

PRODUCT DATA SHEET

Pierce FlexMix Calibration Solution

Product Number: A39239

Lot Number: 3272837

Expiration: July 17, 2027

Summary:

The Thermo Scientific™ Pierce™ FlexMix Calibration Solution is a room-temperature stable, ready-to-use liquid formulation for the calibration of all Thermo Scientific Tribrid™ mass spectrometers. The only additional materials required are a 500µL Hamilton syringe and a liquid infusion line, both supplied with the instrument.

Visual:

Clear, colorless liquid

Components	Accurate Mass (m/z)	Specification (neat)	Results
*LC-MS grade acetonitrile (90% v/v)	--	Purity ≥ 99.9%	Pass
*LC-MS grade water (10% v/v)	--	LC-MS Grade	Pass
LC-MS grade acetic acid	59.0139 ^{b(-)}	Purity ≥ 99.7%	Pass
Imidazole	69.0447 ^{a(+)}	Purity ≥ 99.0%	Pass
Triethylamine	102.1277 ^{a(+)}	Purity ≥ 99.5%	Pass
Trifluoroacetic acid (TFA)	112.9856 ^{b(-)}	Purity ≥ 99.5%	Pass
Tetramethylpiperidine	142.1590 ^{a(+)}	Purity ≥ 97.5%	Pass
Pentafluoropropionic acid	162.9824 ^{b(-)}	Purity ≥ 97.0%	Pass
Caffeine	195.0876 ^{a(+)}	Purity ≥ 97.0%	Pass
Hexamethoxyphosphazene	322.0481 ^{a(+)}	Purity ≥ 99.0%	Pass
Perfluorooctanoic acid	362.9696 ^{b(-)}	Purity ≥ 96.0%	Pass
MRFA	524.2649 ^{a(+)}	Purity ≥ 98%	Pass
2,4,6-Tris(heptafluoropropyl)-1,3,5-triazine	601.9779 ^{c(-)}	Purity ≥ 95.0%	Pass
Hexakis(2,2-difluoroethoxy) phosphazene	622.0290 ^{a(+)}	Purity ≥ 97.0%	Pass
Hexakis(2,2,3,3-tetrafluoropropoxy) phosphazene	922.0098 ^{a(+)} , 1033.9881 ^{d(-)}	Purity ≥ 95.0%	Pass
Ultramark 1621	See note below	Purity ≥ 95.0%	Pass
Hexakis(1h,1h,7h-perfluoroheptoxy) phosphazene	2121.9331 ^{a(+)} , 2233.9115 ^{d(-)}	Purity ≥ 95.0%	Pass
Hexakis(1h,1h,9h-perfluorononyloxy) phosphazene	2721.8948 ^{a(+)} , 2833.8731 ^{d(-)}	Purity ≥ 95.0%	Pass

^a[M+H]⁺

^b[M-H]⁻

^c[M+OH]⁻

^d[M+TFA]⁻

*Combined concentration of all other components listed is less than 1% w/v

Note: Ultramark 1622 is a well-defined mixture of compounds producing a well-defined peak envelope in the range of 900-2200 m/z in the positive and negative ion modes.

Important Product Information:

- For best results, use a dedicated syringe and infusion line.
- Before and after calibration, flush the syringe and infusion line with 1:1 water/acetonitrile solution to clean.
- Turn on the mass spectrometer and wait for it to enter ready state.
- Infuse the calibration solution and optimize spray conditions until a spray stability of ≤ 15% RSD is achieved before initiating calibration routine.

