

Acquisition Method Info

Operator Name	SYSTEM (SYSTEM)	Creation Date	2024-02-22 10:48:11-05:00
Created By	SYSTEM (SYSTEM)	Last Modification Date	2024-04-03 09:35:05-04:00
Last Modified By	SYSTEM (SYSTEM)		
Method Name	FINAL THC 022224.m		
Method Path	D:\Projects\TOX Lab\Methods\FINAL THC 022224.m (Version: NA)		
Method Description			
Pre Run Script			
Post Run Script			
Est. Run Time	18.00		
Device List			
	Multisampler		
	Binary Pump		
	Column Comp.		
	TQ		

Name: Multisampler **Module:** G7167A

Sampling Speed

Draw Speed	100.0 $\mu\text{L}/\text{min}$
Eject Speed	400.0 $\mu\text{L}/\text{min}$
Wait Time After Drawing	1.2 s

Injection

Needle Wash Mode	Standard Wash
Injection Volume	20.00 µL

Standard Needle Wash

Needle Wash Mode	Flush Port
Duration	3 s

High Throughput

Injection Valve to Bypass for Delay Volume Reduction

Sample Flush-Out Factor

Overlapped Injection

Overlap Injection Enabled	No
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Needle Height Position

Draw Position Offset	0.0 mm
Use Vial/Well Bottom Sensing	No

Stoptime

Stoptime Mode	Time set
Stoptime	15.00 min

Posttime

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Posttime Mode Time set
Posttime 2.00 min
[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 15.00 min

Posttime

Posttime Mode Time set
Posttime 2.00 min

Solvent Composition

	Channel	Solvent 1	Name 1	Solvent 2	Name 2	Selected	Used	Percent (%)
1	A	H2O		H2O		Ch. 1	Yes	25.0 %
2	B	MeOH		H2O		Ch. 1	Yes	75.0 %

Timetable

	Time (min)	A (%)	B (%)	Flow (mL/min)	Pressure (bar)
1	Start. Cond. min	25.0 %	75.0 %	0.300 mL/min	600.00 bar
2	5.00 min	25.0 %	75.0 %	0.400 mL/min	600.00 bar
3	7.00 min	25.0 %	75.0 %	0.500 mL/min	600.00 bar
4	10.00 min	18.0 %	82.0 %	0.500 mL/min	600.00 bar
5	14.00 min	2.0 %	98.0 %	0.500 mL/min	600.00 bar
6	14.01 min	25.0 %	75.0 %	0.500 mL/min	600.00 bar
7	15.00 min	25.0 %	75.0 %	0.300 mL/min	600.00 bar

Name: Column Comp. Module: G7116A

Left Temperature Control

Left Temp. Control Mode Temperature Set
Left Temperature 55.0 °C
[Enable Analysis Left Temperature](#)

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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 1 (Port 1 -> 6)
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	On
Time filter window	0.07 min

Stop Time

Stop Mode	By Pump Time
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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

