Supplementary Material: Mass Spectrometry Instrument Settings

Orbitrap Fusion Method

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Summary
Global Settings
             Use Ion Source Settings from Tune = False
             Method Duration (min)= 133
             Ion Source Type = NSI
             Sweep Gas (Arb) = 0
             Ion Transfer Tube Temp (°C) = 275
             APPI Lamp = Not in use
             Positive Spray Voltage (V):
                  Start (min)|
                                   Voltage (V)
                       0|
                                       1900
                Negative Spray Voltage (V):
                  Start (min)|
                                   Voltage (V)
                       0|
                                         01
             Pressure Mode = Standard
             Default Charge State = 1
Experiment 1
             Start Time (min) = 17
             End Time (min) = 133
             Cycle Time (sec) = 5
                Scan MasterScan
                                 MSn Level = 1
                                 Use Wide Quad Isolation = True
                                 Detector Type = Orbitrap
                                 Orbitrap Resolution = 120K
                                 Mass Range =Normal
                                 Scan Range (m/z) = 375-1575
                                 Maximum Injection Time (ms) = 50
                                 AGC Target = 500000
                                 Microscans = 1
                                 RF Lens (%) = 60
```

Use ETD Internal Calibration = False

Source Fragmentation = False

DataType = Centroid Polarity = Positive Scan Description =

Filter MIPS

MIPS Mode =Peptide

Filter Intensity Threshold

Maximum Intensity = 1E+20 Use Signal Intensity Range =False Minimum Intensity = 50000

Filter Charge State

Include undetermined charge states = False

Include charge state(s) = 2-6

Include charge states 25 and higher = False

Filter Dynamic Exclusion

Exclude after n times = 1
Exclusion duration (s) = 45
Mass Tolerance = ppm
Mass tolerance low = 10
Mass tolerance high = 10
Exclude isotopes = True

Perform dependent scan on single charge state per precursor only = False

Filter Targeted Exclusion MassList

Ignore charge state requirement for unassigned ions = False

>>>>> Mass List Table <<<<<<<

m/z| z| CompoundName|

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Data Dependent Properties

Data Dependent Mode= Cycle Time

Scan Event 1

Scan ddMSnScan

MSn Level = 2

Isolation Mode = Quadrupole

Isolation Window = 0.8

Use Isolation m/z Offset = False

Multi-notch Isolation = False

Scan Range Mode = Auto Normal

FirstMass = 120

Scan Priority= 1

ActivationType = HCD

Is Stepped Collision Energy On = False

Stepped Collision Energy (%) = 5

Collision Energy (%) = 34

Is EThcD Active = False

Detector Type = IonTrap
Ion Trap Scan Rate = Rapid
Maximum Injection Time (ms) = 35
AGC Target = 10000
Inject ions for all available parallelizable time = True
Microscans = 1
Use ETD Internal Calibration = False
DataType = Centroid
Polarity = Positive
Source Fragmentation = False
Scan Description =