Storage:

Upon receipt store at room temperature

Compatible with these Thermo Scientific™ Instruments:

Orbitrap Fusion™ MS

Orbitrap Fusion™ Lumos™ MS

Orbitrap ID-X MS

Orbitrap Tribrid™ Series 3.1 Instrument Control Software (or later)

Additional information:

For MSDS please visit

www.thermoscientific.com/pierce

For calibration procedure use:

Orbitrap Tribrid Series Getting Started Guide (June 2018)

Technical Support:

For hardware related support: 1-800-532-4752

For reagent support: 1-800-874-3723

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Analysis	Specification	Results
Positive Mode Target Ions (m/z) 69, 102, 142, 195, 322, 524, 622, 922, 1122, 1222, 1322, 1422, 1522, 1622, 1722, 1822, 2122, and 2722 m/z.	All calibration ions are present in the spectrum	Pass
Negative Mode Target Ions (m/z) 113, 163, 363, 602, 1034, 1234, 1334, 1434, 1534, 1634, 1734, 1834, 1934, 2234, and 2834 m/z	All calibration ions are present in the spectrum	Pass
Positive Mode Target Ions (m/z) 69, 102, 142, 195, 322, 524, 622, 922, 1522, 2122, and 2722 m/z	Ratio to Reference is between 0.5 and 2.0 for all ions listed below in positive ion mode: 69, 102, 142, 195, 322, 524, 622, 922, 1522, 2122, and 2722 m/z	Pass
Negative Mode Target Ions (m/z) 113, 163, 363, 602, 1034, 1534, 2234, and 2834 m/z	Ratio to Reference is between 0.5 and 2.0 for all ions listed below in negative ion mode: 113, 163, 363, 602, 1034, 1534, 2234, and 2834 m/z	Pass
Positive Mode Target Ions (m/z) 69, 102, 142, 195, 322, 524, 622, 922, 1122, 1222, 1322, 1422, 1522, 1622, 1722, 1822, 2122, 2722 Negative Mode Target Ions (m/z) 113, 163, 363, 602, 1034, 1234, 1334, 1434, 1534, 1634, 1734, 1834, 1934, 2234, 2834	Contaminant ions are not > 30% of the intensity of the target reference peak within +/- 10 m/z in both positive and negative mode*.	Pass

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Timothy Morton, Sr. Quality Chemist, Mass Spectrometry