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	Compound group	Compound name	Compound formula	Ion species	CAS	z	Monoisotopic mass	ISTD?	Precursor (m/z)	MS1 res	Product (m/z)	MS2 res	Dwell (ms)	Fragmentor (V)	CAV (V)	CE (V)	Polarity
1		delta-9 THC-OH D3	C21H27O3D3	(M+H)+		1		Yes	334.2 m/z	Unit	316.2 m/z	Unit	50 ms	117 V	5 V	12 V	+
2		delta-9 THC-OH D3	C21H27O3D3	(M+H)+		1		Yes	334.2 m/z	Unit	196.1 m/z	Unit	50 ms	117 V	3 V	27 V	+
3		delta-9 THC-OH D3	C21H27O3D3	(M+H)+		1		Yes	334.2 m/z	Unit	123 m/z	Unit	50 ms	117 V	5 V	40 V	+
4		delta-9 THC-OH D3	C21H27O3D3	(M+H)+		1		Yes	334.2 m/z	Unit	105 m/z	Unit	50 ms	117 V	3 V	40 V	+
5		delta-9 THC-OH	C21H30O3	(M+H)+		1		No	331.2 m/z	Unit	313.2 m/z	Unit	50 ms	117 V	3 V	12 V	+
6		delta-9 THC-OH	C21H30O3	(M+H)+		1		No	331.2 m/z	Unit	123 m/z	Unit	50 ms	117 V	3 V	40 V	+
7		delta-9 THC D3	C21H27O2D3	(M+H)+		1		Yes	318.2 m/z	Unit	196.1 m/z	Unit	50 ms	133 V	3 V	25 V	+
8		delta-9 THC D3	C21H27O2D3	(M+H)+		1		Yes	318.2 m/z	Unit	135.1 m/z	Unit	50 ms	133 V	3 V	21 V	+
9		delta-9 THC D3	C21H27O2D3	(M+H)+		1		Yes	318.2 m/z	Unit	123 m/z	Unit	50 ms	133 V	3 V	40 V	+
10		delta-9 THC	C21H30O2	(M+H)+		1		No	315.2 m/z	Unit	193.1 m/z	Unit	50 ms	123 V	3 V	25 V	+
11		delta-9 THC	C21H30O2	(M+H)+		1		No	315.2 m/z	Unit	135.1 m/z	Unit	50 ms	123 V	3 V	21 V	+
12		delta-9 THC	C21H30O2	(M+H)+		1		No	315.2 m/z	Unit	123.1 m/z	Unit	50 ms	123 V	3 V	39 V	+
13		delta-9 THC-COOH D3	C21H25D3O4	(M-H)-		1		Yes	346.2 m/z	Unit	302.2 m/z	Unit	50 ms	150 V	3 V	25 V	-
14		delta-9 THC-COOH D3	C21H25D3O4	(M-H)-		1		Yes	346.2 m/z	Unit	248.2 m/z	Unit	50 ms	150 V	3 V	35 V	-
15		delta-9 THC-COOH D3	C21H25D3O4	(M-H)-		1		Yes	346.2 m/z	Unit	194.1 m/z	Unit	50 ms	150 V	3 V	36 V	-
16		delta-9 THC-COOH	C21H28O4	(M-H)-		1		No	343.2 m/z	Unit	299.2 m/z	Unit	50 ms	150 V	3 V	25 V	-
17		delta-9 THC-COOH	C21H28O4	(M-H)-		1		No	343.2 m/z	Unit	245.2 m/z	Unit	50 ms	150 V	3 V	35 V	-
18		delta-9 THC-COOH	C21H28O4	(M-H)-		1		No	343.2 m/z	Unit	191.1 m/z	Unit	50 ms	150 V	3 V	36 V	-

Source Parameter

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	Parameter Id	Positive Value	Negative Value
1	Gas Temperature (°C)	300	300
2	Gas Flow (L/min)	10	10
3	Nebulizer (psi)	45	45
4	Capillary Voltage (V)	3500	3500
5	Sheath Gas Temperature (°C)	375	375
6	Sheath Gas Flow (L/min)	12	12
7	Nozzle Voltage (V)	500	500

Optimizer Settings

Optimizer Compound Settings

Precursor abundance threshold	500
Product ion abundance threshold	50
MRM abundance threshold	10
Optimizer Dwell Time	5 ms
Maximum number of product ions	3
Product ion low m/z cut-off	Enabled

	Name	Option	From	To	Step Size
1	Fragmentor (V)	Find product ions from defined range	100	150	10
2	Collision Energy	Find product ions from defined range	12	40	4

Optimizer Source Settings

Optimization mode	EIC
Determine parameter range from method source setpoints	On

Source parameters

	Name	Pre-wait (min)	Replicate(s)	Step Wait (min)	From	To	Step Size
1	Nebulizer (psi)	0	1	0	43	47	1

Source parameters (Voltage)

	Name	Pre-wait (min)	Replicate(s)	Step Wait (min)	From (Positive)	To (Positive)	Step Size (Positive)	From (Negative)	To (Negative)	Step Size (Negative)
1	Capillary Voltage (V)	0	1	0	3100	3900	200	3100	3900	200

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Chromatogram

	Chromatogram Type	Label
1	TIC	TIC

Timetable

	Start Time (min)	Timetable Type	Timetable Value
1	0	Diverter Valve	To Waste
2	3.3	Diverter Valve	To MS
3	11.5	Diverter Valve	To Waste

PostRun Diverter Valve Switch

Diverter Valve

PostRun Diverter Valve Position

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