Model | |
| Choice of Peak Model | Intact Protein |
| Resolution at 400 m/z | |
| Raw File Specific | 6187 |
| Generate XIC for Each Component | |
| Calculate XIC | False |

| Advanced Parameters ( ReSpect™) | |
|---|---|
| Charge State Distribution | |
| Model Mass Range | 10000 - 120000 |
| Charge State Range | 5 - 40 |
| Minimum Adjacent Charges (low & high model mass) | 3 - 3 |
| Noise Parameters | |
| Rel. Abundance Threshold (%) | 15 |
| Deconvolution Quality | |
| Quality Score Threshold | 0 |
| Choice of Peak Model | |
| Target Mass | 120000 Da |
| Peak Model Parameters | |
| Number of Peak Models | 1 |
| Left/Right Peak Shape | 2:2 |
| Peak Filter Parameters | |
| Peak Detection Minimum Significance Measure | 1 Standard Deviations |
| Peak Detection Quality Measure | 95% |
| Specialized Parameters | |
| Peak Model Width Factor | 1 |
| Intensity Threshold Scale | 0.01 |
| Deconvolution Parameters | |
| Noise Compensation | True |
| Charge Carrier | H |
| Negative Charge | False |

| Source Spectra Parameters | |
|---|---|
| Source Spectra Method | Sliding Windows |
| Sliding Windows Definition | |
| RT Range | 0.020 - 0.260 minutes |
| Target Avg Spectrum Width | 0.05 minutes |
| Target Avg Spectrum Offset Scan | 1 |
| Sliding Windows Merging Parameters | |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 minutes |
| Min. Number of Detected Intervals | 3 |

## Deconvoluted Spectrum



| Sliding Windows ReSpect Masses Table | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Row Number | Average Mass | Sum Intensity | Relative Abundance | Fractional Abundance | Score | Number of Charge States | Charge State Distribution | Number of Detected Intervals | Mass Std Dev | PPM Std Dev | Delta Mass | Scan Range | Start Time (min) | Stop Time (min) | Apex RT |
| 1 | 28428.52 | 1711541.75 | 100.00 | 70.77 | 23.86 | 4 | 5 - 8 | 9 | 0.60 | 20.96 | 0.00 | 1 - 10 | 0.023 | 0.237 | 0.130 |
| 2 | 18336.19 | 257555.72 | 15.05 | 10.65 | 16.77 | 3 | 6 - 8 | 8 | 1.70 | 92.50 | -10092.33 | 1 - 10 | 0.023 | 0.237 | 0.173 |
| 3 | 51711.96 | 186325.26 | 10.89 | 7.70 | 26.05 | 5 | 13 - 17 | 6 | 2.03 | 39.30 | 23283.44 | 4 - 10 | 0.087 | 0.237 | 0.216 |
| 4 | 31889.50 | 174095.60 | 10.17 | 7.20 | 15.17 | 3 | 10 - 12 | 6 | 1.65 | 51.75 | 3460.98 | 1 - 8 | 0.023 | 0.194 | 0.087 |
| 5 | 42643.41 | 88801.55 | 5.19 | 3.67 | 21.36 | 4 | 12 - 15 | 3 | 2.52 | 59.05 | 14214.88 | 1 - 8 | 0.023 | 0.194 | 0.173 |

**Supplemental File 7:** Biopharma Finder search parameters and outputs for LESA mass spectrum shown in Fig 2C. (Kidney medulla, 10 mM ammonium acetate, 0.125% C8E4).

