Thermo EASY-LC method print for Thermo

Sample pickup:

Volume [μ l] : 4.00 Flow [μ l / min] : 10.00 Volume [µl]

Sample loading:_

Volume [μ l] : 10.00 Flow [μ l / min] : (unspecified)

Max. pressure [Bar] : 750.00

Gradient:

| Time [mm:ss] | Duration [mm:ss] | Flow [nl/min] | Mixture [%B] |
|--------------|------------------|---------------|--------------|
| 00:00 | 00:00 | 250.00 | 2.00 |
| 05:00 | 05:00 | 250.00 | 8.00 |
| 80:00 | 75:00 | 250.00 | 28.00 |
| 90:00 | 10:00 | 250.00 | 44.00 |
| 95:00 | 05:00 | 250.00 | 100.00 |
| 98:00 | 03:00 | 300.00 | 100.00 |
| 101:00 | 03:00 | 300.00 | 2.00 |
| 104:00 | 03:00 | 300.00 | 2.00 |
| 107:00 | 03:00 | 300.00 | 100.00 |
| 110:00 | 03:00 | 300.00 | 100.00 |

Pre-column equilibration:

Volume [μ l] : 0.00 Flow [μ l / min] : (unspecified)

Max. pressure [Bar] : 750.00

Analytical column equilibration:

Volume [μ l] : 3.00 Flow [μ l / min] : (unspecified) Max. pressure [Bar] : 750.00

Autosampler wash:

Flush volume [μ l] : 100.00

Method Summary

Method Settings

Application Mode: Peptide Method Duration (min): 110

Global Parameters

Ion Source

Ion Source Type: NSI Spray Voltage: Static Positive Ion (V): 2000 Negative Ion (V): 600 Sweep Gas (Arb): 0

Ion Transfer Tube Temp (°C): 280 Use Ion Source Settings from Tune: False

FAIMS Mode: Not Installed

MS Global Settings

Infusion Mode: Liquid Chromatography

Expected LC Peak Width (s): 25 Advanced Peak Determination: True

Default Charge State: 3

Internal Mass Calibration: EASY-IC™

Mode: Run Start

Experiment#1 [6x6]

Start Time (min): 0 End Time (min): 110

Master Scan:

SIM

Multiplex lons: True

Maximum number of multiplexed ions: 6

Define Multiplexing Groups (MSX ID): User-defined

Q1 Offset: Off

Orbitrap Resolution: 30000

RF Lens (%): 40 AGC Target: Custom

Normalized AGC Target (%): 1000 Maximum Injection Time Mode: Custom Maximum Injection Time (ms): 10

Microscans: 1
Data Type: Centroid
Polarity: Positive

Source Fragmentation: Disabled

Loop Control: All Scan Description:

Time Mode: Unscheduled

| SIM Scan | SIM Scan | | | | | | | |
|-----------|----------|-------------|--------------------|-------------------------|--------|------------------|--|--|
| Compound | Formula | Adduct | Precursor (m/z) | Precursor Charge (z) | MSX ID | Scan Width (m/z) | | |
| Boxcar1-1 | | (no adduct) | 408.9358 | 1 | 1 | 17 | | |
| Boxcar1-2 | | (no adduct) | 425.9435 | 1 | 2 | 17 | | |
| Boxcar1-3 | | (no adduct) | 441.9508 | 1 | 3 | 15 | | |
| Boxcar1-4 | | (no adduct) | 456.9576 | 1 | 4 | 15 | | |
| Boxcar1-5 | | (no adduct) | 471.4642 | 1 | 5 | 14 | | |
| Boxcar1-6 | | (no adduct) | 484.9703 | 1 | 6 | 13 | | |
| Boxcar2-1 | | (no adduct) | 498.4765 | 1 | 1 | 14 | | |
| Boxcar2-2 | | (no adduct) | 511.9826 | 1 | 2 | 13 | | |
| Boxcar2-3 | | (no adduct) | 524.9885 | 1 | 3 | 13 | | |
| Boxcar2-4 | | (no adduct) | 537.9944 | 1 | 4 | 13 | | |
| Boxcar2-5 | | (no adduct) | 551.0004 | 1 | 5 | 13 | | |
| Boxcar2-6 | | (no adduct) | 563.506 | 1 | 6 | 12 | | |
| Boxcar3-1 | | (no adduct) | 576.0117 | 1 | 1 | 13 | | |
| Boxcar3-2 | | (no adduct) | 589.0176 | 1 | 2 | 13 | | |
| Boxcar3-3 | | (no adduct) | 602.0236 | 1 | 3 | 13 | | |
| Boxcar3-4 | | (no adduct) | 615.0294 | 1 | 4 | 13 | | |
| Boxcar3-5 | | (no adduct) | 628.0354 | 1 | 5 | 13 | | |

