

Acquisition Experiment Report

File: x:\qtof\2020\anna\daten november und dezember 2020\agii std 01.raw

Header

Acquired File Name: AGII Std 01
Acquired Date: 30-Oct-2020
Acquired Time: 14:45:47
Job Code: AGII check
Task Code:
User Name:
Laboratory Name:
Instrument:
Conditions:
Submitter:
SampleID:
Bottle Number: 1:A,3
Description: AGII 10 pmol pro microl

Instrument Calibration:

Calibration File:

Parameters

MS1 Static: None

MS1 Scanning:

Mass: 120 Da to 1285 Da.

Resolution: 0.0/0.0

Ion Energy: 0.0

Reference File: ESI_GFP_MSMS

Acquisition File: CALIBRATION_20201020

MS1 Scan Speed Compensation: None

Calibration Time: 11:33

Calibration Date: 10/20/20

Coefficients

MS1 Static: None

Function 1: $-0.000000001430*x^4 + 0.000000167597*x^3 + -0.000006605132*x^2 + 1.000173022246*x +-0.002112432820$, Root Mass

Function 2: $-0.000000001430*x^4 + 0.000000167597*x^3 + -0.000006605132*x^2 + 1.000173022246*x +-0.002112432820$, Root Mass

Parameters for C:\MassLynx\Wartung2020.PRO\ACQUDB\AGII Test 10 min.EXP

Created by Masslynx v4.0

Temperature Correction	Disabled
EDC Delay Coefficient	1.3000
EDC Delay Offset	-1.0000
T0Constant	-50
Maldi Laser Firing Rate	1.0
Maldi Plate Speed	1.0
Maldi Laser Energy	250.0
Maldi Pattern Filename	c:\Masslynx\Spiral_96.ptn

Experimental Instrument Parameters

Instrument Parameter Filename

C:\MassLynx\Wartung2020.PRO\ACQUDB\Service20201020.ipr

Polarity ES+

Analyser V Mode

Np Multiplier	0.70	
Resolution	10000	
Trigger Threshold	700	
Signal Threshold	80	
Veff	5509.00	
Lteff	1400.0	
T0Constant	-50.0	
Capillary (kV)	3.5	
Sampling Cone	40.0	
Extraction Cone	2.5	
Ion Guide	3.0	
Source Temperature (°C)	100	
Desolvation Temperature (°C)		320
Cone Gas Flow (L/Hr)	30.0	
Desolvation Gas Flow (L/Hr)		500.0
LM Resolution	4.9	
HM Resolution	15.0	
Ion Energy	1.8	
Pre-filter	2.0	
Collision Energy	4.0	
Collision Cell Entrance	2.0	
Collision Cell Exit	-10.0	
Collision Gas Flow	0.50	
Ion Guide Gas Flow (ml/min)		0.00
Detector	2250	
Pusher Interval (µS)	45	
Pusher Width	4	
Acceleration1	80.0	
Acceleration2	200.0	
Aperture2	70.0	
Transport1	70.0	
Transport2	70.0	
Steering	0.0	
Tube Lens	77	
Pusher	935.0	
Pusher Offset	-1.27	
Puller	745.0	
Multiplier	650	
Collector	15	
CollectorPulse	10.0	
StopperPulse	10.0	
Entrance	75	
CollisionCellStaticOffset		120
Offset2	0.00	
TOF	9.10	
Reflectron	2.16	
Vacuum Lock	1.87e-3	
Backing	1.72e0	
Ion Guide	5.12e2	
Quadrupole	OFF	
Collision Cell	3.61e-3	
TOF	9.54e-7	
Ion Guide RF Offset		300

Ion Guide RF Gain 0
 Ion Guide RF Limit 360
 Collision Cell RF Offset 360
 Collision Cell RF Gain 0
 Collision Cell RF Limit 380
 MS Profile Type Profile
 MSProfileMass1 400
 MSProfileDwellTime1 25
 MSProfileRampTime1 25
 MSProfileMass2 500
 MSProfileDwellTime2 25
 MSProfileRampTime2 25
 MSProfileMass3 600

Function Parameters - Function 1 - TOF MS FUNCTION

Scan Time (sec) 1.000
 Interscan Time (sec) 0.100
 Start Mass 100.0
 End Mass 1300.0
 Start Time (mins) 0.00
 End Time (mins) 10.00
 Data Format Continuum
 Use Tune Page Cone Voltage YES
 Use Tune Page Collision Energy NO
 Collision Energy (eV) 4.0
 Sensitivity Normal
 Dynamic Range Normal
 Calibration Dynamic 2

Function Parameters - Function 2 - TOF MSMS FUNCTION

Scan Time (sec) 1.000
 Interscan Time (sec) 0.100
 Set Mass 523.8
 Start Mass 65.0
 MSMS End Mass 1100.0
 Start Time (mins) 0.00
 End Time (mins) 10.00
 Data Format Continuum
 Use Tune Page Cone Voltage YES
 Use Tune Page Collision Energy NO
 Collision Energy Ramp Start (eV) 12.0
 Collision Energy Ramp End (eV) 18.0
 Sensitivity Normal
 Dynamic Range Normal
 Calibration Dynamic 2

ACE Experimental Record

----- Run method parameters -----

-- PUMP --

Waters GI Pump

1 -----

[B06NPB147N]

Application Mode: Direct Injection

Pump Type: BSM1

Run Time: 10.00 min

Solvent Selection A: A1

Solvent Selection B: B1

Seal Wash: 5.0 min

Switch 1: No Change

Switch 2: No Change

Switch 3: No Change

Chart Out 1: System Pressure

Chart Out 2: %B

Run Events: No

[Analytical Gradient Table]