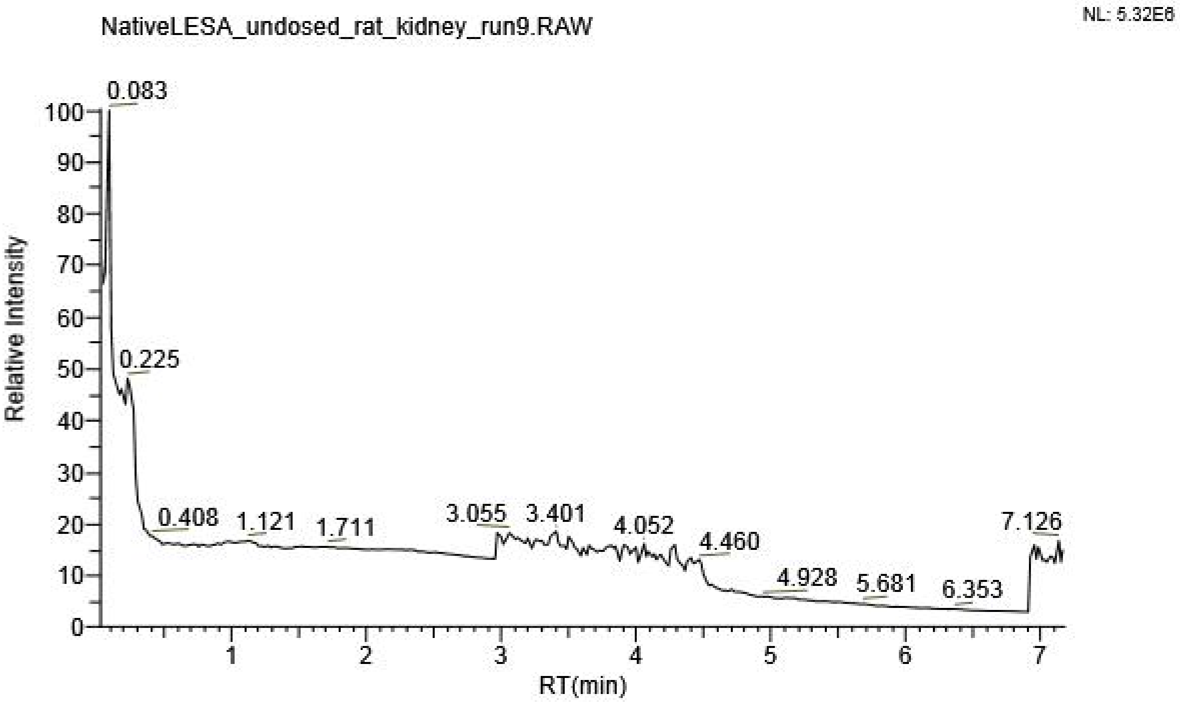
# BioPharma Finder Report

Created: 08/04/2019 14:41:38

| Sample Information | |
|---|---|
| Raw File Name | C:\Xcalibur\Data\ms2LESA\NativeLESA_undosed_rat_kidney_run9.RAW |
| Instrument Method | |
| Vial | |
| Injection Volume (µL) | 0 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 0 |

| Chromatogram Parameters | |
|---|---|
| Use Restricted Time | False |
| Time Limits | 0.023 - 7.169 minutes |
| Scan Range | 1 - 334 |
| m/z Range | 2000 - 20000 |
| Chromatogram Trace Type | TIC |
| Sensitivity | High |
| Rel. Intensity Threshold (%) | 1 |