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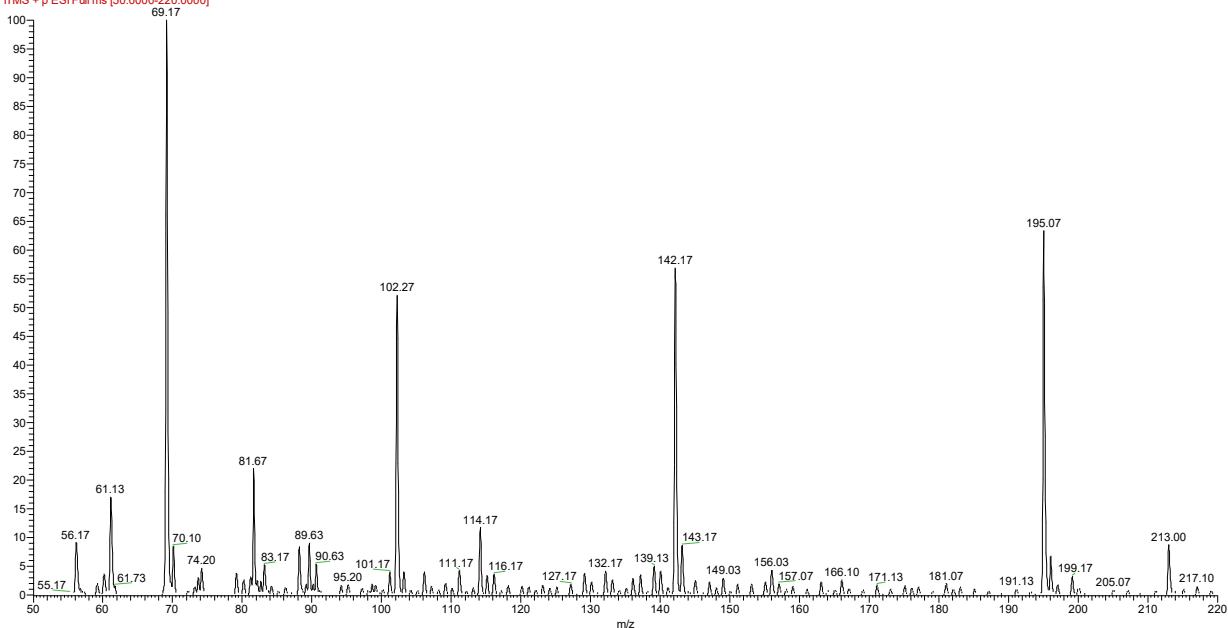
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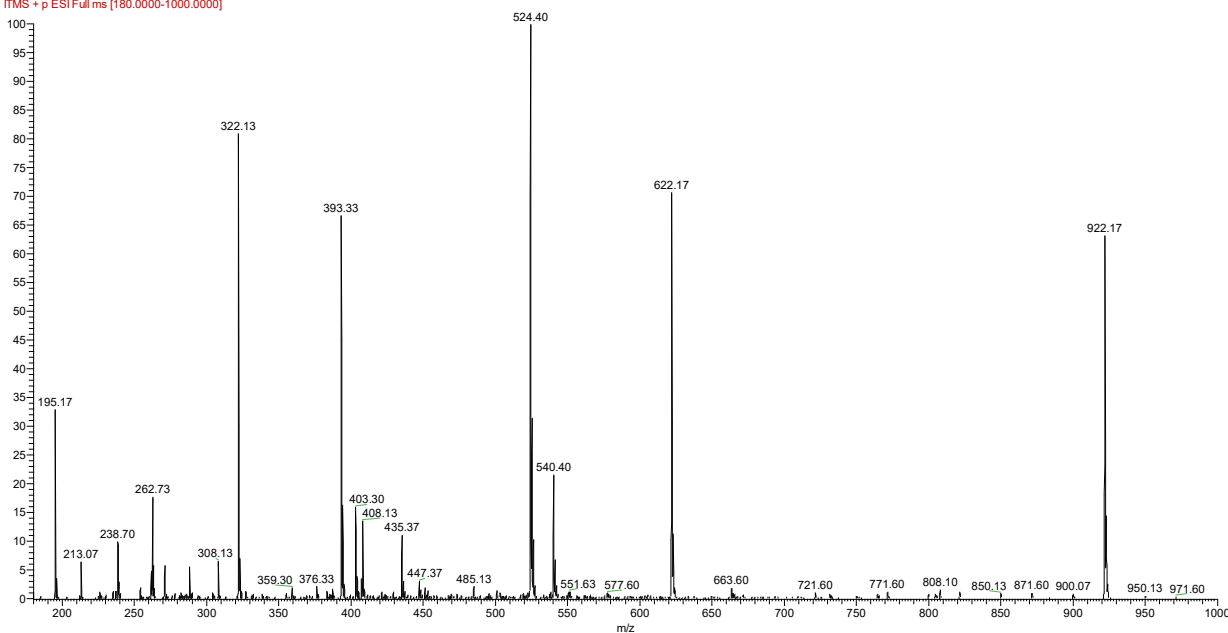
Positive Ion Mode (Ion Trap, Normal Scan Mode), 50-220 m/z

3257270_F#1-5986 RT: 0.00-1.00 AV: 1297 NL: 9.37E5
F: ITMS + p ESI Full ms [50.0000-220.0000]



Positive Ion Mode (Ion Trap, Normal Scan Mode), 180-1000 m/z

3257270_F#1-5986 RT: 1.00-2.00 AV: 829 NL: 9.76E5
F: ITMS + p ESI Full ms [180.0000-1000.0000]