| Boxcar3-6 | (no adduct) | 641.0413 | 1 | 6 | 13 |
|-----------|-------------|----------|---|---|----|
| Boxcar4-1 | (no adduct) | 654.5474 | 1 | 1 | 14 |
| Boxcar4-2 | (no adduct) | 668.0536 | 1 | 2 | 13 |
| Boxcar4-3 | (no adduct) | 681.5597 | 1 | 3 | 14 |
| Boxcar4-4 | (no adduct) | 695.566 | 1 | 4 | 14 |
| Boxcar4-5 | (no adduct) | 709.5724 | 1 | 5 | 14 |
| Boxcar4-6 | (no adduct) | 724.079 | 1 | 6 | 15 |
| Boxcar5-1 | (no adduct) | 739.5861 | 1 | 1 | 16 |
| Boxcar5-2 | (no adduct) | 756.0936 | 1 | 2 | 17 |
| Boxcar5-3 | (no adduct) | 773.1013 | 1 | 3 | 17 |
| Boxcar5-4 | (no adduct) | 790.6093 | 1 | 4 | 18 |
| Boxcar5-5 | (no adduct) | 808.6174 | 1 | 5 | 18 |
| Boxcar5-6 | (no adduct) | 827.6261 | 1 | 6 | 20 |
| Boxcar6-1 | (no adduct) | 848.1354 | 1 | 1 | 21 |
| Boxcar6-2 | (no adduct) | 870.1454 | 1 | 2 | 23 |
| Boxcar6-3 | (no adduct) | 894.1563 | 1 | 3 | 25 |
| Boxcar6-4 | (no adduct) | 920.6683 | 1 | 4 | 28 |
| Boxcar6-5 | (no adduct) | 949.6815 | 1 | 5 | 30 |
| Boxcar6-6 | (no adduct) | 982.6965 | 1 | 6 | 36 |

Experiment#2 [1x20]

Start Time (min): 0 End Time (min): 110

Master Scan:

SIM

Multiplex lons: True

Maximum number of multiplexed ions: 20

Define Multiplexing Groups (MSX ID): User-defined

Q1 Offset: Off

Orbitrap Resolution: 60000

RF Lens (%): 40
AGC Target: Custom

Normalized AGC Target (%): 1000 Maximum Injection Time Mode: Custom Maximum Injection Time (ms): 1.25

Microscans: 1 Data Type: **Centroid** Polarity: **Positive**

Source Fragmentation: Disabled

Loop Control: All Scan Description:

Time Mode: Unscheduled

| SIM Scan | | | | | | |
|----------|---------|-------------|--------------------|-------------------------|--------|------------------|
| Compound | Formula | Adduct | Precursor (m/z) | Precursor Charge (z) | MSX ID | Scan Width (m/z) |
| Boxcar1 | | (no adduct) | 415.9389 | 1 | 1 | 31 |
| Boxcar2 | | (no adduct) | 444.9522 | 1 | 1 | 27 |
| Boxcar3 | | (no adduct) | 470.964 | 1 | 1 | 25 |
| Boxcar4 | | (no adduct) | 495.9753 | 1 | 1 | 25 |
| Boxcar5 | | (no adduct) | 519.9862 | 1 | 1 | 23 |
| Boxcar6 | | (no adduct) | 542.9967 | 1 | 1 | 23 |
| Boxcar7 | | (no adduct) | 566.0072 | 1 | 1 | 23 |
| Boxcar8 | | (no adduct) | 589.0176 | 1 | 1 | 23 |
| Boxcar9 | | (no adduct) | 612.0281 | 1 | 1 | 23 |
| Boxcar10 | | (no adduct) | 635.5388 | 1 | 1 | 24 |
| Boxcar11 | | (no adduct) | 659.5497 | 1 | 1 | 24 |
| Boxcar12 | | (no adduct) | 684.0608 | 1 | 1 | 25 |
| Boxcar13 | | (no adduct) | 709.5724 | 1 | 1 | 26 |
| Boxcar14 | | (no adduct) | 737.0849 | 1 | 1 | 29 |
| Boxcar15 | | (no adduct) | 766.5983 | 1 | 1 | 30 |
| Boxcar16 | | (no adduct) | 798.1127 | 1 | 1 | 33 |
| Boxcar17 | | (no adduct) | 832.6284 | 1 | 1 | 36 |
| Boxcar18 | | (no adduct) | 871.1459 | 1 | 1 | 41 |
| Boxcar19 | | (no adduct) | 916.1664 | 1 | 1 | 49 |

| Boxcar20 | (no adduct) | 970.6912 | 1 | 1 | 60 | |
|----------|-------------|----------|---|---|----|---|
| | , , | 1 | | | | 1 |

Experiment#3 [1x12]

Start Time (min): 0 End Time (min): 110

Master Scan:

SIM

Multiplex lons: True

Maximum number of multiplexed ions: 12

Define Multiplexing Groups (MSX ID): User-defined

Q1 Offset: Off

Orbitrap Resolution: 60000

RF Lens (%): 40 AGC Target: Custom

Normalized AGC Target (%): 1000 Maximum Injection Time Mode: Custom

Maximum Injection Time (ms): 2

Microscans: 1
Data Type: Centroid
Polarity: Positive

Source Fragmentation: Disabled

Loop Control: All Scan Description:

Time Mode: Unscheduled

| SIM Scan | SIM Scan | | | | | | | |
|----------|----------|-------------|--------------------|-------------------------|--------|------------------|--|--|
| Compound | Formula | Adduct | Precursor (m/z) | Precursor Charge (z) | MSX ID | Scan Width (m/z) | | |
| Boxcar1 | | (no adduct) | 424.9431 | 1 | 1 | 49 | | |
| Boxcar2 | | (no adduct) | 470.4638 | 1 | 1 | 42 | | |
| Boxcar3 | | (no adduct) | 511.4824 | 1 | 1 | 40 | | |
| Boxcar4 | | (no adduct) | 550.5001 | 1 | 1 | 38 | | |
| Boxcar5 | | (no adduct) | 589.0176 | 1 | 1 | 39 | | |
| Boxcar6 | | (no adduct) | 628.0354 | 1 | 1 | 39 | | |

| Boxcar7 | (no adduct) | 668.0536 | 1 | 1 | 41 |
|----------|-------------|----------|---|---|----|
| Boxcar8 | (no adduct) | 710.0726 | 1 | 1 | 43 |
| Boxcar9 | (no adduct) | 756.5938 | 1 | 1 | 50 |
| Boxcar10 | (no adduct) | 809.6179 | 1 | 1 | 56 |
| Boxcar11 | (no adduct) | 872.1463 | 1 | 1 | 69 |
| Boxcar12 | (no adduct) | 953.6834 | 1 | 1 | 94 |

Experiment#4 [1x6]

Start Time (min): 0 End Time (min): 110

Master Scan:

SIM

Multiplex lons: True

Maximum number of multiplexed ions: 6

Define Multiplexing Groups (MSX ID): User-defined

Q1 Offset: Off

Orbitrap Resolution: 60000

RF Lens (%): 40 AGC Target: Custom

Normalized AGC Target (%): 1000 Maximum Injection Time Mode: Custom

Maximum Injection Time (ms): 4

Microscans: 1
Data Type: Centroid
Polarity: Positive

Source Fragmentation: Disabled

Loop Control: All Scan Description:

Time Mode: Unscheduled

| SIM Scan | | | | | | | |
|----------|---------|-------------|--------------------|-------------------------|--------|------------------|--|
| Compound | Formula | Adduct | Precursor (m/z) | Precursor Charge (z) | MSX ID | Scan Width (m/z) | |
| Boxcar1 | | (no adduct) | 445.9526 | 1 | 1 | 91 | |

| Boxcar2 | (no adduct) | 530.491 | 1 | 1 | 78 |
|---------|-------------|----------|---|---|-------|
| Boxcar3 | (no adduct) | 608.5265 | 1 | 1 | 78 |
| Boxcar4 | (no adduct) | 689.5634 | 1 | 1 | 84 |
| Boxcar5 | (no adduct) | 784.6065 | 1 | 1 | 106 |
| Вохсагб | (no adduct) | 919.1677 | 1 | 1 | 163.1 |

Experiment#5 [1x3]

Start Time (min): 0 End Time (min): 110

Master Scan:

SIM

Multiplex lons: True

Maximum number of multiplexed ions: 3

Define Multiplexing Groups (MSX ID): User-defined

Q1 Offset: Off

Orbitrap Resolution: 60000

RF Lens (%): 40 AGC Target: Custom

Normalized AGC Target (%): 1000 Maximum Injection Time Mode: Custom

Maximum Injection Time (ms): 8

Microscans: 1 Data Type: **Centroid** Polarity: **Positive**

Source Fragmentation: Disabled

Loop Control: All Scan Description:

Time Mode: Unscheduled

| SIM Scan | SIM Scan | | | | | | |
|----------|----------|-------------|--------------------|-------------------------|--------|---------------------|--|
| Compound | Formula | Adduct | Precursor (m/z) | Precursor Charge (z) | MSX ID | Scan Width (m/z) | |
| Boxcar1 | | (no adduct) | 484.9703 | 1 | 1 | 169 | |
| Boxcar2 | | (no adduct) | 650.5455 | 1 | 1 | 162 | |

| Boxcar3 | (no adduct) | 866.1436 | 1 | 1 | 269.1 |
|---------|-------------|----------|---|---|-------|
| | | | | | |

Experiment#6 [SIM Scan]

Start Time (min): 0 End Time (min): 110

Master Scan:

SIM

Multiplex lons: False Scan Width (m/z): 600

Q1 Offset: Off

Orbitrap Resolution: 60000

RF Lens (%): 50
AGC Target: Custom

Normalized AGC Target (%): 1000 Maximum Injection Time Mode: Custom Maximum Injection Time (ms): 24

Microscans: 1 Data Type: **Centroid** Polarity: **Positive**

Source Fragmentation: Disabled

Loop Control: All Scan Description:

Time Mode: Unscheduled

| SIM Scan | | | | |
|----------|---------|-------------|-----------------|----------------------|
| Compound | Formula | Adduct | Precursor (m/z) | Precursor Charge (z) |
| MRFA | | (no adduct) | 700 | 1 |