

Instrument Method: Metabolomics_pHILIC_Parkville_v1.meth

Thermo Scientific SII for Xcalibur Method

---- Overview ----

Name: New Instrument Method

Comment:

Run time: 32.000 [min]

Instrument: Analytical on thermo-hruqoh18

Description:

---- Script ----

```
initial      Instrument Setup
              Sampler.InjectWash: Both
              Sampler.WashSpeed: 8.000 [µl/s]
              Sampler.WashVolume: 50.000 [µl]
              Sampler.SampleHeight: 0.000 [mm]
              Sampler.WasteSpeed: 8.000 [µl/s]
              Sampler.DispenseDelay: 0.000 [s]
              Sampler.DispSpeed: 5.000 [µl/s]
              Sampler.DrawSpeed: 5.000 [µl/s]
              Sampler.DrawDelay: 3.000 [s]
              Sampler.InjectMode: Normal
              Sampler.PumpDevice: "Pump"
              Sampler.LoopWashFactor: 2.000
              Sampler.TempCtrl: On
              Sampler.Temperature.Nominal: 4.0 [°C]
              Sampler.ReadyTempDelta: 1.0 [°C]
              Sampler.Temperature.LowerLimit: 4.0 [°C]
              Sampler.Temperature.UpperLimit: 45.0 [°C]
              ColumnOven.TempCtrl: On
              ColumnOven.Temperature.Nominal: 25.0 [°C]
              ColumnOven.Temperature.LowerLimit: 5.0 [°C]
              ColumnOven.Temperature.UpperLimit: 110.0 [°C]
              ColumnOven.EquilibrationTime: 0.5 [min]
              ColumnOven.ReadyTempDelta: 5.0 [°C]
              ColumnOven.Cooler_TempCtrl: Off
              ColumnOven.Column_A.ActiveColumn: No
              ColumnOven.Column_A.SystemPressure: "Pump"
              ColumnOven.Column_B.ActiveColumn: No
              ColumnOven.Column_B.SystemPressure: "Pump"
              PumpModule.Pump.%A.Equate: "20mM AC pH9"
              PumpModule.Pump.%B.Equate: "Acetonitrile"
              PumpModule.Pump.%C.Equate: "%C"
              PumpModule.Pump.Pressure.LowerLimit: 0 [bar]
              PumpModule.Pump.Pressure.UpperLimit: 550 [bar]
              PumpModule.Pump.MaximumFlowRampUp: 6.000 [ml/min²]
              PumpModule.Pump.MaximumFlowRampDown: 6.000 [ml/min²]
0.000 [min] Inject Preparation
              Wait Sampler.Ready And ColumnOven.Ready And PumpModule.Pump.Ready
0.000 [min] Inject
              Sampler.Inject
              Sampler.Relay_3.On
```

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```
Thermo Scientific SII for Xcalibur Method
0.000 [min] Start Run
      ColumnOven.ColumnOven_Temp.AcqOn
      ColumnOven.Cooler_Temp.AcqOn
      PumpModule.Pump.Pump_Pressure.AcqOn
0.000 [min] Run
      PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
      PumpModule.Pump.%B.Value: 80.0 [%]
      PumpModule.Pump.%C.Value: 0.0 [%]
      PumpModule.Pump.%D.Value: 0.0 [%]
      PumpModule.Pump.Curve: 5
0.100 [min]
      Sampler.Relay_3.Off
15.000 [min]
      PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
      PumpModule.Pump.%B.Value: 50.0 [%]
      PumpModule.Pump.%C.Value: 0.0 [%]
      PumpModule.Pump.%D.Value: 0.0 [%]
      PumpModule.Pump.Curve: 5
18.000 [min]
      PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
      PumpModule.Pump.%B.Value: 5.0 [%]
      PumpModule.Pump.%C.Value: 0.0 [%]
      PumpModule.Pump.%D.Value: 0.0 [%]
      PumpModule.Pump.Curve: 5
21.000 [min]
      PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
      PumpModule.Pump.%B.Value: 5.0 [%]
      PumpModule.Pump.%C.Value: 0.0 [%]
      PumpModule.Pump.%D.Value: 0.0 [%]
      PumpModule.Pump.Curve: 5
24.000 [min]
      PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
      PumpModule.Pump.%B.Value: 80.0 [%]
      PumpModule.Pump.%C.Value: 0.0 [%]
      PumpModule.Pump.%D.Value: 0.0 [%]
      PumpModule.Pump.Curve: 5
32.000 [min]
      PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
      PumpModule.Pump.%B.Value: 80.0 [%]
      PumpModule.Pump.%C.Value: 0.0 [%]
      PumpModule.Pump.%D.Value: 0.0 [%]
      PumpModule.Pump.Curve: 5
32.000 [min] Stop Run
      ColumnOven.ColumnOven_Temp.AcqOff
      ColumnOven.Cooler_Temp.AcqOff
      PumpModule.Pump.Pump_Pressure.AcqOff
```

Method of Q Exactive

Overall method settings

Global Settings

Use lock masses off
 Lock mass injection -
 Chrom. peak width (FWHM) 30 s

Time

Method duration 32.00 min

Customized Tolerances (+/-)

Lock Masses -
 Inclusion -
 Exclusion -
 Neutral Loss -
 Mass Tags -
 Dynamic Exclusion 10.0 ppm

Experiments

Full MS - SIM

General

Runtime 0 to 32 min
 Polarity positive
 In-source CID 0.0 eV

Full MS - SIM

Microscans 1
 Resolution 35,000
 AGC target 1e6
 Maximum IT 50 ms
 Number of scan ranges 1
 Scan range 85 to 1275 m/z
 Spectrum data type Profile

Full MS - SIM

General

Runtime 0 to 32 min
 Polarity negative
 In-source CID 0.0 eV

Full MS - SIM

Microscans 1
 Resolution 35,000
 AGC target 1e6
 Maximum IT 50 ms
 Number of scan ranges 1
 Scan range 85 to 1275 m/z
 Spectrum data type Profile

Setup

General

Switch Count 0
Base Tunefile C:\Xcalibur\methods\300uL_70-1050_posneg.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 True
Start in 1-2 True
Switch Count 0

Divert Valve B

General

Used False
Start in 1-2 True
Switch Count 0

Lock Masses

2 entries

Mass	Polarity	Start	End	Comment
[m/z]		[min]	[min]	
217.10465	Positive			
255.23295	Negative			