Time(min) Flow Rate(uL/min) %A %B Curve

1. Initial 8.000 90.0 10.0

2. 8.00 8.000 10.0 90.0 6

3. 8.50 8.000 10.0 90.0 6

4. 8.60 8.000 90.0 10.0 6

5. 10.00 8.000 90.0 10.0 6

Analytical Low Pressure Limit: 0 psi

Analytical High Pressure Limit: 5500 psi

Solvent Name A: Water

Solvent Name B: Acetonitrile

Comment:

System Pressure Data Channel: Yes

Flow Rate Data Channel: No

%A Data Channel: No

%B Data Channel: Yes

Primary A Pressure Data Channel: No

Accumulator A Pressure Data Channel: No

Primary B Pressure Data Channel: No

Accumulator B Pressure Data Channel: No

Degasser Pressure Data Channel: No

[Trapping Gradient Table]

Time(min) Flow Rate(uL/min) %A %B Curve

1. Initial 15.000 99.0 1.0 Initial

Percentage of first solvent(B): 100.0

Percentage of first solvent(A): 100.0

Used for Load Ahead: No

Sample Loading Time: 1.00 min

Trapping Pump: No

Disable Flow Ramps: No

SM Multiload: No

3 -----

Aux Solvent Manager

Run Time: 10.00 min

Application Mode: Direct Injection

Seal Wash: 5.0 min

Analytical Pump A...

AuxSolventName: Water
AuxFlowSource: A1
Aux Low Pressure Limit: 0 psi
Aux High Pressure Limit: 10000 psi
Analytical Pump B...
AuxSolventName: Water
AuxFlowSource: B1
Aux Low Pressure Limit: 0 psi
Aux High Pressure Limit: 10000 psi
Trapping Pump A...
AuxSolventName: Water
AuxFlowSource: 1
Aux Low Pressure Limit: 0 psi
Aux High Pressure Limit: 10000 psi
Trapping Pump B...
AuxSolventName: Water
AuxFlowSource: 1
Aux Low Pressure Limit: 0 psi
Aux High Pressure Limit: 10000 psi
[Analytical Pump A Flow Table]
Time(min) Flow Rate(mL/min)
1. Initial 1.000
[Analytical Pump B Flow Table]
Time(min) Flow Rate(mL/min)
1. Initial 1.000
[Trapping Pump A Flow Table]
Time(min) Flow Rate(mL/min)
1. Initial 0.600
[Trapping Pump B Flow Table]
Time(min) Flow Rate(mL/min)
1. Initial 0.600
Percentage of first solvent(B): 100.0
Percentage of first solvent(A): 100.0
Used for Load Ahead: No
Sample Loading Time: 1.00 min
Trapping Pump: No
Disable Flow Ramps: No
SM Multiload: No
Method Comments...
Comment: Method updated.

-- END PUMP --

-- AUTOSAMPLER --

Waters Acquity AutoSampler
Run Time: 10.00 min
Comment:
Load Ahead: Disabled
Injection Mode: Partial Loop
Loop Offline: Disable
Weak Wash Solvent Name: Water
Weak Wash Volume: 500 uL
Strong Wash Solvent Name: Acetonitrile

Strong Wash Volume: 500 uL
Target Column Temperature: 30.0 C
Column Temperature Alarm Band: Disabled
Target Sample Temperature: 6.0 C
Sample Temperature Alarm Band: Disabled
Full Loop Overfill Factor: Automatic
Syringe Draw Rate: Automatic
Needle Placement: Automatic
Pre-Aspirate Air Gap: Automatic
Post-Aspirate Air Gap: Automatic
Column Temperature Data Channel: Yes
Ambient Temperature Data Channel: No
Sample Temperature Data Channel: No
Sample Organizer Temperature Data Channel: No
Sample Pressure Data Channel: No
Switch 1: No Change
Switch 2: No Change
Switch 3: No Change
Switch 4: No Change
Chart Out: Sample Pressure
Sample Temp Alarm: Disabled
Column Temp Alarm: Disabled
Run Events: No
Needle Overfill Flush: Automatic
No Injection: Disabled
iKey Cool Down: 2.0

Sample Run Injection Parameter

Injection Volume (ul) - 1.00
-- END AUTOSAMPLER --

----- oOo -----

End of experimental record.

----- Waters GI Pump Postrun Report -----

----- oOo -----

----- Waters Acquity SM Postrun Report -----

Software Version: 1.53.1398

Firmware Version: 1.53.369 (Mar 12 2014)

Checksum: 0x3d8b1239

Serial Number: B06NPS133N

Sample Syringe Size: 100.0

Sample Loop Size: 5.0

Needle Size: 15.0

Minimum Sample Temperature: 6.0

Maximum Sample Temperature: 6.0

Average Sample Temperature: 6.0

Minimum Column Temperature: 30.0

Maximum Column Temperature: 30.0

Average Column Temperature: 30.0

Measured Loop Volume: 5.930

Measured Loop Volume No Pressure: 6.080

----- oOo -----

Function 1

Scans in function: 270
Cycle time (secs): 1.100
Scan duration (secs): 1.000
Inter Scan Delay (secs): 0.100
Start and End Time(mins): 0.000 to 10.000
Ionization mode: ES+
Data type: Accurate Mass
Function type: TOF MS
Mass range: 100 to 1300

Function 2

Scans in function: 270
Cycle time (secs): 1.100
Scan duration (secs): 1.000
Inter Scan Delay (secs): 0.100
Start and End Time(mins): 0.000 to 10.000
Ionization mode: ES+
Data type: Accurate Mass
Function type: TOF Daughter
Mass range: 65 to 1100
Collision Energy: 0.0