Chromatogram

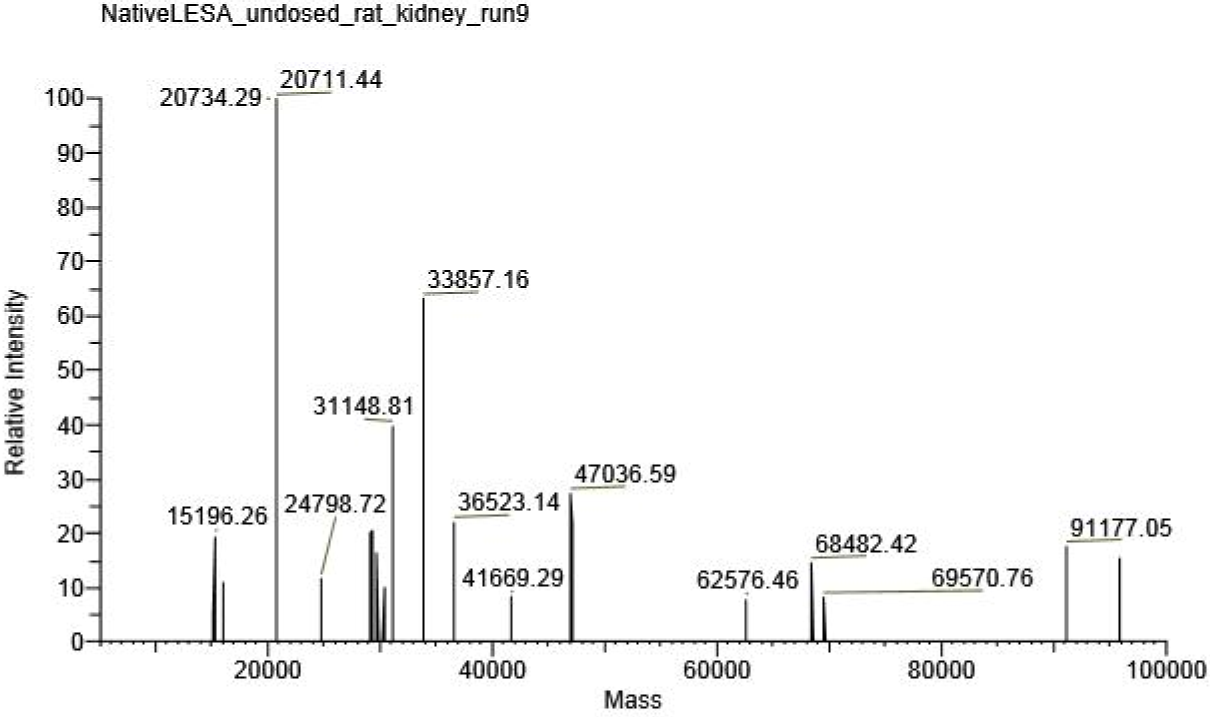


| Main Parameters ( ReSpect™ ) | |
|---|---|
| Deconvolution Results Filter | |
| Output Mass Range | 5000 - 100000 |
| Deconvoluted Spectra Display Mode | Isotopic Profile (new) |
| Charge State Distribution | |
| Deconvolution Mass Tolerance | 25 ppm |
| Choice of Peak Model | |
| Choice of Peak Model | Intact Protein |
| Resolution at 400 m/z | |
| Raw File Specific | 6187 |
| Generate XIC for Each Component | |
| Calculate XIC | False |

| Advanced Parameters ( ReSpect™) | |
|---|---|
| Charge State Distribution | |
| Model Mass Range | 10000 - 120000 |
| Charge State Range | 5 - 40 |
| Minimum Adjacent Charges (low & high model mass) | 3 - 3 |
| Noise Parameters | |
| Rel. Abundance Threshold (%) | 15 |
| Deconvolution Quality | |
| Quality Score Threshold | 0 |
| Choice of Peak Model | |
| Target Mass | 120000 Da |
| Peak Model Parameters | |
| Number of Peak Models | 1 |
| Left/Right Peak Shape | 2:2 |
| Peak Filter Parameters | |
| Peak Detection Minimum Significance Measure | 1 Standard Deviations |
| Peak Detection Quality Measure | 95% |
| Specialized Parameters | |
| Peak Model Width Factor | 1 |
| Intensity Threshold Scale | 0.01 |
| Deconvolution Parameters | |
| Noise Compensation | True |
| Charge Carrier | H |
| Negative Charge | False |

| Source Spectra Parameters | |
|---|---|
| Source Spectra Method | Sliding Windows |
| Sliding Windows Definition | |
| RT Range | 0.300 - 3.300 minutes |
| Target Avg Spectrum Width | 0.2 minutes |
| Target Avg Spectrum Offset Scan | 1 |
| Sliding Windows Merging Parameters | |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 minutes |
| Min. Number of Detected Intervals | 40 |

