Compound Discoverer Data Processing

Select Spectra

Parameter	Value
Precursor Selection	Use MS(n - 1) Precursor
Lower RT Limit	0.2
Upper RT Limit	21
First Scan	0
Last Scan	0
Ignore Specified Scans	
Lowest Charge State	0
High Sharge State	0
Min. Precursor Mass	100 Da
Max. Precursot Mass	5000 Da
Total Intensity Threshold	0
Minimum Peak Count	1
Mass Analyzer	Any
MS Order	Any
Activation Type	Any
Min. Collision Energy	0
Max. Collision Energy	1000
Scan Type	Is Full
Polarity Mode	(Not specified)
S/N Threshold (FT-only)	1.5
Unrecognized Charge Replacement	1
Unrecognized Mass Analyzer Replacement	FTMS
Unrecognized MS Order Replacements	MS1
Unrecognized Activation Type Replacements	HCD
Unrecognized Polarity Replacements	+
Unrecognized MS Resolution Replacements	60000
Unrecognized MSn Resolution Replacements	15000

Detect Unknown Compounds

Parameter	Value
Mass Tolerance (ppm)	7.5
Intensity Tolerance (%)	100
S/N Threshold	3
Min. Peak Intensity	100000
Ions	[M+H]+1; [M+TFA-H]-1
Min. Element Counts	C H
Max. Element Counts	C100 H190 N10 Na2 O15 P2 S2
Filter Peaks	TRUE
Max. Peak Width [min]	1
Remove Singlets	TRUE
Min # Scans per Peak	6
Min # Isotopes	4

Group Unknown Compounds

Parameter	Value
Mass Tolerance	7.5
RT Tolerance [min]	0.2
Rule #1	Unspecified
Rule #2	Unspecified
Preferred MS Order	MS1
Preferred Ion	[M+H]+1, [M+TFA-H]-1

Fill Gaps

Parameter	Value
Mass Tolerance	7.5
S/N Threshold	1.5
Use Real Peak Detection	TRUE

Align Retention Times

Parameter	Value
Alignment Model	Adaptive Curve
Alignment Fallback	Use Linear Model
Maximum Shift [min]	0.6
Shift Reference File	TRUE
Mass Tolerance	7.5
Remove Outlier	TRUE

Mark Background Compounds

Parameter	Value
Max. Sample/Blank	3
Max. Blank/Sample	0
Hide Background	True