Acquisition Method Report

Agilent Technologies

Acquisition Method Info

Method Name	Daytam AA method.m
Method Path	D:\MassHunter\Methods\Daytam AA method.m
Method Description	6460 Triple Quad LC/MS ESI with Agilent Jet Stream Technology Positive MRM Reserpine Checkout

Device List

- HiP Sampler
- Quat. Pump
- Column Comp.
- QQQ

MS QQQ Mass Spectrometer

Ion Source	AJS ESI	Tune File	D:\MassHunter\Tune\QQQ\G6460C\atunes.TUNE.XML
Stop Mode	No Limit/As Pump	Stop Time (min)	2.0
Time Filter	On	Time Filter Width (min)	0.1

Time Segments

Index	Start Time (min)	Scan Type	Ion Mode	Div Valve	Delta EMV	Store
1	0	MRM	ESI+Agilent Jet Stream	To Waste	0	No
2	1.5	MRM	ESI+Agilent Jet Stream	To MS	0	Yes
3	5.5	MRM	ESI+Agilent Jet Stream	To Waste	0	No

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	Unit/Enh (6490)	200	Unit/Enh (6490)	200	135	0	7	Positive

Scan Parameters

Data Stg	Threshold
Centroid	0

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	150	150
Gas Flow (l/min)	11	11
Nebulizer (psi)	40	40
SheathGasHeater	400	400
SheathGasFlow	11	11
Capillary (V)	2000	0
VCharging	0	0

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
DL-Cystine IS	Yes	244.9	Unit/Enh (6490)	153.9	Unit/Enh (6490)	5	90	8	7	Positive
L-Cystine	No	241	Unit/Enh (6490)	74.2	Unit/Enh (6490)	5	100	24	7	Positive
L-Tyriptophan IS	Yes	210.1	Unit/Enh (6490)	192.1	Unit/Enh (6490)	5	90	4	7	Positive
L-Tryptophan	No	205.1	Unit/Enh (6490)	188.1	Unit/Enh (6490)	5	80	1	7	Positive
L-Tyrosine IS	Yes	192.1	Unit/Enh (6490)	145.2	Unit/Enh (6490)	5	80	8	7	Positive
L-Tyrosine	No	182.1	Unit/Enh (6490)	165	Unit/Enh (6490)	5	100	1	7	Positive
L-Citrulline IS	Yes	177.2	Unit/Enh (6490)	160.2	Unit/Enh (6490)	5	90	4	7	Positive
L-Arginine IS	Yes	177.2	Unit/Enh (6490)	70.2	Unit/Enh (6490)	5	110	20	7	Positive
L-Citrulline	No	176.4	Unit/Enh (6490)	159.3	Unit/Enh (6490)	5	80	3	7	Positive