Deconvoluted Spectrum



### Sliding Windows ReSpect Masses Table

| Row Number | Average Mass | Sum Intensity | Relative Abundance | Fractional Abundance | Score | Number of Charge States | Charge State Distribution | Number of Detected Intervals | Mass Std Dev | PPM Std Dev | Delta Mass | Scan Range | Start Time (min) | Stop Time (min) | Apex RT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 20711.44 | 19849421.89 | 100.00 | 22.00 | 22.63 | 4 | 5 - 8 | 138 | 0.63 | 30.29 | 0.00 | 15 - 161 | 0.307 | 3.299 | 2.383 |
| 2 | 33857.16 | 12522848.07 | 63.09 | 13.88 | 23.91 | 6 | 7 - 12 | 137 | 1.55 | 45.76 | 13145.73 | 16 - 161 | 0.327 | 3.299 | 2.200 |
| 3 | 47036.59 | 5397511.39 | 27.19 | 5.98 | 24.33 | 6 | 9 - 14 | 107 | 3.48 | 73.91 | 26325.15 | 40 - 161 | 0.815 | 3.299 | 2.749 |
| 4 | 20734.29 | 5151119.87 | 25.95 | 5.71 | 18.78 | 4 | 5 - 8 | 99 | 0.43 | 20.74 | 22.86 | 23 - 146 | 0.469 | 2.994 | 2.037 |
| 5 | 31148.81 | 5146309.42 | 25.93 | 5.70 | 21.48 | 5 | 7 - 11 | 85 | 2.07 | 66.36 | 10437.37 | 16 - 161 | 0.327 | 3.299 | 1.854 |
| 6 | 36523.14 | 4335162.62 | 21.84 | 4.80 | 15.54 | 3 | 11 - 13 | 100 | 1.07 | 29.29 | 15811.70 | 35 - 160 | 0.714 | 3.279 | 1.039 |
| 7 | 29206.24 | 4050590.31 | 20.41 | 4.49 | 26.29 | 5 | 6 - 10 | 109 | 1.68 | 57.39 | 8494.81 | 25 - 161 | 0.510 | 3.299 | 2.403 |
| 8 | 15196.26 | 3813644.23 | 19.21 | 4.23 | 17.10 | 3 | 5 - 7 | 102 | 0.58 | 38.46 | -5515.18 | 17 - 154 | 0.347 | 3.157 | 2.403 |
| 9 | 91177.05 | 3467631.17 | 17.47 | 3.84 | 22.89 | 4 | 29 - 32 | 93 | 4.21 | 46.19 | 70465.61 | 27 - 155 | 0.551 | 3.177 | 1.670 |
| 10 | 29326.39 | 3235284.87 | 16.30 | 3.59 | 23.00 | 5 | 6 - 10 | 93 | 1.86 | 63.57 | 8614.96 | 33 - 161 | 0.673 | 3.299 | 3.116 |
| 11 | 29735.99 | 3232881.38 | 16.29 | 3.58 | 15.26 | 6 | 6 - 12 | 55 | 1.69 | 56.70 | 9024.55 | 35 - 147 | 0.714 | 3.014 | 1.691 |
| 12 | 95852.40 | 3050618.05 | 15.37 | 3.38 | 15.62 | 4 | 24 - 27 | 65 | 5.02 | 52.41 | 75140.96 | 40 - 150 | 0.815 | 3.075 | 1.752 |
| 13 | 31146.56 | 2932689.72 | 14.77 | 3.25 | 25.64 | 6 | 6 - 11 | 43 | 2.38 | 76.49 | 10435.13 | 42 - 159 | 0.856 | 3.258 | 2.342 |
| 14 | 68482.42 | 2868304.85 | 14.45 | 3.18 | 18.49 | 3 | 17 - 19 | 78 | 2.36 | 34.43 | 47770.98 | 15 - 106 | 0.307 | 2.179 | 0.673 |
| 15 | 24798.72 | 2298792.11 | 11.58 | 2.55 | 18.71 | 4 | 6 - 9 | 77 | 1.04 | 42.02 | 4087.28 | 23 - 158 | 0.469 | 3.238 | 1.284 |
| 16 | 15952.35 | 2157903.03 | 10.87 | 2.39 | 20.72 | 3 | 5 - 7 | 74 | 0.46 | 28.75 | -4759.09 | 58 - 158 | 1.182 | 3.238 | 2.403 |
| 17 | 30305.48 | 1965608.27 | 9.90 | 2.18 | 20.90 | 7 | 6 - 12 | 58 | 1.44 | 47.64 | 9594.05 | 43 - 150 | 0.877 | 3.075 | 2.485 |
| 18 | 41669.29 | 1640651.37 | 8.27 | 1.82 | 22.08 | 5 | 8 - 12 | 54 | 2.92 | 69.97 | 20957.86 | 18 - 147 | 0.368 | 3.014 | 1.956 |
| 19 | 69570.76 | 1610236.26 | 8.11 | 1.78 | 14.18 | 3 | 21 - 23 | 46 | 5.44 | 78.18 | 48859.32 | 66 - 146 | 1.345 | 2.994 | 2.729 |
| 20 | 62576.46 | 1514752.34 | 7.63 | 1.68 | 14.13 | 4 | 15 - 18 | 49 | 4.11 | 65.69 | 41865.02 | 15 - 160 | 0.307 | 3.279 | 1.548 |

**Supplemental File 8:** Biopharma Finder search parameters and outputs for LESA mass spectrum obtained from a separate medulla location. (Kidney medulla, 10 mM ammonium acetate, 0.125% C8E4).