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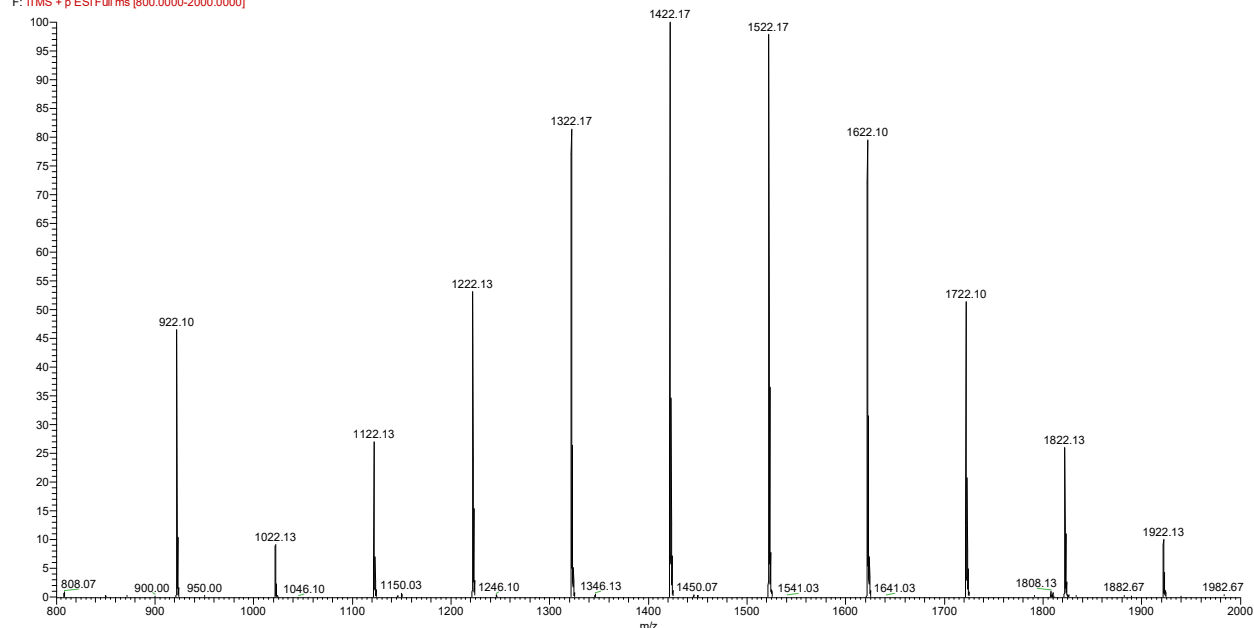
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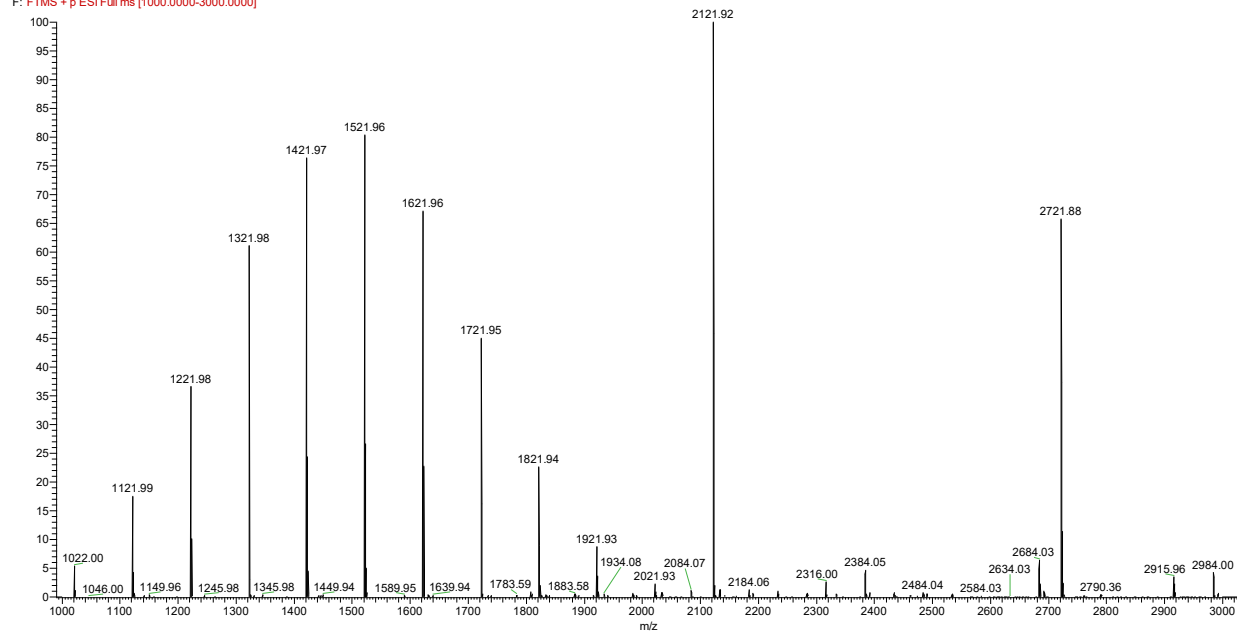
Positive Ion Mode (Ion Trap, Normal Scan Mode), 800-2000 m/z