Acquisition Method Report

Agilent Technologies

Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
L-Arginine	No	175.2	Unit/Enh (6490)	70.2	Unit/Enh (6490)	5	110	20	7	Positive
L-Phenylalanine IS	Yes	175.1	Unit/Enh (6490)	129.1	Unit/Enh (6490)	5	100	8	7	Positive
3-Methyl-L-Histidine IS	Yes	173.2	Unit/Enh (6490)	127.2	Unit/Enh (6490)	5	80	10	7	Positive
3-Methyl-L-Histidine	No	170.1	Unit/Enh (6490)	124.1	Unit/Enh (6490)	5	100	10	7	Positive
L-Phenylalanine	No	166.1	Unit/Enh (6490)	120.1	Unit/Enh (6490)	5	80	6	7	Positive
DL-5-Hydroxylysine	No	163.1	Unit/Enh (6490)	128.1	Unit/Enh (6490)	5	90	6	7	Positive
L-Histidine	No	156.1	Unit/Enh (6490)	110.1	Unit/Enh (6490)	5	100	8	7	Positive
L-Methionine IS	Yes	153.1	Unit/Enh (6490)	107.2	Unit/Enh (6490)	5	80	6	7	Positive
L-Lysine IS	Yes	151.1	Unit/Enh (6490)	88.1	Unit/Enh (6490)	5	90	16	7	Positive
L-Methionine	No	150.1	Unit/Enh (6490)	104.1	Unit/Enh (6490)	5	80	4	7	Positive
L-Glutamic acid IS	Yes	150.1	Unit/Enh (6490)	85.2	Unit/Enh (6490)	5	80	12	7	Positive
L-Glutamine IS	Yes	148.1	Unit/Enh (6490)	85.1	Unit/Enh (6490)	5	80	14	7	Positive
L-Glutamic acid	No	148.1	Unit/Enh (6490)	84.2	Unit/Enh (6490)	5	80	12	7	Positive
L-Lysine	No	147.1	Unit/Enh (6490)	84.2	Unit/Enh (6490)	5	80	12	7	Positive
L-Glutamine	No	147.1	Unit/Enh (6490)	84.2	Unit/Enh (6490)	5	80	12	7	Positive
L-Leucine IS	Yes	142.2	Unit/Enh (6490)	96.3	Unit/Enh (6490)	5	90	6	7	Positive
L-Ornithine IS	Yes	138.2	Unit/Enh (6490)	74.2	Unit/Enh (6490)	5	80	16	7	Positive
L-Aspartic acid IS	Yes	137.1	Unit/Enh (6490)	91.2	Unit/Enh (6490)	5	90	5	7	Positive
L-asparagine IS	Yes	135	Unit/Enh (6490)	89.1	Unit/Enh (6490)	5	80	4	7	Positive
L-Aspartic acid	No	134.1	Unit/Enh (6490)	74.1	Unit/Enh (6490)	5	90	10	7	Positive
L-ornithine	No	133.2	Unit/Enh (6490)	70.3	Unit/Enh (6490)	5	80	14	7	Positive
L-asparagine	No	133.1	Unit/Enh (6490)	74.2	Unit/Enh (6490)	5	70	10	7	Positive
L-isoleucine	No	132.2	Unit/Enh (6490)	69.2	Unit/Enh (6490)	5	100	14	7	Positive
Trans-4-hydroxy L-proline	No	132.2	Unit/Enh (6490)	68.2	Unit/Enh (6490)	5	90	20	7	Positive
L-Leucine	No	132.2	Unit/Enh (6490)	43.3	Unit/Enh (6490)	5	100	24	7	Positive
DL-Valine IS	Yes	126.1	Unit/Enh (6490)	80.2	Unit/Enh (6490)	5	80	8	7	Positive
Taurine	No	126.1	Unit/Enh (6490)	44.3	Unit/Enh (6490)	5	110	14	7	Positive
L-Proline IS	Yes	122.1	Unit/Enh (6490)	75.2	Unit/Enh (6490)	5	90	14	7	Positive
L-Threonine IS	Yes	121.1	Unit/Enh (6490)	75	Unit/Enh (6490)	5	80	6	7	Positive
L-Threonine	No	120.2	Unit/Enh (6490)	74.2	Unit/Enh (6490)	5	80	4	7	Positive
L-Valine	No	118.2	Unit/Enh (6490)	72.2	Unit/Enh (6490)	5	80	4	7	Positive
L-Norvaline	No	118.1	Unit/Enh (6490)	72.1	Unit/Enh (6490)	5	90	5	7	Positive
L-Proline	No	116.2	Unit/Enh (6490)	70.2	Unit/Enh (6490)	5	90	12	7	Positive
L-Serine IS	Yes	109.1	Unit/Enh (6490)	63	Unit/Enh (6490)	5	90	8	7	Positive
L-Serine	No	106.2	Unit/Enh (6490)	60.2	Unit/Enh (6490)	5	80	4	7	Positive
L-2-aminobutyric acid	No	104.2	Unit/Enh (6490)	58.3	Unit/Enh (6490)	5	80	4	7	Positive
3-Amino isobutyric acid	No	104.1	Unit/Enh (6490)	86.2	Unit/Enh (6490)	5	100	2	7	Positive

