==== Overall Status: ====:

Status: Instrument status Ok

Performance: Ok

====== Ion Source: ======:

Spray Voltage (V) 2985.9

Spray Current (µA) 21.50

Capillary Temperature (°C) 343.08

Sheath gas flow rate 50.06

Aux gas flow rate 15.02

Sweep gas flow rate 1.06

Aux. Temperature (°C) 448.13

====== Ion Optics: ======:

Capillary Voltage (V) -0.7

Bent Flatapole DC (V) -6.2

Inj Flatapole DC (V) -8.3

Trans Multipole DC (V) -4.1

HCD Multipole DC (V) -0.3

RF0 and RF1 Amp (V) 753.4

RF0 and RF1 Freq (kHz) 3282.000

RF2 and RF3 Amp (V) 0.7

RF2 and RF3 Freq (kHz) 3980.000

Inter Flatapole DC (V) -7.06

Quad Exit DC (V) 15.16

C-Trap Entrance Lens DC (V) 59.83

C-Trap RF Amp (V) 1009.5

C-Trap RF Freq (kHz) 3.213

C-Trap RF Curr (A) 0.143

C-Trap Exit Lens DC (V) 59.97

HCD Exit Lens DC (V) -35.38

====== Vacuum: ======:

Fore Vacuum Sensor (mbar) 1.64

High Vacuum Sensor (mbar) 3.64e-09

UHV Sensor (mbar) 2.41e-10

Source TMP Speed 1000.0

UHV TMP Speed 1000.0

===== Temperatures: =====:

Analyzer Temperature (°C) 30.87

Ambient Temperature (°C) 26.8

Ambient Humidity (%) 0.0

Source TMP Motor Temperature 51.0

Source TMP Bottom Temperatur 41.0

UHV TMP Motor Temperature (° 36.0

IOS Heatsink Temp. (°C) 31.0

HVPS Peltier Temp. (°C) 35.42

Quad. Det. Temp. (°C) 37.82

==== Diagnostic Data: ====

Performance ld 28.418

Performance me 1020.246

Performance cy: 55011.708

CTCD mV -61.25

5\_Glucose\_2 #1 RT: 0.0066

Total Ion Current: 719537920.00

Scan Low Mass: 70.00

Scan High Mass: 1000.00

Scan Start Time (min): 1.00

Scan Number: 186

Base Peak Intensity: 64228748.00

Base Peak Mass: 203.05

Scan Mode: FTMS + c ESI Full lock ms [70.00-1000.00]

Q Exactive Orbitrap Data:

=========================

Multiple Injection: ii

Multi Inject Info: IT=5;5

AGC: On

Micro Scan Count: 1

Scan Segment: 1

Scan Event: 1

Master Index: 0

Charge State: 0

Monoisotopic M/Z: 0.0000

Ion Injection Time (ms): 10.095

Max. Ion Time (ms): 200.00

FT Resolution: 70000

MS2 Isolation Width: 930.00

AGC Target: 3000000

Analyzer Temperature: 30.85

=== Mass Calibration: ===:

Conversion Parameter B: 67807167.1490

Conversion Parameter C: 18239587.3141

Temperature Comp. (ppm): -6.67

RF Comp. (ppm): 0.05

Space Charge Comp. (ppm): -1.45

Resolution Comp. (ppm): -0.23

Number of Lock Masses: 3

Lock Mass #1 (m/z): 371.1012

Lock Mass #2 (m/z): 391.2843

Lock Mass #3 (m/z): 445.1200

LM Search Window (ppm): 15.0

Number of LM Found: 1

Last Locking (sec): 0.0

LM Correction (ppm): 1.36

=== Ion Optics Settings: ===:

S-Lens RF Level: 40.00

S-Lens Voltage (V): 25.00

Skimmer Voltage (V): 15.00

Inject Flatopole Offset (V): 8.00

Bent Flatapole DC (V): 6.00

MP2 and MP3 RF (V): 326.00

Gate Lens Voltage (V): 5.63

C-Trap RF (V): 700.0

==== Diagnostic Data: ====:

Intens Comp Factor: 1.4000

Res. Dep. Intens: 1.308

CTCD NumF: 0

CTCD Comp: 0.411

CTCD ScScr: 0.686

RawOvFtT: 2629696.8

LC FWHM parameter: 5.0

Rod: 11

PS Inj. Time (ms): 1.632

AGC PS Mode: 1

AGC PS Diag: 701000

HCD Energy eV: 0.000

AGC Fill: 1.00

Injection t0: -0.007

t0 FLP: 73.07

Access Id: 0

Analog Input 1 (V): 0.000

Analog Input 2 (V): 0.000

=== Tune Data: ===:

Spray Voltage (+): 3500.00

Spray Voltage (-): 3300.00

Capillary Temperature (+ or +-): 300.00

Capillary Temperature (-): 320.00

Sheath Gas (+ or +-): 50.00

Sheath Gas (-): 10.00

Aux Gas (+ or +-): 15.00

Aux Gas (-): 0.00

Spare Gas (+ or +-): 1.00

Spare Gas (-): 0.00

Max Spray Current (+): 100.00

Max Spray Current (-): 100.00

Probe Heater Temp. (+ or +-): 450.00

Probe Heater Temp. (-): 30.00

S-Lens RF Level: 40.00

Ion Source: HESI

=== Calibration Data: ===:

Mass Cal. (+) age (d): 6.26

Mass Cal. (-) age (d): 0.31

Isolation Cal. (+) age (d): 32.1

Isolation Cal. (-) age (d): 32.0

Amplifier Gain: 1000.000

Mass Calibration Parameter (0): 7.90000000e+01

Mass Calibration Parameter (1): 1.00000000e+02

Mass Calibration Parameter (2): -1.53807381e-09

Mass Calibration Parameter (3): 1.37779579e+09

Mass Calibration Parameter (4): 2.45620169e-12

Mass Calibration Parameter (5): 1.37779579e+09

Mass Calibration Parameter (6): -8.13626641e-10

Mass Calibration Parameter (7): 1.37780686e+09

Mass Calibration Parameter (8): 1.24235795e-12

Mass Calibration Parameter (9): 1.37780686e+09

Mass Calibration Parameter (10): -1.14000000e-06

Mass Calibration Parameter (11): 0.00000000e+00

Mass Calibration Parameter (12): -1.14000000e-06

Mass Calibration Parameter (13): 0.00000000e+00

Mass Calibration Parameter (14): -8.85685936e-13

Mass Calibration Parameter (15): 1.37779583e+09

Mass Calibration Parameter (16): -7.73823109e-13

Mass Calibration Parameter (17): 1.37780690e+09

Mass Calibration Parameter (18): -6.27040137e-11

Mass Calibration Parameter (19): 1.37779582e+09

Mass Calibration Parameter (20): -1.10823481e-10

Mass Calibration Parameter (21): 1.37780688e+09

Mass Calibration Parameter (22): 0.00000000e+00

Mass Calibration Parameter (23): 0.00000000e+00

Mass Calibration Parameter (24): 0.00000000e+00

Mass Calibration Parameter (25): 0.00000000e+00

Mass Calibration Parameter (26): 0.00000000e+00

Mass Calibration Parameter (27): 0.00000000e+00

Mass Calibration Parameter (28): 0.00000000e+00

Mass Calibration Parameter (29): 0.00000000e+00

Mass Calibration Parameter (30): 4.20000000e+01

Mass Calibration Parameter (31): 1.00000000e+00

Mass Calibration Parameter (32): 1.00000000e+00

Mass Calibration Parameter (33): 0.00000000e+00

Mass Calibration Parameter (34): 2.98999478e+01

Mass Calibration Parameter (35): 9.70804143e+05

Mass Calibration Parameter (36): 9.70804143e+04

Mass Calibration Parameter (37): 1.28000000e+03

Mass Calibration Parameter (38): 2.56000000e+02

Mass Calibration Parameter (39): 1.38003290e+09

Mass Calibration Parameter (40): 6.00000000e+00

Mass Calibration Parameter (41): 1.38066190e+02

Mass Calibration Parameter (42): 7.00797830e+02

Mass Calibration Parameter (43): 1.95087652e+02

Mass Calibration Parameter (44): 5.89552280e+02

Mass Calibration Parameter (45): 5.24264964e+02

Mass Calibration Parameter (46): 3.59635973e+02

Mass Calibration Parameter (47): 1.22199064e+03

Mass Calibration Parameter (48): 2.35561990e+02

Mass Calibration Parameter (49): 1.42197786e+03

Mass Calibration Parameter (50): 2.18369911e+02

Mass Calibration Parameter (51): 1.62196509e+03

Mass Calibration Parameter (52): 2.04464813e+02

Mass Calibration Parameter (53): 1.00000000e+00

Mass Calibration Parameter (54): 1.00000000e+00

Mass Calibration Parameter (55): 1.00000000e+00

Mass Calibration Parameter (56): 3.05285907e+01

Mass Calibration Parameter (57): 1.02348760e+06

Mass Calibration Parameter (58): 1.02348760e+05

Mass Calibration Parameter (59): 2.40000000e+03

Mass Calibration Parameter (60): 2.56000000e+02

Mass Calibration Parameter (61): 1.38054670e+09

Mass Calibration Parameter (62): 8.00000000e+00

Mass Calibration Parameter (63): 2.65147903e+02

Mass Calibration Parameter (64): 5.05724724e+02

