

#### PRODUCT DATA SHEET

#### Pierce FlexMix Calibration Solution

Product Number: A39239 Lot Number: 3261374 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 <sup>b(-)</sup>	Purity ≥ 99.7%	Pass
Imidazole	69.0447 <sup>a(+)</sup>	Purity ≥ 99.0%	Pass
Triethylamine	102.1277 <sup>a(+)</sup>	Purity ≥ 99.5%	Pass
Trifluoroacetic acid (TFA)	112.9856 <sup>b(-)</sup>	Purity ≥ 99.5%	Pass
Tetramethylpiperidine	142.1590 <sup>a(+)</sup>	Purity ≥ 97.5%	Pass
Pentafluoropropionic acid	162.9824 <sup>b(-)</sup>	Purity ≥ 97.0%	Pass
Caffeine	195.0876a(+)	Purity ≥ 97.0%	Pass
Hexamethoxyphosphazene	322.0481a(+)	Purity ≥ 99.0%	Pass
Perfluoroheptanoic acid	362.9696 <sup>b(-)</sup>	Purity ≥ 96.0%	Pass
MRFA	524.2649 <sup>(a)+</sup>	Purity ≥ 98%	Pass
2,4,6-Tris(heptafluoropropyl)- 1,3,5-triazine	601.9779 <sup>c(-)</sup>	Purity ≥ 95.0%	Pass
Hexakis(2,2-difluoroethoxy) phosphazene	622.0290 <sup>a(+)</sup>	Purity ≥ 97.0%	Pass
Hexakis(2,2,3,3- tetrafluoropropoxy) phosphazene	922.0098 <sup>a(+)</sup> , 1033.9881 <sup>d(-)</sup>	Purity ≥ 95.0%	Pass
Ultramark 1621	See note below	Purity ≥ 95.0%	Pass
Hexakis(1h,1h,7h- perfluoroheptoxy) phosphazene	2121.9331 <sup>a(+)</sup> , 2233.9115 <sup>d(-)</sup>	Purity ≥ 95.0%	Pass
Hexakis(1h,1h,9h- perfluorononyloxy) phosphazene	2721.8948 <sup>a(+)</sup> , 2833.8731 <sup>d(-)</sup>	Purity ≥ 95.0%	Pass

a[M+H]+

**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<sup>™</sup> MS

Orbitrap Fusion<sup>TM</sup> Lumos<sup>TM</sup> MS

Orbitrap ID-X MS

Orbitrap Tribrid<sup>™</sup> 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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<sup>&</sup>lt;sup>b</sup>[M-H]⁻

c[M+OH]<sup>-</sup> c[M+TFA]-

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



Analysis	Specification	Results
Positive Mode Target lons (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 <i>m/z</i>	63, 363, 602, 1034,1234, 1334, 1434, 1534,  All calibration ions are present in the spectrum	
Positive Mode Target Ions (m/z) 69, 102, 142, 195, 322, 524, 622, 922, 1522, 2122, and 2722 m/z	02, 142, 195, 322, 524, 622, 922, 1522, 2122, and 69, 102, 142, 195, 322, 524, 622, 922, 1522, 2122,	
Negative Mode Target lons (m/z) 113, 163, 363, 602, 1034, 1534, 2234, and 2834 <i>m/z</i>	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 <i>m/z</i>	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

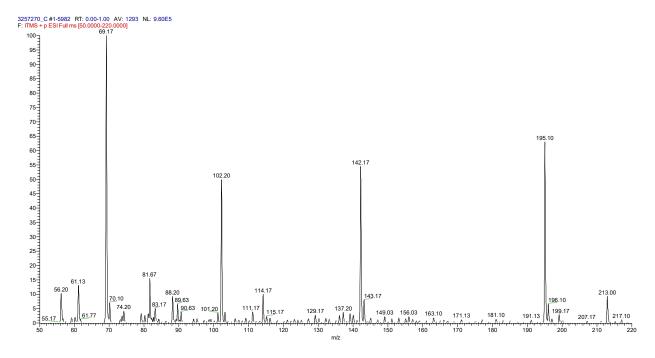


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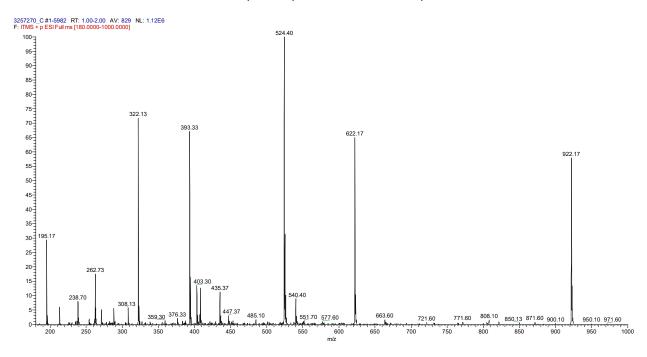
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# Positive Ion Mode (Ion Trap, Normal Scan Mode), 50-220 m/z