Cpd Name	ISTD?	Prec Ion	MS1 Res	Prod Ion	MS2 Res	Dwell	Frag (V)	CE (V)	Cell Acc (V)	Polarity
Gamma-aminobutyric acid	No	104	Unit/Enh (6490)	87.1	Unit/Enh (6490)	5	80	6	7	Positive
L-Alanine IS	Yes	94.1	Unit/Enh (6490)	48.2	Unit/Enh (6490)	5	90	6	7	Positive
L-Alanine	No	90.2	Unit/Enh (6490)	44.2	Unit/Enh (6490)	5	80	4	7	Positive
Beta-Alanine	No	90.1	Unit/Enh (6490)	72.1	Unit/Enh (6490)	5	80	2	7	Positive
Sarcosine	No	90.1	Unit/Enh (6490)	44.2	Unit/Enh (6490)	5	90	8	7	Positive
L-Glycine IS	Yes	78.2	Unit/Enh (6490)	31.3	Unit/Enh (6490)	5	90	4	7	Positive
L-Glycin	No	76.2	Unit/Enh (6490)	30.1	Unit/Enh (6490)	5	80	1	7	Positive
Ethanolamine	No	62.1	Unit/Enh (6490)	44.2	Unit/Enh (6490)	5	80	4	7	Positive

Scan Parameters

Data Stg	Threshold
Centroid	0

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	150	150
Gas Flow (l/min)	11	11
Nebulizer (psi)	40	40
SheathGasHeater	400	400
SheathGasFlow	11	11
Capillary (V)	2000	0
VCharging	0	0

Time Segment 3

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	Unit/Enh (6490)	200	Unit/Enh (6490)	200	135	0	7	Positive

Scan Parameters

Data Stg	Threshold
Centroid	0

Source Parameters

Parameter	Value (+)	Value (-)
Gas Temp (°C)	150	150
Gas Flow (l/min)	11	11
Nebulizer (psi)	40	40
SheathGasHeater	400	400
SheathGasFlow	11	11
Capillary (V)	2000	0
VCharging	0	0

Chromatograms

Chrom Type	Label	Offset	Y-Range
TIC	TIC	0	10000000

Instrument Curves

Actual

Name: HiP Sampler Model: G4226A

Auxiliary	
Draw Speed	200.0 µL/min
Eject Speed	200.0 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	3.00 µL
Needle Wash	
Needle Wash Location	Flush Port
Wash Time	2.0 s
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

Acquisition Method Report

Agilent Technologies

Name: Quat. Pump Model: G4204A

Flow	0.700 mL/min
Use Solvent Types	No
Low Pressure Limit	0.00 bar
High Pressure Limit	600.00 bar
Max. Flow Ramp Up	100.000 mL/min²
Primary Channel	Automatic
Max. Flow Ramp Down	100.000 mL/min²
Stroke	
Automatic Stroke Calculation	Yes
Compress	
Compressibility Mode	No Compensation
Mixer Selection	
Selected Mixer	Use Mixer if installed
Blend Assist	
Enabled	No
Stop Time	
Stoptime Mode	Time set
Stoptime	10.00 min
Post Time	
Posttime Mode	Off

Solvent Composition

	Channel	Ch. 1 Solv.	Name 1	Used	Percent
1	A	100.0 % Water V.03		Yes	22.00 %
2	B	100.0 % Acetonitrile V.03		Yes	78.00 %
3	C			No	
4	D			No	

Timetable

	Time	A	B	C	D	Flow	Pressure
1	1.00 min	22.00 %	78.00 %	0.00 %	0.00 %	0.700 mL/min	--- bar
2	4.00 min	70.00 %	30.00 %	0.00 %	0.00 %	0.700 mL/min	--- bar
3	5.00 min	70.00 %	30.00 %	0.00 %	0.00 %	0.700 mL/min	--- bar
4	5.10 min	22.00 %	78.00 %	0.00 %	0.00 %	0.700 mL/min	--- bar
5	9.00 min	22.00 %	78.00 %	0.00 %	0.00 %	0.700 mL/min	--- bar

Name: Column Comp. Model: G1316A

Left Temperature Control	
Temperature Control Mode	Temperature Set
Temperature	30.0 °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	Combined
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