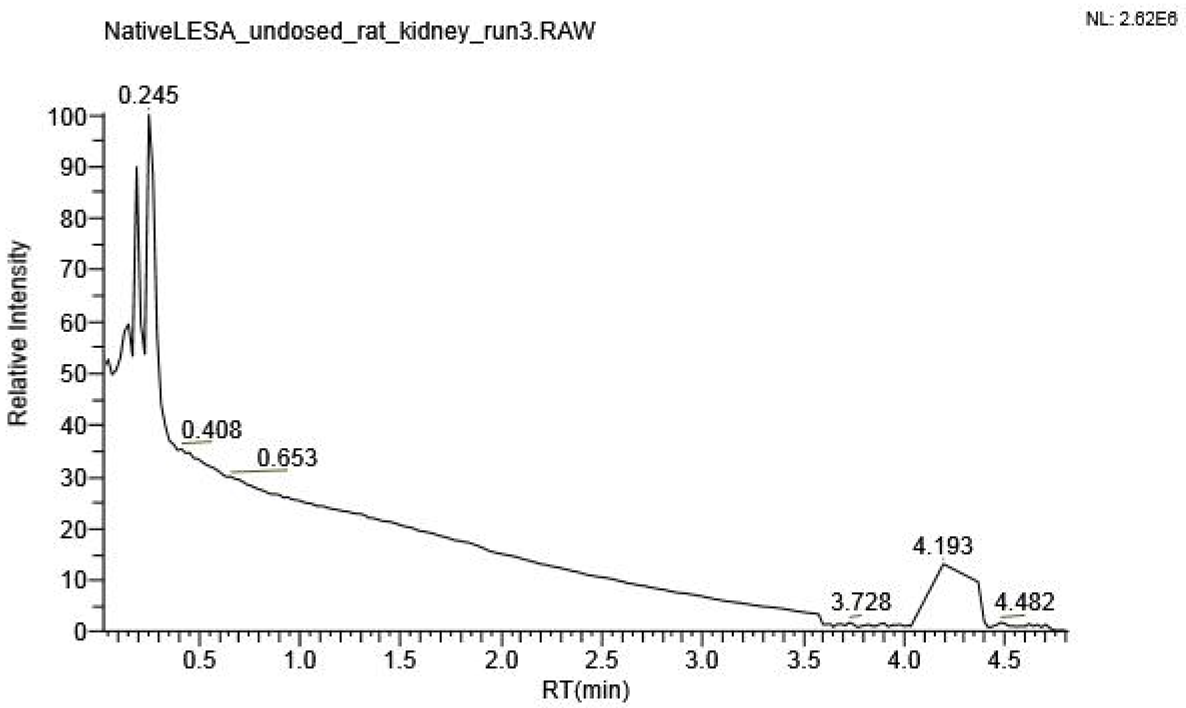
# BioPharma Finder Report

Created: 08/04/2019 14:48:25

| Sample Information | |
|---|---|
| Raw File Name | C:\Xcalibur\Data\ms2LESA\NativeLESA_undosed_rat_kidney_run3.RAW |
| Instrument Method | |
| Vial | |
| Injection Volume (µL) | 0 |
| Sample Weight | 0 |
| Sample Volume (µL) | 0 |
| ISTD Amount | 0 |
| Dil Factor | 0 |

| Chromatogram Parameters | |
|---|---|
| Use Restricted Time | False |
| Time Limits | 0.023 - 7.169 minutes |
| Scan Range | 1 - 334 |
| m/z Range | 2000 - 20000 |
| Chromatogram Trace Type | TIC |
| Sensitivity | High |
| Rel. Intensity Threshold (%) | 1 |

