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Thermo Scientific SII for Xcalibur Method

---- Overview ----
Name: New Instrument Method
Comment:
Run time: 17.000 [min]
Instrument: GVDLZ42_1 on gvdlz42
Description:
---- Script ----
initial     Instrument Setup
            Sampler.InjectWash: Both
            Sampler.WashSpeed: 5.000 [µl/s]
            Sampler.WashVolume: 20.000 [µl]
            Sampler.SampleHeight: 2.000 [mm]
            Sampler.WasteSpeed: 5.000 [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: 10.0 [°C]
            Sampler.ReadyTempDelta: 1.0 [°C]
            Sampler.Temperature.LowerLimit: 4.0 [°C]
            Sampler.Temperature.UpperLimit: 45.0 [°C]
            ColumnOven.TempCtrl: On
            ColumnOven.Temperature.Nominal: 40.0 [°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"
            PumpModule.Pump.%A.Equate: "0.02% FA 4mM NH4Fo Water"
            PumpModule.Pump.%B.Equate: "0.02% FA 4mM NH4Fo Methanol"
            PumpModule.Pump.%C.Equate: "%C"
            PumpModule.Pump.%D.Equate: "ACN"
            PumpModule.Pump.Pressure.LowerLimit: 20 [bar]
            PumpModule.Pump.Pressure.UpperLimit: 1000 [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
0.000 [min] Start Run
            ColumnOven.ColumnOven_Temp.AcqOn
```

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            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: 0.0 [%]
            PumpModule.Pump.%C.Value: 95.0 [%]
            PumpModule.Pump.%D.Value: 5.0 [%]
            PumpModule.Pump.Curve: 5
9.000 [min]
            PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
            PumpModule.Pump.%B.Value: 0.0 [%]
            PumpModule.Pump.%C.Value: 5.0 [%]
            PumpModule.Pump.%D.Value: 95.0 [%]
            PumpModule.Pump.Curve: 5
10.000 [min]
            PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
            PumpModule.Pump.%B.Value: 0.0 [%]
            PumpModule.Pump.%C.Value: 0.0 [%]
            PumpModule.Pump.%D.Value: 100.0 [%]
            PumpModule.Pump.Curve: 5
13.000 [min]
            PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
            PumpModule.Pump.%B.Value: 0.0 [%]
            PumpModule.Pump.%D.Value: 100.0 [%]
            PumpModule.Pump.Curve: 5
            PumpModule.Pump.%C.Value: 0.0 [%]
13.500 [min]
            PumpModule.Pump.Flow.Nominal: 0.300 [ml/min]
            PumpModule.Pump.%B.Value: 0.0 [%]
            PumpModule.Pump.%C.Value: 95.0 [%]
            PumpModule.Pump.%D.Value: 5.0 [%]
            PumpModule.Pump.Curve: 5
17.000 [min] Stop Run
            ColumnOven.ColumnOven_Temp.AcqOff
            ColumnOven.Cooler_Temp.AcqOff
            PumpModule.Pump.Pump_Pressure.AcqOff
```

Method of Q Exactive HF

Overall method settings

Global Settings		
Use lock masses	best	
Lock mass injection	–	
Chrom. peak width (FWHM)	15	s
Time		
Method duration	15.00	min
Customized Tolerances (+/-)		
Lock Masses	–	
Inclusion	–	
Exclusion	–	
Neutral Loss	–	
Mass Tags	–	
Dynamic Exclusion	–	

Experiments

Full MS / dd-MS² (TopN)

General		
Runtime	0 to 12	min
Polarity	negative	
In-source CID	0.0	eV
Default charge state	1	
Inclusion	on	
Exclusion	–	
Tags	–	
Full MS		
Microscans	1	
Resolution	60,000	
AGC target	3e6	
Maximum IT	100	ms
Number of scan ranges	1	
Scan range	70 to 960	m/z
Spectrum data type	Profile	
dd-MS² / dd-SIM		
Microscans	1	
Resolution	30,000	
AGC target	1e5	
Maximum IT	50	ms
Loop count	5	
MSX count	1	
TopN	5	
Isolation window	4.0	m/z
Isolation offset	0.0	m/z
Scan range	200 to 2000	m/z
Fixed first mass	–	

