Acquisition Method Report

Agilent Technologies

Acquisition Method Info

Method Name	Joan_silvia_MRM_HILIC_01102019_5ul.m
Method Path	D:\MassHunter\Methods\Joan_silvia_MRM_HILIC_01102019_5ul.m
Method Description	Veure volulm i dilució de la mostra

Device List
  HiP Sampler
  Binary Pump
  Column Comp.
  QQQ

MS QQQ Mass Spectrometer

Ion Source	AJS ESI	Tune File	D:\MassHunter\Tune\QQQ\G6490A\atunes.TUNE.XML
Stop Mode	No Limit/As Pump	Stop Time (min)	1
Time Filter	On	Time Filter Width (min)	0.07

Time Segments

Index	Start Time (min)	Scan Type	Ion Mode	Div Valve	Delta EMV	Store
1	0	MRM	ESI+Agilent Jet Stream	To Waste	300	Yes
2	0.35	MRM	ESI+Agilent Jet Stream	To MS	300	Yes
3	6	MRM	ESI+Agilent Jet Stream	To MS	300	Yes

Time Segment 1

Scan Segments

Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
Compound 1	No	350	Wide / Unit (6490)	200	Wide / Unit (6490)	10	380	0	5	Positive

Scan Parameters

Data Stg	Threshold
Centroid	0

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	270	270
Gas Flow (l/min)	15	15
Nebulizer (psi)	35	35
SheathGasHeater	400	400
SheathGasFlow	11	11
Capillary (V)	3000	3000
VCharging	1000	1500

Ion Funnel Parameters

Pos High Pressure RF	130	Neg High Pressure RF	110
Pos Low Pressure RF	100	Neg Low Pressure RF	60

Time Segment 2

Scan Segments

Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
NADPH_1	No	746	Wide / Unit (6490)	729	Wide / Unit (6490)	10	380	15	5	Positive
NADPH_2	No	746	Wide / Unit (6490)	302	Wide / Unit (6490)	10	380	30	5	Positive
NADP_2	No	744	Wide / Unit (6490)	622	Wide / Unit (6490)	10	380	12	5	Positive
NADP_1	No	744	Wide / Unit (6490)	604	Wide / Unit (6490)	10	380	12	5	Positive
NADH_2	No	666	Wide / Unit (6490)	137	Wide / Unit (6490)	10	380	52	5	Positive
NADH_1	No	666	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	40	5	Positive
NAD	No	664	Wide / Unit (6490)	428	Wide / Unit (6490)	10	380	24	5	Positive
NAD	No	664	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	60	5	Positive
SAH_3	No	385	Wide / Unit (6490)	250	Wide / Unit (6490)	10	380	4	5	Positive
SAH_2	No	385	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	24	5	Positive
SAH_1	No	385	Wide / Unit (6490)	88	Wide / Unit (6490)	10	380	60	5	Positive
methionine_2	No	150	Wide / Unit (6490)	104	Wide / Unit (6490)	10	380	6	5	Positive
methionine_1	No	150	Wide / Unit (6490)	56	Wide / Unit (6490)	10	380	12	5	Positive
homocysteine_1	No	136	Wide / Unit (6490)	90	Wide / Unit (6490)	10	380	8	5	Positive
homocysteine_2	No	136	Wide / Unit (6490)	56	Wide / Unit (6490)	10	380	16	5	Positive
alpha_KG_1	No	145	Wide / Unit (6490)	101	Wide / Unit (6490)	10	380	4	5	Negative
alpha_KG_2	No	145	Wide / Unit (6490)	57	Wide / Unit (6490)	10	380	8	5	Negative

Scan Parameters

Data Stg	Threshold
Centroid	0

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	270	270
Gas Flow (l/min)	15	15
Nebulizer (psi)	35	35
SheathGasHeater	400	400
SheathGasFlow	11	11
Capillary (V)	3000	3000
VCharging	1000	1500

Ion Funnel Parameters

Pos High Pressure RF	130	Neg High Pressure RF	110
Pos Low Pressure RF	100	Neg Low Pressure RF	60

