

Compound Discoverer Parameters

Parameter	Value
Precursor Selection	Use MS(n - 1) Precursor
Lower RT Limit	0.4
Upper RT Limit	0
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	Any
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 Resolutino Replacements	15000

Detect Unknown Compounds

Parameter	Value
Mass Tolerance (ppm)	10 ppm
Intensity Tolerance (%)	100
S/N Threshold	3
Min. Peak Intensity	100000
Ions	[M+H] ⁺ 1; [M-H] ⁻ 1
Min. Element Counts	C H C100 H190 N10
Max. Element Counts	Na2 O15 P2 S2

Group Unknown Compounds

Parameter	Value
Mass Tolerance	10 ppm
RT Tolerance [min]	0.2
Rule #1	Unspecified
Rule #2	Unspecified
Preferred MS Order	MS1
Preferred Ion	[M+H] ⁺ 1

Fill Gaps

Parameter	Value
Mass Tolerance	10 ppm
RT Tolerance [min]	0.2
S/N Threshold	1.5

Mark Background Compounds

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