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

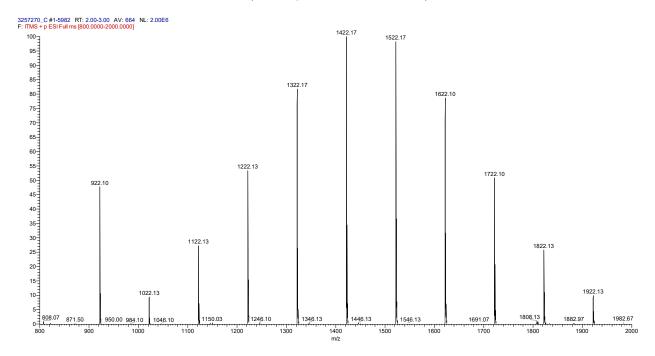


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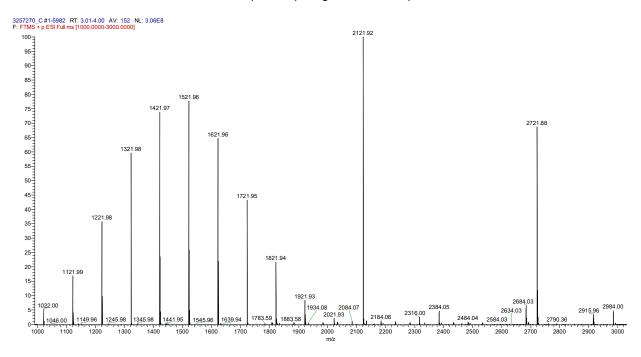
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# Positive Ion Mode (Ion Trap, Normal Scan Mode), 800-2000 m/z



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

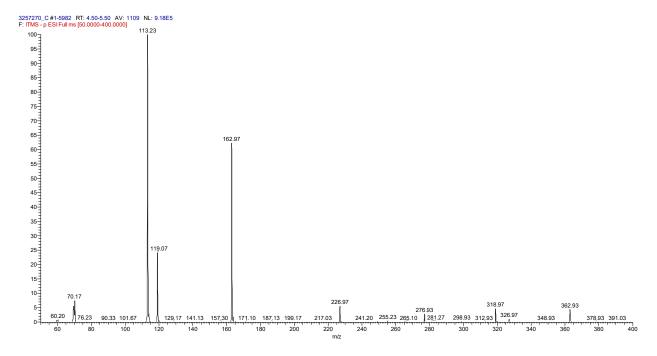


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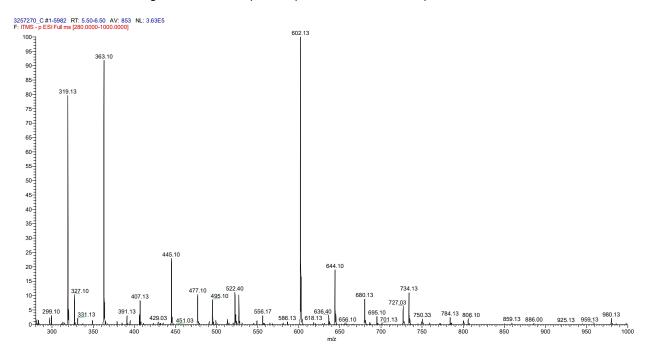
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# Negative Ion Mode (Ion Trap, Normal Scan Mode), 50-400 m/z



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

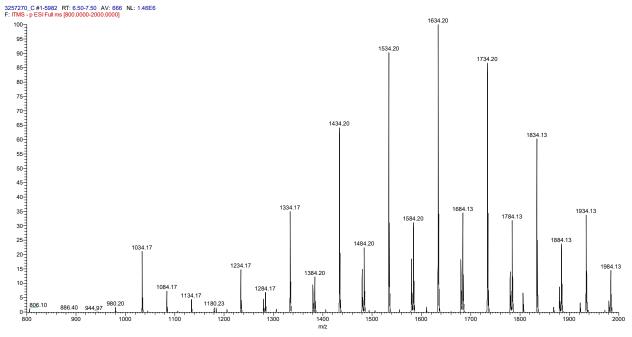


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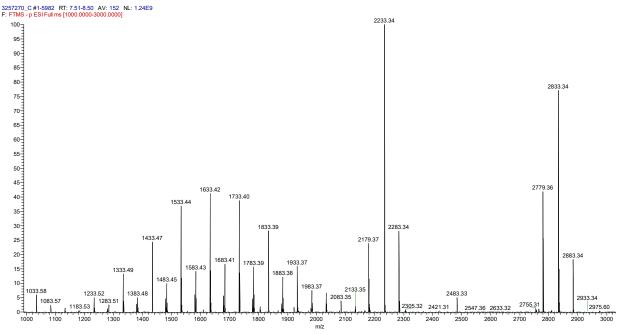
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# Negative Ion Mode (Ion Trap, Normal Scan Mode), 800-2000 m/z



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



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

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