3257270_F#1-5986 RT: 2.00-3.00 AV: 664 NL: 2.00E6
F: FTMS + p ESI Full ms [800.0000-2000.0000]



Positive Ion Mode (Orbitrap, High Scan Mode), 1000-3000 m/z

3257270_F#1-5986 RT: 3.01-4.00 AV: 152 NL: 3.02E8
F: FTMS + p ESI Full ms [1000.0000-3000.0000]



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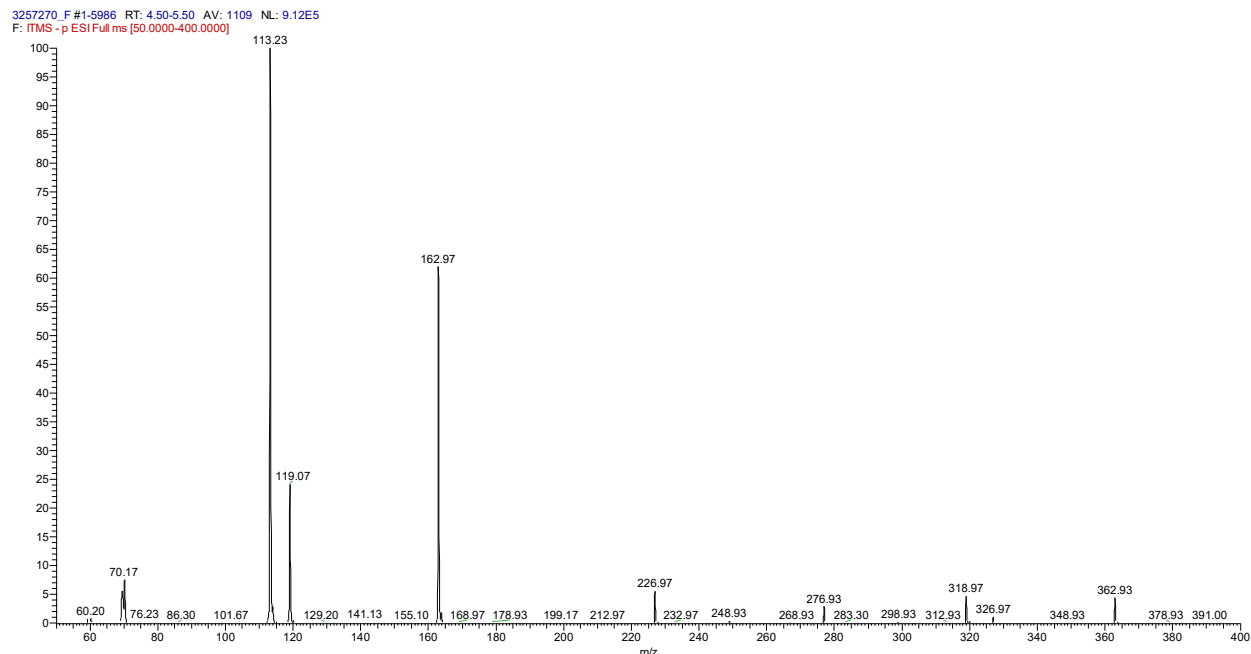
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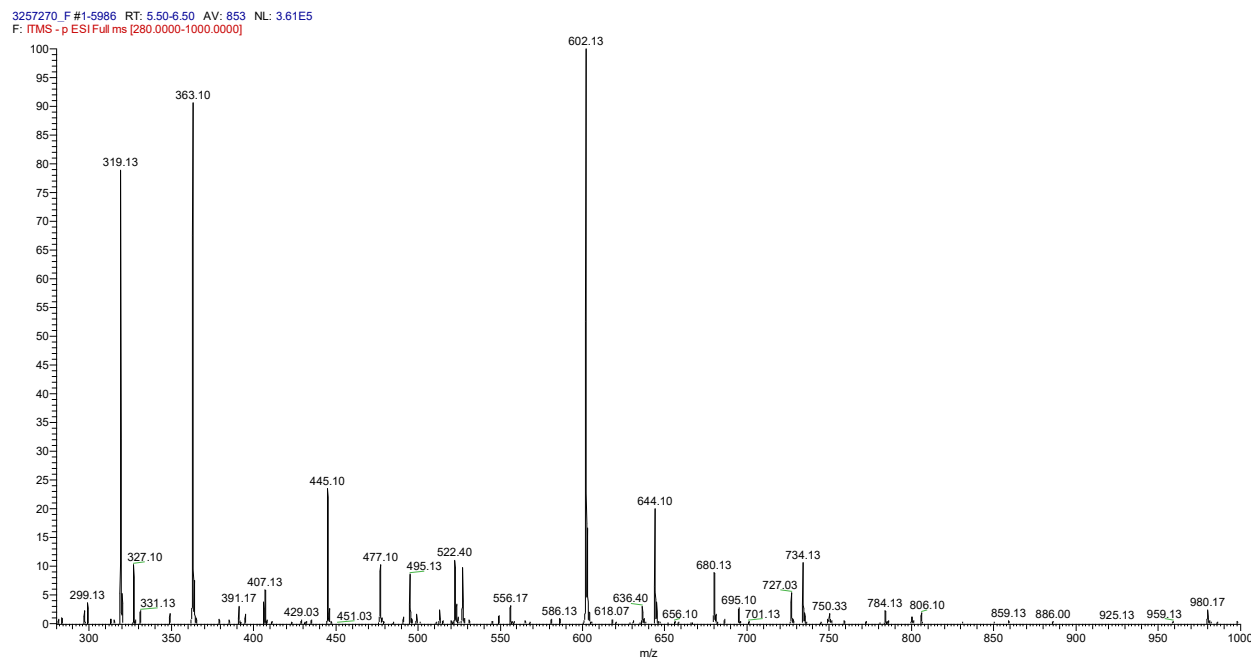
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Negative Ion Mode (Ion Trap, Normal Scan Mode), 50-400 m/z



