Acquisition Method Report

Agilent

Acquisition Method Info

Operator Name	SYSTEM (SYSTEM)
Created By	SYSTEM (SYSTEM)
Last Modified By	SYSTEM (SYSTEM)
Method Name	GHB.m
Method Path	D:\Projects\TOX Lab\Methods\GHB.m (Version: NA)
Method Description	
Pre Run Script	
Post Run Script	
Est. Run Time	5.00

Creation Date	2024-08-01 10:17:28-04:00
Last Modification Date	2024-08-02 11:56:43-04:00

Device List

- Multisampler
- Binary Pump
- Column Comp.
- TQ

Name: Multisampler **Module:** G7167A

Sampling Speed	
Draw Speed	100.0 µL/min
Eject Speed	400.0 µL/min
Wait Time After Drawing	1.2 s
Injection	
Needle Wash Mode	Standard Wash
Injection Volume	5.00 µL
Standard Needle Wash	
Needle Wash Mode	Flush Port
Duration	3 s
High Throughput	
Injection Valve to Bypass for Delay Volume Reduction	No
Sample Flush-Out Factor	5.0
Overlapped Injection	
Overlap Injection Enabled	No
Needle Height Position	
Draw Position Offset	0.0 mm
Use Vial/Well Bottom Sensing	No
Stoptime	
Stoptime Mode	Time set
Stoptime	4.00 min
Posttime	

Posttime Mode	Off
Use Injector Program	
Use Injector Program	No

Name: Binary Pump **Module:** G7112B

Flow	0.300 mL/min
Use Solvent Types	Yes
Low Pressure Limit	0.00 bar
High Pressure Limit	600.00 bar
Maximum Flow Gradient	100.000 mL/min²
Stroke A	
Automatic Stroke Calculation A	Yes
Stroke B	
Automatic Stroke Calculation B	Yes
Stoptime	
Stoptime Mode	Time set
Stoptime	4.00 min
Posttime	
Posttime Mode	Off

Solvent Composition

	Channel	Solvent 1	Name 1	Solvent 2	Name 2	Selected	Used	Percent (%)
1	A	H20		H20		Ch. 2	Yes	95.0 %
2	B	H20		MeOH		Ch. 2	Yes	5.0 %

Timetable

	Time (min)	A (%)	B (%)	Flow (mL/min)	Pressure (bar)
1	Start. Cond. min	95.0 %	5.0 %	0.300 mL/min	600.00 bar
2	3.00 min	92.0 %	8.0 %	0.300 mL/min	600.00 bar
3	3.01 min	95.0 %	5.0 %	0.300 mL/min	600.00 bar
4	4.00 min	95.0 %	5.0 %	0.300 mL/min	600.00 bar

Name: Column Comp. **Module:** G7116A

Left Temperature Control	
Left Temp. Control Mode	Temperature Set
Left Temperature	30.0 °C
Enable Analysis Left Temperature	
Enable Analysis Left Temperature On	Yes
Enable Analysis Left Temperature Value	0.8 °C
Left Temp. Equilibration Time	0.0 min
Right Temperature Control	
Right temperature Control Mode	Combined

Enable Analysis Right Temperature

Enable Analysis Right Temperature On	Yes
Enable Analysis Right Temperature Value	0.8 °C
Right Temp. Equilibration Time	0.0 min

Enforce column for run

Enforce column for run is enabled	No

Thermal equilibration devices

Enforce left thermal equilibration device	No
Enforce right thermal equilibration device	No

Stoptime

Stoptime Mode	As Pump/Injector

Posttime

Posttime Mode	Off

Timetable

Valve Position	Position 2 (Port 1 -> 2)
Position Switch After Run	Do not switch

Name: TQ Mass Spectrometer **Module:** G6475A

General

Tune File	atunes.tune
Ion Source	AJS ESI
Optimized Method	Off
Last Compound Optimized Time	
Last Source Optimized Time	
Time Filter Enabled	Off

Stop Time

Stop Mode	By Pump Time

Time Segment

	Start Time (min)	Scan Type	Detector Gain Factor (+)	Detector Gain Factor (-)	Store Data
1	0	MRM	1	1	Yes

Time Segment 1

Scan Type: MRM

	Compound group	Compound name	Compound formula	Ion species	CAS	z	Monoisotopic mass (m/z)	ISTD?	Precursor (m/z)	MS1 res	Product (m/z)	MS2 res	Dwell (ms)	Fragmentor (V)	CAV (V)	CE (V)	Polarity
1		GHB-D6	C4HD6O3	(M+H)+		1	109.1 m/z	No	110.1 m/z	Unit	92 m/z	Unit	100 ms	60 V	4 V	5 V	+
2		GHB-D6	C4HD6O3	(M+H)+		1	109.1 m/z	No	110.1 m/z	Unit	49 m/z	Unit	100 ms	60 V	4 V	20 V	+
3		GHB	C4H8O3	(M+H)+		1	104 m/z	No	105 m/z	Unit	87 m/z	Unit	100 ms	60 V	4 V	5 V	+
4		GHB	C4H8O3	(M+H)+		1	104 m/z	No	105 m/z	Unit	45 m/z	Unit	100 ms	60 V	4 V	20 V	+

	Compound group	Compound name	Compound formula	Ion species	CAS	z	Monoisotopic mass (m/z)	ISTD?	Precursor (m/z)	MS1 res	Product (m/z)	MS2 res	Dwell (ms)	Fragmentor (V)	CAV (V)	CE (V)	Polarity
5		GBL	C4H6O2	(M+H)+		1	86 m/z	No	87 m/z	Unit	45 m/z	Unit	100 ms	70 V	4 V	15 V	+
6		GBL	C4H6O2	(M+H)+		1	86 m/z	No	87 m/z	Unit	43 m/z	Unit	100 ms	70 V	4 V	10 V	+

Source Parameter

	Parameter Id	Positive Value	Negative Value
1	Gas Temperature (°C)	300	300
2	Gas Flow (L/min)	13	13
3	Nebulizer (psi)	35	35
4	Capillary Voltage (V)	4000	4000
5	Sheath Gas Temperature (°C)	250	250
6	Sheath Gas Flow (L/min)	11	11
7	Nozzle Voltage (V)	1500	1500

Optimizer Settings

Optimizer Compound Settings

Precursor abundance threshold 5000

Product ion abundance threshold 500

MRM abundance threshold 100

Optimizer Dwell Time 130 ms

Maximum number of product ions 4

Product ion low m/z cut-off Disabled

	Name	Option	From	To	Step Size
1	Fragmentor (V)	Find product ions from defined range	110	140	10
2	Collision Energy	Find product ions from defined range	0	20	4

Chromatogram

	Chromatogram Type	Label
1	TIC	TIC

Timetable

	Start Time (min)	Timetable Type	Timetable Value
1	0	Diverter Valve	To Waste
2	1.4	Diverter Valve	To MS
3	2.6	Diverter Valve	To Waste

Advanced override settings

Positive

	Parameter	Override Tune	Dynamic Mass (m/z)	Tune Setting	Override Value
1	HED (kV)	No	m/z	Standard	Large molecule

Negative

Name: **DA - Intelligent Reflex Parameters**

Intelligent Reflex Enabled	No