Chromatogram

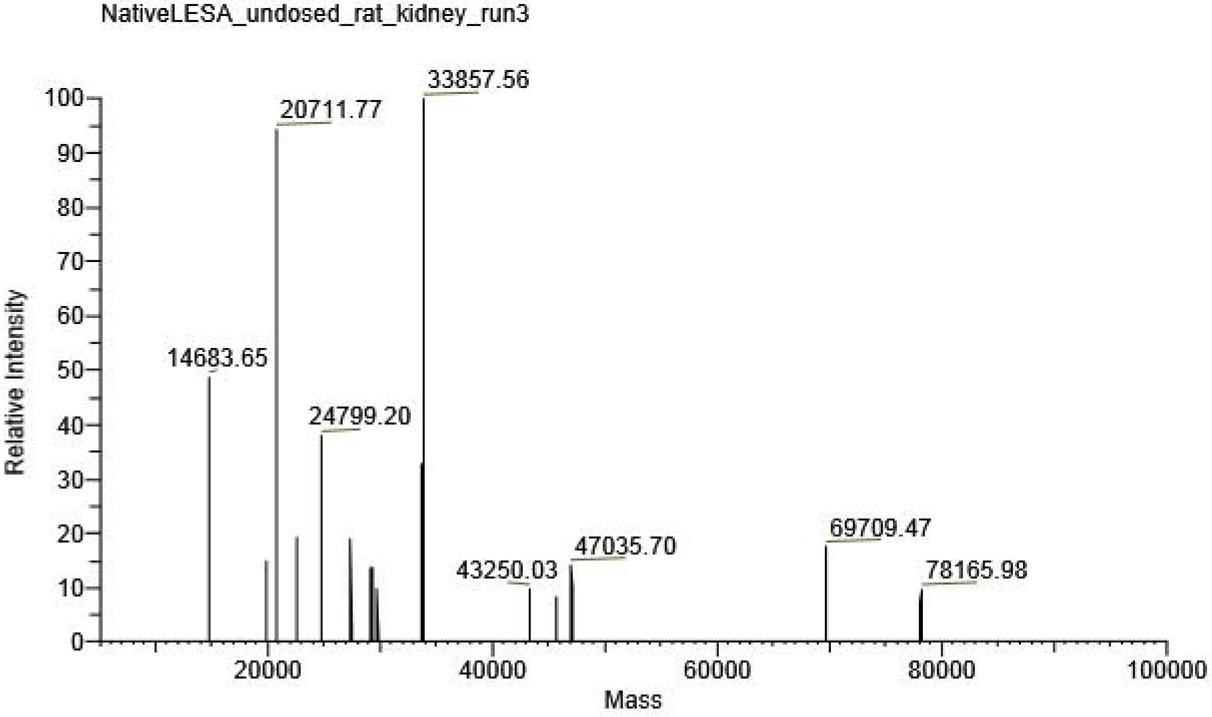


| Main Parameters ( ReSpect™ ) | |
|---|---|
| Deconvolution Results Filter | |
| Output Mass Range | 5000 - 100000 |
| Deconvoluted Spectra Display Mode | Isotopic Profile (new) |
| Charge State Distribution | |
| Deconvolution Mass Tolerance | 30 ppm |
| Choice of Peak Model | |
| Choice of Peak Model | Intact Protein |
| Resolution at 400 m/z | |
| Raw File Specific | 6187 |
| Generate XIC for Each Component | |
| Calculate XIC | False |

| Advanced Parameters ( ReSpect™) | |
|---|---|
| Charge State Distribution | |
| Model Mass Range | 10000 - 120000 |
| Charge State Range | 5 - 40 |
| Minimum Adjacent Charges (low & high model mass) | 3 - 3 |
| Noise Parameters | |
| Rel. Abundance Threshold (%) | 15 |
| Deconvolution Quality | |
| Quality Score Threshold | 0 |
| Choice of Peak Model | |
| Target Mass | 120000 Da |
| Peak Model Parameters | |
| Number of Peak Models | 1 |
| Left/Right Peak Shape | 2:2 |
| Peak Filter Parameters | |
| Peak Detection Minimum Significance Measure | 1 Standard Deviations |
| Peak Detection Quality Measure | 95% |
| Specialized Parameters | |
| Peak Model Width Factor | 1 |
| Intensity Threshold Scale | 0.01 |
| Deconvolution Parameters | |
| Noise Compensation | True |
| Charge Carrier | H |
| Negative Charge | False |

| Source Spectra Parameters | |
|---|---|
| Source Spectra Method | Sliding Windows |
| Sliding Windows Definition | |
| RT Range | 0.500 - 3.000 minutes |
| Target Avg Spectrum Width | 0.2 minutes |
| Target Avg Spectrum Offset Scan | 1 |
| Sliding Windows Merging Parameters | |
| Merge Tolerance | 30 ppm |
| Max RT Gap | 0.5 minutes |
| Min. Number of Detected Intervals | 40 |

