

Acquisition Method Info

Method Name	metabolite_ESI_+VE_MSMS.m
Method Path	D:\MassHunter\Methods\2024\metabolite_ESI_+VE_MSMS.m
Method Description	Default Method

- Device List
- HiP Sampler
 - Binary Pump
 - Column Comp.
 - DAD
 - Q-TOF

TOF/Q-TOF Mass Spectrometer

Component Name	MS Q-TOF	Component Model	G6550A
Ion Source	Dual AJS ESI	Stop Time (min)	30.00
Can wait for temp.	Enable	Fast Polarity	N/A
MS Abs. threshold	200	MS Rel. threshold(%)	0.010
MS/MS Abs. threshold	5	MS/MS Rel. threshold(%)	0.010
Tune File	Autotune.tun		

Time Segments

Time Segment #	Start Time (min)	Diverter Valve State	Storage Mode	Ion Mode
1	0	MS	Both	Dual AJS ESI

Time Segment 1

Acquisition Mode AutoMS2

MS Min Range (m/z)	100
MS Max Range (m/z)	1200
MS Scan Rate (spectra/sec)	1.00
MS/MS Scan Rate (spectra/sec)	1.00
Isolation Width MS/MS	Medium (~4 amu)

Ramped Collision Energy

Charge	Slope	Offset
1	8	-2.6
2	6	-2.6
3	4	-2.6

Auto MS/MS Preferred/Exclude Table

Mass	Delta Mass (ppm)	Charge	Type	Retention Time (min)	Delta Ret. Time (min)	Isolation Width	Collision Energy
197.8075	500	1	Exclude	0		Medium (~4 amu)	

Precursor Selection

Max Precursors Per Cycle	10
Threshold (Abs)	10000
Threshold (Rel)(%)	0.010
Precursor abundance based scan speed	Yes
Target (counts/spectrum)	25000.000
Use MS/MS accumulation time limit	Yes
Use dynamic precursor rejection	No
Purity Stringency (%)	100.000
Purity Cutoff (%)	30.000
Isotope Model	Common
Active exclusion enabled	Yes
Active exclusion excluded after (spectra)	1
Active exclusion released after (min)	0.20
Sort precursors	By abundance only

Charge State Preference

Selected

Charges

1

2

Unk

Source Parameters

Parameter	Value
Gas Temp (°C)	250
Gas Flow (l/min)	13
Nebulizer (psig)	35
SheathGasTemp	300
SheathGasFlow	11

Scan Segments

Scan Seg #	Ion Polarity	Collision Energy
1	Positive	0

Scan Segment 1

Scan Source Parameters

Parameter	Value
VCap	3500
Nozzle Voltage (V)	1000
Fragmentor	175
Skimmer1	65
OctopoleRFPeak	750

ReferenceMasses

Ref Mass Enabled	Disabled
Ref Nebulizer (psig)	

Chromatograms

Chrom Type	Label	Offset	Y-Range
TIC	TIC	15	10000000

Name: HiP Sampler Model: G4226A

Auxiliary

Draw Speed	100.0 µL/min
Eject Speed	100.0 µL/min
Draw Position Offset	0.0 mm
Wait Time After Drawing	2.0 s
Sample Flush Out Factor	5.0
Vial/Well bottom sensing	Yes

Injection

Injection Mode	Injection with needle wash
Injection Volume	5.00 µL
Needle Wash	
Needle Wash Location	Flush Port
Wash Time	3.0 s

High throughput

Automatic Delay Volume Reduction	No
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Overlapped Injection

Enable Overlapped Injection	No
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Valve Switching

Valve Movements	0
Valve Switch Time 1	
Switch Time 1 Enabled	Yes
Switch Time 1	0.01 min
Valve Switch Time 2	
Switch Time 2 Enabled	No
Valve Switch Time 3	
Switch Time 3 Enabled	No
Valve Switch Time 4	
Switch Time 4 Enabled	No

Stop Time

Stoptime Mode	As pump/No limit
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Post Time

Posttime Mode	Off
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Name: Binary Pump **Model:** G4220B

Flow 0.300 mL/min
Use Solvent Types Yes
Stroke Mode Synchronized
Low Pressure Limit 0.00 bar
High Pressure Limit 1200.00 bar
Max. Flow Ramp Up 100.000 mL/min²
Max. Flow Ramp Down 100.000 mL/min²
Expected Mixer No check

Stroke A

Automatic Stroke Calculation A Yes

Stop Time

Stoptime Mode Time set
Stoptime 35.00 min

Post Time

Posttime Mode Off

Solvent Composition

	Channel	Ch. 1 Solv.	Name 1	Ch2 Solv.	Name 2	Selected	Used	Percent
1	A	100.0 % Water V.02	0.1% FA in water	100.0 % Water V.02	0.1% FA in water	Ch. 2	Yes	90.00 %
2	B	100.0 % Acetonitrile V.03		100.0 % Acetonitrile V.02		Ch. 2	Yes	10.00 %

Timetable

	Time	A	B	Flow	Pressure
1	0.50 min	90.00 %	10.00 %	0.300 mL/min	1200.00 bar
2	20.00 min	0.00 %	100.00 %	0.300 mL/min	1200.00 bar
3	30.00 min	0.00 %	100.00 %	0.300 mL/min	1200.00 bar
4	31.00 min	90.00 %	10.00 %	0.300 mL/min	1200.00 bar
5	35.00 min	90.00 %	10.00 %	0.300 mL/min	1200.00 bar

Name: Column Comp. **Model:** G1316C

Ready when front door open Yes

Left Temperature Control

Temperature Control Mode Temperature Set
Temperature 40.00 °C

Enable Analysis Left Temperature

Enable Analysis Left Temperature On Yes
Enable Analysis Left Temperature Value 0.80 °C

Right Temperature Control

Right temperature Control Mode Temperature Set
Right temperature 40.00 °C

Enable Analysis Right Temperature

Enable Analysis Right Temperature On Yes
Enable Analysis Right Temperature Value 0.80 °C

Stop Time

Stoptime Mode As pump/injector

Post Time

Posttime Mode Off

Name: DAD

Model: G4212B

Peakwidth >0.10 min (2.0 s response time) (2.5 Hz)
UV Lamp Required No

Analog Output 1

Analog 1 Zero Offset 5 %
Analog 1 Attenuation 1000 mAU

Signals

Prepare Mode

Margin for negative Absorbance 100 mAU

Autobalance

Autobalance Prerun Yes
Autobalance Postrun No

Spectrum

Spectrum Range WL from 190.0 nm
Spectrum Range WL to 640.0 nm
Spectrum Step 2.0 nm
Spectrum Store All

Stoptime

Stoptime Mode As pump/injector

Posttime

Posttime Mode Off

Signals

Signal table

	Use Sig.	Signal	Wavelength	Bandwidth	Use Ref.	Ref Wavel.	Ref Bandw.
1	Yes	Signal A	254.0 nm	4.0 nm	Yes	360.0 nm	100.0 nm
2	Yes	Signal B	254.0 nm	4.0 nm	No		
3	Yes	Signal C	290.0 nm	4.0 nm	Yes	360.0 nm	100.0 nm
4	Yes	Signal D	280.0 nm	4.0 nm	Yes	360.0 nm	100.0 nm
5	Yes	Signal E	272.0 nm	4.0 nm	Yes	360.0 nm	100.0 nm
6	No	Signal F					
7	No	Signal G					
8	No	Signal H					