Time Segment 3

Acquisition Method Report

Agilent Technologies

Scan Segments

Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
Ac_CoA_3	No	810	Wide / Unit (6490)	428	Wide / Unit (6490)	10	380	25	5	Positive
Ac_CoA_1	No	810	Wide / Unit (6490)	303	Wide / Unit (6490)	10	380	36	5	Positive
Ac_CoA_2	No	810	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	60	5	Positive
NADPH_1	No	746	Wide / Unit (6490)	729	Wide / Unit (6490)	10	380	15	5	Positive
NADPH_2	No	746	Wide / Unit (6490)	302	Wide / Unit (6490)	10	380	30	5	Positive
NADP_2	No	744	Wide / Unit (6490)	622	Wide / Unit (6490)	10	380	12	5	Positive
NADP_1	No	744	Wide / Unit (6490)	604	Wide / Unit (6490)	10	380	12	5	Positive
NADH_2	No	666	Wide / Unit (6490)	137	Wide / Unit (6490)	10	380	52	5	Positive
NADH_1	No	666	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	40	5	Positive
NAD	No	664	Wide / Unit (6490)	428	Wide / Unit (6490)	10	380	24	5	Positive
NAD	No	664	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	60	5	Positive
ATP_1	No	508	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	44	5	Positive
ATP_2	No	508	Wide / Unit (6490)	97	Wide / Unit (6490)	10	380	40	5	Positive
SAM_3	No	399	Wide / Unit (6490)	298	Wide / Unit (6490)	10	380	4	5	Positive
SAM_1	No	399	Wide / Unit (6490)	250	Wide / Unit (6490)	10	380	12	5	Positive
SAM_2	No	399	Wide / Unit (6490)	97	Wide / Unit (6490)	10	380	32	5	Positive
SAH_3	No	385	Wide / Unit (6490)	250	Wide / Unit (6490)	10	380	4	5	Positive
SAH_2	No	385	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	24	5	Positive
SAH_1	No	385	Wide / Unit (6490)	88	Wide / Unit (6490)	10	380	60	5	Positive
AMP_1	No	348	Wide / Unit (6490)	136	Wide / Unit (6490)	10	380	15	5	Positive
AMP_2	No	348	Wide / Unit (6490)	97	Wide / Unit (6490)	10	380	30	5	Positive
homocysteine_1	No	136	Wide / Unit (6490)	90	Wide / Unit (6490)	10	380	8	5	Positive
homocysteine_2	No	136	Wide / Unit (6490)	56	Wide / Unit (6490)	10	380	16	5	Positive
isocitrate_1	No	191	Wide / Unit (6490)	117	Wide / Unit (6490)	10	380	10	5	Negative
isocitrate_2	No	191	Wide / Unit (6490)	73	Wide / Unit (6490)	10	380	20	5	Negative
alpha_KG_1	No	145	Wide / Unit (6490)	101	Wide / Unit (6490)	10	380	4	5	Negative
alpha_KG_2	No	145	Wide / Unit (6490)	57	Wide / Unit (6490)	10	380	8	5	Negative

Scan Parameters

Data Stg	Threshold
Centroid	0

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	270	270
Gas Flow (l/min)	15	15
Nebulizer (psi)	35	35
SheathGasHeater	400	400
SheathGasFlow	11	11
Capillary (V)	3000	3000
VCharging	1000	1500

Ion Funnel Parameters

Pos High Pressure RF	130	Neg High Pressure RF	110
Pos Low Pressure RF	100	Neg Low Pressure RF	60

Chromatograms

Chrom Type	Label	Offset	Y-Range
TIC	TIC	0	10000000

Acquisition Method Report

Agilent Technologies

Instrument Curves
 Actual

Name: HiP Sampler **Model:** G4226A

Auxiliary
Draw Speed	50.0 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	Standard injection
Injection Volume	5.00 µL

High throughput
Automatic Delay Volume Reduction	No
Overlapped Injection	
Enable Overlapped Injection	No

Valve Switching
Valve Movements	0
Valve Switch Time 1	
Switch Time 1 Enabled	No
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

Post Time
Posttime Mode	Off

Name: Binary Pump **Model:** G4220A

Flow	0.400 mL/min
Use Solvent Types	Yes
Stroke Mode	Synchronized
Low Pressure Limit	0.00 bar
High Pressure Limit	900.00 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	13.00 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.03		100.0 % Water V.03		Ch. 1	Yes	2.00 %
2	B	100.0 % Acetonitrile V.03		100.0 % Acetonitrile V.03		Ch. 1	Yes	98.00 %

Timetable

	Time	A	B	Flow	Pressure
1	2.00 min	2.00 %	98.00 %	0.400 mL/min	900.00 bar
2	9.00 min	60.00 %	40.00 %	0.400 mL/min	900.00 bar
3	9.50 min	2.00 %	98.00 %	0.400 mL/min	900.00 bar
4	13.00 min	2.00 %	98.00 %	0.400 mL/min	900.00 bar

Acquisition Method Report

<div style="float:right">**Agilent Technologies**</div>

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

Valve Position	Position 1 (Port 1 -> 2)
Ready when front door open	Yes

Left Temperature Control

Temperature Control Mode	Temperature Set
Temperature	25.0 °C

   Enable Analysis Left Temperature

Enable Analysis Left Temperature On	Yes
Enable Analysis Left Temperature Value	0.8 °C

Right Temperature Control

Right temperature Control Mode	Temperature Set
Right temperature	25.0 °C

   Enable Analysis Right Temperature

Enable Analysis Right Temperature On	Yes
Enable Analysis Right Temperature Value	0.8 °C

Stop Time

Stoptime Mode	As pump/injector

Post Time

Posttime Mode	Off