(N)CE / stepped (N)CE	nce: 10, 30, 60
Spectrum data type	Profile
dd Settings	
Minimum AGC target	8.00e3
Intensity threshold	1.6e5
Apex trigger	–
Charge exclusion	–
Multiple charge states	all
Peptide match	preferred
Exclude isotopes	on
Dynamic exclusion	10.0 s
If idle ..	do not pick others

Full MS – SIM

General

Runtime	0 to 12 min
Polarity	negative
In-source CID	0.0 eV
Full MS – SIM	
Microscans	1
Resolution	60,000
AGC target	3e6
Maximum IT	200 ms
Number of scan ranges	1
Scan range	70 to 1050 m/z
Spectrum data type	Profile

Setup

Tunefiles

General

Switch Count	2
Base Tunefile	C:\Xcalibur\methods\2021-07-29 PFAS High temp.mstune

Element 1

At	0.60 min
New Tunefile	C:\Xcalibur\methods\2021-07-29 PFAS High temp.mstune

Element 2

At	1.46 min
New Tunefile	C:\Xcalibur\methods\2021-07-29 PFAS High temp.mstune

Contact Closure

General

Used	False
Start in Closed	True
Switch Count	0

Syringe

General

Used	False
Start in OFF	True

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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  False
Switch Count      1
```

Element 1

```
At            12.00 min
Switches to     1-6
```

Divert Valve B

General

```
Used          False
Start in 1-2   True
Switch Count      0
```

Lock Masses

(no entries)

Inclusion List

55 entries

Mass [m/z]	Formula [M]	Species	CS [z]	Polarity	Start [min]	End [min]	(N)CE	MSX ID	Comment
212.97870				Negative	3.50	4.50			
326.97440				Negative	5.00	6.00			
312.97300				Negative	5.10	6.10			
298.94290				Negative	5.20	6.20			
328.96800				Negative	5.30	6.30			
262.97600				Negative	4.50	5.50			
362.97600				Negative	5.70	6.70			
348.93980				Negative	5.80	6.80			
376.96900				Negative	5.80	6.80			
426.96810				Negative	6.00	7.00			
412.96670				Negative	6.10	7.10			
398.93660				Negative	6.30	7.30			
462.96360				Negative	6.50	7.50			
448.93350				Negative	6.80	7.80			
526.96260				Negative	6.80	7.80			
555.95200				Negative	7.00	8.00			
512.96020				Negative	7.00	8.00			
498.93070				Negative	7.10	8.10			
569.96780				Negative	7.50	8.50			
530.89720				Negative	7.40	8.40			

562.95720	Negative	7.40	8.40
548.92740	Negative	7.50	8.50
583.98360	Negative	7.70	8.70
568.96420	Negative	7.70	8.70
598.92440	Negative	7.80	8.80
630.88990	Negative	8.00	9.00
612.95420	Negative	7.70	8.70
662.95130	Negative	8.10	9.10
712.94830	Negative	8.40	9.40
698.91820	Negative	8.50	9.50
812.94210	Negative	8.90	9.90
912.93300	Negative	9.10	10.20
216.99230	Negative	3.50	4.50
329.99330	Negative	4.90	5.90
267.99280	Negative	4.50	5.50
317.98970	Negative	5.10	6.10
301.95310	Negative	5.20	6.20
331.97800	Negative	5.20	6.20
366.98310	Negative	5.70	6.70
428.97470	Negative	5.90	6.90
420.99350	Negative	6.10	7.10
401.94670	Negative	6.30	7.30
471.99360	Negative	6.70	8.70
528.96860	Negative	6.80	7.80
518.98030	Negative	8.00	9.00
506.95700	Negative	7.10	8.10
572.98670	Negative	7.50	8.50
569.98070	Negative	7.40	8.40
589.01500	Negative	7.70	8.70
614.96090	Negative	7.70	8.70
714.95480	Negative	8.40	9.40
215.98880	Negative	3.40	4.40
414.97330	Negative	6.10	7.10
514.96700	Negative	7.00	8.00
502.94390	Negative	7.10	8.10