Negative Ion Mode (Ion Trap, Normal Scan Mode), 280-1000 m/z



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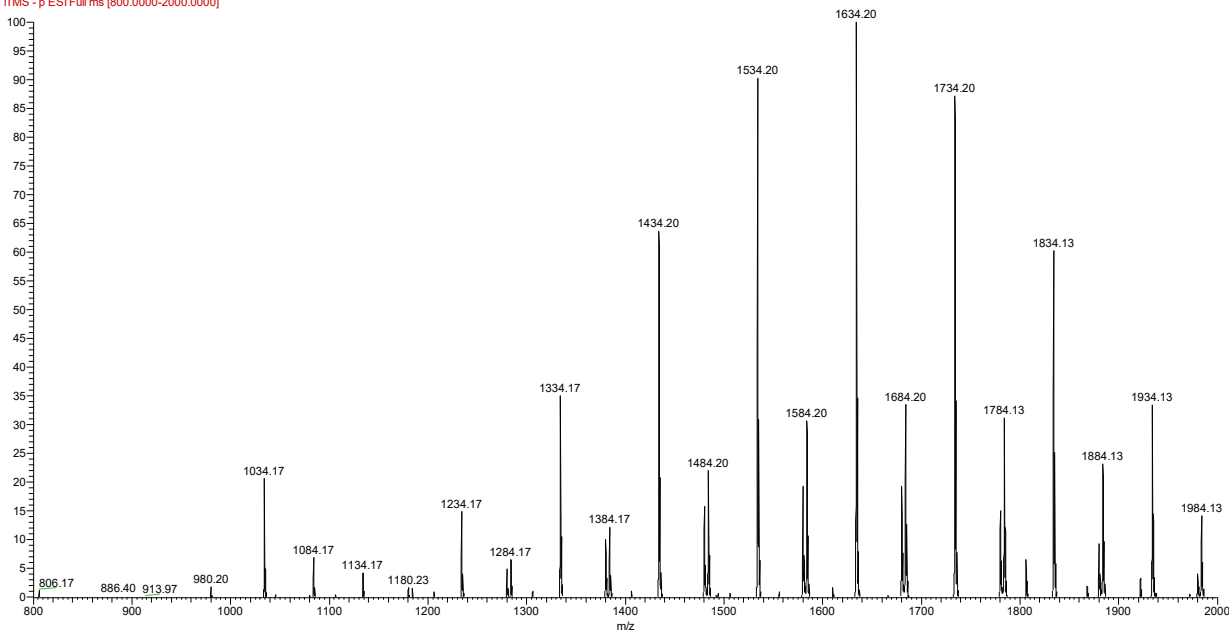
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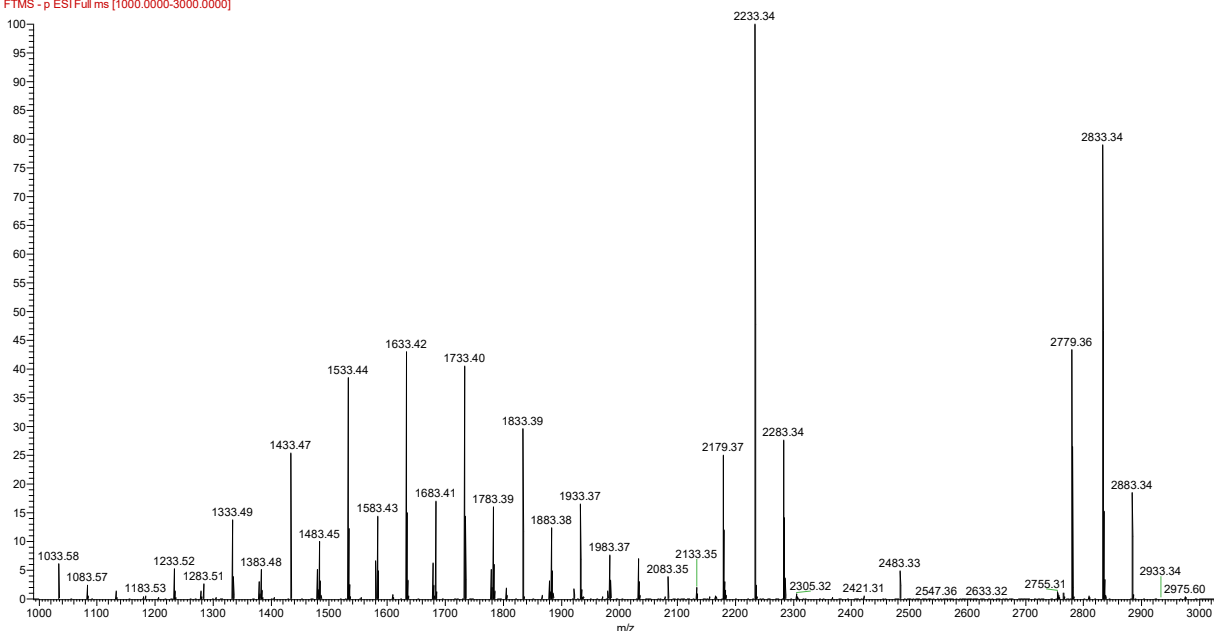
Negative Ion Mode (Ion Trap, Normal Scan Mode), 800-2000 m/z

3257270_F#1-5986 RT: 6.50-7.50 AV: 666 NL: 1.47E6
F: FTMS -p ESI Full ms [800.0000-2000.0000]



Negative Ion Mode (Orbitrap, High Scan Mode), 1000-3000 m/z

3257270_F#1-5986 RT: 7.51-8.50 AV: 152 NL: 1.20E9
F: FTMS -p ESI Full ms [1000.0000-3000.0000]



Spectra were acquired on a Thermo Scientific™ Orbitrap Eclipse Mass Spectrometer

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