## Deconvoluted Spectrum



## Sliding Windows ReSpect Masses Table

| Row Number | Average Mass | Sum Intensity | Relative Abundance | Fractional Abundance | Score | Number of Charge States | Charge State Distribution | Number of Detected Intervals | Mass Std Dev | PPM Std Dev | Delta Mass | Scan Range | Start Time (min) | Stop Time (min) | Apex RT |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 33857.56 | 12656058.89 | 100.00 | 22.05 | 30.47 | 6 | 7 - 12 | 113 | 1.29 | 38.12 | 0.00 | 25 - 146 | 0.510 | 2.994 | 0.612 |
| 2 | 20711.77 | 11932977.46 | 94.29 | 20.79 | 22.73 | 4 | 5 - 8 | 113 | 0.66 | 31.82 | -13145.79 | 25 - 146 | 0.510 | 2.994 | 0.612 |
| 3 | 24799.20 | 4797751.65 | 37.91 | 8.36 | 20.59 | 4 | 6 - 9 | 113 | 0.92 | 36.92 | -9058.36 | 25 - 146 | 0.510 | 2.994 | 0.612 |
| 4 | 14683.65 | 4760163.36 | 37.61 | 8.29 | 16.50 | 3 | 5 - 7 | 96 | 0.31 | 21.36 | -19173.91 | 32 - 142 | 0.653 | 2.912 | 1.365 |
| 5 | 33716.86 | 4135550.76 | 32.68 | 7.20 | 16.57 | 3 | 8 - 10 | 113 | 1.36 | 40.36 | -140.70 | 25 - 146 | 0.510 | 2.994 | 0.938 |
| 6 | 22528.56 | 2426025.40 | 19.17 | 4.23 | 18.05 | 4 | 5 - 8 | 84 | 1.75 | 77.73 | -11329.00 | 31 - 142 | 0.632 | 2.912 | 0.917 |
| 7 | 27374.65 | 2389225.53 | 18.88 | 4.16 | 21.79 | 4 | 6 - 9 | 92 | 1.59 | 57.92 | -6482.91 | 44 - 146 | 0.897 | 2.994 | 1.935 |
| 8 | 69709.47 | 2217647.63 | 17.52 | 3.86 | 14.49 | 3 | 21 - 23 | 82 | 2.88 | 41.25 | 35851.91 | 32 - 131 | 0.653 | 2.688 | 0.917 |
| 9 | 14686.72 | 2028902.20 | 16.03 | 3.53 | 21.67 | 3 | 5 - 7 | 61 | 0.21 | 14.12 | -19170.84 | 64 - 141 | 1.304 | 2.892 | 1.691 |
| 10 | 19872.59 | 1871867.97 | 14.79 | 3.26 | 16.39 | 3 | 6 - 8 | 57 | 0.57 | 28.78 | -13984.96 | 29 - 121 | 0.592 | 2.485 | 1.650 |
| 11 | 47035.70 | 1773721.29 | 14.01 | 3.09 | 27.78 | 6 | 9 - 14 | 56 | 3.31 | 70.43 | 13178.14 | 52 - 146 | 1.060 | 2.994 | 2.017 |
| 12 | 29205.97 | 1715512.18 | 13.55 | 2.99 | 25.04 | 5 | 6 - 10 | 87 | 1.72 | 58.72 | -4651.59 | 25 - 146 | 0.510 | 2.994 | 1.365 |
| 13 | 29734.57 | 1227954.21 | 9.70 | 2.14 | 15.04 | 3 | 10 - 12 | 43 | 2.09 | 70.40 | -4122.99 | 36 - 101 | 0.734 | 2.078 | 1.019 |
| 14 | 43250.03 | 1223301.38 | 9.67 | 2.13 | 19.46 | 3 | 12 - 14 | 49 | 2.09 | 48.40 | 9392.47 | 28 - 109 | 0.571 | 2.240 | 1.162 |
| 15 | 78165.98 | 1202540.78 | 9.50 | 2.10 | 13.95 | 3 | 21 - 23 | 41 | 7.38 | 94.41 | 44308.42 | 33 - 90 | 0.673 | 1.854 | 1.162 |
| 16 | 45659.72 | 1039819.48 | 8.22 | 1.81 | 16.80 | 3 | 10 - 12 | 41 | 3.76 | 82.28 | 11802.16 | 25 - 85 | 0.510 | 1.752 | 0.612 |