Mass Calibration Parameter (65): 5.14284397e+02

Mass Calibration Parameter (66): 3.63124030e+02

Mass Calibration Parameter (67): 1.27999721e+03

Mass Calibration Parameter (68): 2.30170970e+02

Mass Calibration Parameter (69): 1.37999083e+03

Mass Calibration Parameter (70): 2.21675076e+02

Mass Calibration Parameter (71): 1.47998444e+03

Mass Calibration Parameter (72): 2.14055474e+02

Mass Calibration Parameter (73): 1.57997805e+03

Mass Calibration Parameter (74): 2.07171174e+02

Mass Calibration Parameter (75): 1.67997166e+03

Mass Calibration Parameter (76): 2.00911061e+02

Mass Calibration Parameter (77): 1.77996528e+03

Mass Calibration Parameter (78): 1.95186177e+02

Mass Calibration Parameter (79): 0.00000000e+00

Mass Calibration Parameter (80): 0.00000000e+00

Mass Calibration Parameter (81): 0.00000000e+00

Mass Calibration Parameter (82): 0.00000000e+00

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Mass Calibration Parameter (115): 0.00000000e+00

Mass Calibration Parameter (116): 0.00000000e+00

Mass Calibration Parameter (117): 0.00000000e+00

Mass Calibration Parameter (118): 0.00000000e+00

Mass Calibration Parameter (119): 0.00000000e+00

CTCD Scale (+): 1.451

CTCD Scale (-): 3.440

CTCD Para (+): 0.800

CTCD Para (-): 0.500

Detect Delay: 5.50

Relais Delay: 5.00

Res.-Dep. Delay: 10.00

Quad DC (+,0): 5.517

Quad DC (+,1): -0.001

Quad DC (-,0): -5.860

Quad DC (-,1): 0.001

Quad OTK (+,0): 0.811

Quad OTK (+,1): -0.098

Quad OTK (-,0): 11.743

Quad OTK (-,1): 0.079

Quad Para A: 0.000

Quad Para B: 0.000

Quad Para C: 0.000

CLT GND Voltage (+): 20.10

CLT GND Voltage (-): 16.45

CLT Offset Voltage (+): 1650.0

CLT Offset Voltage (-): 1650.0

CLT Push Voltage (+): 150.0

CLT Push Voltage (-): 150.0

CLT Pull Voltage (+): 300.0

CLT Pull Voltage (-): 300.0

Lens 6 Voltage (+): 630.0

Lens 6 Voltage (-): 630.0

Z-Lens 3 Voltage (+): 230.0

Z-Lens 3 Voltage (-): 230.0

De-Inject Voltage (+): 40.0

De-Inject Voltage (-): 40.0

De-Measure Voltage (+): 470.0

De-Measure Voltage (-): 470.0

CE-Inject Voltage (+): 3800.0

CE-Inject Voltage (-): 3800.0

=== Configuration Data: ===:

Preamp Protect Mode: 0

TMP Sweep Mode: 0

Temp Sensor Mode: 0

=== Identification: ===:

SW Version: 2.2-164600/2.2.1.1646

Model: Q Exactive

Instrument: Exactive S... slot #809

Hardware Id: 001999C9156E

Method of Q Exactive

OVERALL METHOD SETTINGS

Global Settings

use lock masses best

Chrom. peak width (FWHM) 5 s

Time

Method duration 12.00 min

Experiment

FULL MS — SIM

General

Runtime 0 to 12 min

Polarity positive

In-source CID 0.0 eV

Full MS — SIM

Microscans 1

Resolution 70,000

AGC target 3e6

Maximum IT 200 ms

Number of scan ranges 1

Scan range 70 to 1000 m/z

Spectrum data type Centroid

Setup

TUNEFILES

General

Switch Count 0

Base Tunefile C:\Xcalibur\methods\Rainey\Rainey-HighFlow-Slens-40.mstune

CONTACT CLOSURE

General

Used False

Start in Closed True

Switch Count 0

SYRINGE

General

Used False

Start in OFF True

Stop at end of run False

Switch Count 0

Pump setup

Syringe type Hamilton

Flow rate 3.000 µL/min

Inner diameter 2.303 mm

Volume 250 µL

DIVERT VALVE A

General

Used False

Start in 1-2 True

Switch Count 0

DIVERT VALVE B

General

Used False

Start in 1-2 True

Switch Count 0

LOCK MASSES

3 entries

Mass Polarity Start End Comment

[m/z] [min] [min]

391.28429 Positive

371.10124 Positive

445.12003 Positive

INCLUSION LIST

(no entries)

EXCLUSION LIST

(no entries)

NEUTRAL LOSSES

(no entries)

MASS TAGS

(no entries)

Sample Name:

Comments: Ratio

Study:

Client:

Laboratory:

Company:

Phone:

Instrument Method: C:\Xcalibur\methods\Rob\Rob\_IROA\_Short.meth

Processing Method:

Vial: BA4

Injection Volume (µl): 3.00

Sample Weight: 0.00

Sample Volume (µl): 0.00

ISTD Amount: 0.00

Dil Factor: 1.00